Inaugural–Dissertation

zur Erlangung der Doktorwürde
der
Naturwissenschaftlich–Mathematischen Gesamtfakultät
der
Ruprecht–Karls–Universität Heidelberg

vorgelegt von
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Tag der mündlichen Prüfung:
06. Dezember 2013

Modeling and Analysis of Demand for Commodities and a Case Study of the Petrochemical Market

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Abstract

This thesis aims to establish a demand model for commodities that takes all crucial influencing factors into account. To begin with, we analyze the dependency of the demand on prices, market parameters, and specific characteristics of the customers in order to provide the mathematical framework for a general demand model. In particular, this approach takes account of effects that are caused by price-based substitution of products irrespective of their availability.

Fundamental market models that include supply-demand interactions gain importance in the context of commodity pricing. We explicitly develop demand models for petrochemical products that are applicable within the profit maximization problem of a monopoly in order to determine optimal price and sales decisions. The solvability of the market optimization problem requires additional restrictions on the modeling.

Basically, the model displays the nonlinear demand-price relationship. Model extensions incorporate the changes of macroeconomic indices, which quantify changes in the economic situation. Moreover, our approach to modeling demand comprises the impacts of varying prices of substitutable and complementary products, and establishes a connection to the characteristics of the consumer's side.

Integrating the demand models to real market models necessitates the identification of the demand parameters. We discuss the difficulty to get reliable parameter estimates in the situation of incomplete data and investigate two methods based on additional assumptions in order to estimate the demand parameters. For the demand model that includes the dependency on the price and macroeconomic indices, a heuristic methodology firstly determines parameters based on market simulations. The second approach creates an inequality constrained parameter identification problem, where the constraints reflect additional assumptions on the shape of the demand model function. This problem can be solved using the generalized Gauss-Newton method.

Zusammenfassung

Ziel dieser Arbeit ist es, ein Nachfragemodell für Rohstoffe aufzustellen, das alle wesentlichen Einflussfaktoren berücksichtigt. Zu Anfang analysieren wir die Abhängigkeit der Nachfrage von Preisen, Marktparametern und spezifischen Eigenschaften der Abnehmer, um die mathematischen Rahmenbedingungen für eine allgemeine Nachfragemodellierung festzulegen. Insbesondere berücksichtigt unser Ansatz Effekte, die durch preisbasierte Substitution ungeachtet der Verfügbarkeit der Waren entstehen.

Fundamentalmarktmodelle, die das Zusammenwirken von Angebot und Nachfrage abbilden, gewinnen im Rahmen der Preisfindung für Rohstoffe an Bedeutung. Mit dem Ziel optimale Preis- und Absatzmengenentscheidungen für petrochemische Produkte zu bestimmen, entwickeln wir explizit Nachfragemodelle, die sich zur Einbettung in das Profitmaximierungsproblem eines Monopolisten eignen. Dabei sind zusätzliche Bedingungen an die Modellierung erforderlich, um die Lösbarkeit des Marktoptimierungsproblems sicherzustellen.

Grundsätzlich stellt das Modell den nichtlinearen Zusammenhang zwischen Preis und Nachfrage dar. Modellerweiterungen beinhalten makroökonomische Kennzahlen, die die Änderung der Wirtschaftslage quantifizieren. Darüber hinaus erfasst unser Modellansatz für die Nachfrage die Wirkung von Preisänderungen bei Substituten und komplementären Produkten und stellt eine Verbindung zu den Eigenschaften der Abnehmerseite her.

Die Eingliederung der Nachfragemodelle in reale Marktmodelle erfordert die Identifikation der Nachfrageparameter. Wir erörtern die Problematik einer verlässlichen Parameterschätzung angesichts unvollständiger Daten und untersuchen zwei Methoden, die auf zusätzlichen Annahmen basieren, um die Nachfrageparameter zu schätzen. Für das Nachfragemodell, das die Abhängigkeit von Preis und makroökonomischen Kennzahlen darstellt, bestimmt ein heuristischer Ansatz die Parameter zunächst durch Marktsimulationen. Die zweite Methode erstellt ein Parameteridentifikationsproblem mit Ungleichungsnebenbedingungen, die die zusätzlichen Annahmen über das Verhalten der Nachfragefunktion wiedergeben. Dieses Problem kann mit dem verallgemeinerten Gauss-Newton Verfahren gelöst werden.

Danksagung

An dieser Stelle möchte ich mich bei allen bedanken, die mich während meiner Zeit als Doktorandin an der Universität Heidelberg unterstützt und damit zum Gelingen dieser Arbeit beigetragen haben.
Zuerst möchte ich mich bei meinem Betreuer Prof. Dr. Dr. h.c. mult. Willi Jäger für die Möglichkeit, meine Doktorarbeit in seiner Arbeitsgruppe an der Fakultät für Mathematik und Informatik der Ruprecht-Karls-Universität Heidelberg und am *Interdisziplinären Zentrum für wissenschaftliches Rechnen* zu schreiben, bedanken. Desweiteren möchte ich Danke sagen für die Gespräche und zahlreichen Ratschläge, die wegweisend für den Verlauf meiner Forschung waren, sowie für seine aufmunternden Worte, die mir immer wieder zu neuer Motivation verholfen haben.
Außerdem gilt mein besonderer Dank Prof. Dr. Sebastian Sager von der Otto-von-Guericke Universität Magdeburg für seine Unterstützung und sein Engagement, die mir immer wieder Ansporn gegeben haben. Die gemeinsamen Diskussionen und seine fachlichen Ratschläge haben mir in hohem Maße geholfen, diese Arbeit anzufertigen.
Der Graduiertenschule *HGS Mathcomp* und dem *Interdisziplinären Zentrum für wissenschaftliches Rechnen* bin ich für die finanzielle Unterstützung sehr dankbar. Bei der Graduiertenschule möchte ich mich außerdem für ihr Doktorandenprogramm, das durch Kurse und Vorträge immer wieder Gelegenheit bot, sich mit anderen Doktoranden auszutauschen, bedanken.
Vielen Dank an Lilian Kramer für ihre Hilfsbereitschaft und Geduld. Ohne ihre Unterstützung wäre mir das Erstellen dieser Arbeit schwerer gefallen. Sie hatte stets ein offenes Ohr für all meine Probleme und ihre Vorschläge haben mir oft über kleine Krisen hinweg geholfen.
Der gesamten Arbeitsgruppe *Applied Analysis* möchte ich dafür danken, dass ich meine Doktorarbeit in einer so angenehmen und humorvollen Umgebung schreiben konnte. Vielen Dank an Dr. Anamaria Bodea, Cristian Croitoru, Dr. Stephan Ludwig und Lilian Kramer für den fachlichen Austausch aber auch für die vielen lustigen Unterhaltungen.
Für die organisatorische Hilfe möchte ich mich ganz herzlich bei Ina Scheid und Gabriela Schocke, die immerzu Verständnis für die Anliegen der Doktoranden hatten, bedanken.
Bei Dr. Simon Jäger möchte ich mich für die informativen Treffen, bei denen ich viel über die Besonderheiten der Rohstoffmärkte und die damit verbundenen Modellanforderungen erfahren konnte, bedanken.
Vielen Dank an die Mitglieder der Arbeitsgruppen *Mathematical Algorithmic Optimization* und *Simulation and Optimization* für die konstruktiven Gespräche und Hilfe bei organisatorischen Dingen. Besonders bedanken möchte ich mich bei Holger Diedam für die vielen aufschlussreichen Diskussionen zu Beginn des Projektes und für die Unterstützung bei der Erstellung des Computerprogrammes.

Bei Lilian Kramer, David Dähn, Tobias Pfrommer, Lauren Orwin und Rachel Dryden bedanke ich mich dafür, dass sie Teile dieser Arbeit Korrektur gelesen haben.
Darüber hinaus möchte ich mich recht herzlich bei meinen Freunden Agnes, Anne, Lilli, Nicole, Patti, Simone, David und Tobi für ihre Unterstützung, ihre Aufmunterungen sowie für die manchmal notwendige Erholung während der vielen schönen und lustigen Stunden, die wir gemeinsam verbracht haben, bedanken.
Zum Schluss möchte ich mich bei meiner Familie bedanken. Ganz besonderer Dank gilt meinen Eltern für ihre Unterstützung, ihr Verständnis und für ihre stetigen Ermutigungen. Vielen Dank an die beiden und an meinen Bruder, dass ich immer auf sie zählen kann. Dankeschön auch an Bernd, Iris, Norbert und Evi für ihre Unterstützung und ihre Herzlichkeit.

Contents

1 Introduction

The formation of demand is one of the most complex mechanisms in commodity markets and its modeling still poses several challenges. Nevertheless, modeling the connections of demand and its essential influencing factors is of high interest for researchers, as well as for market participants seeking guidance with respect to production planning, pricing and trading strategies, and risk management. Regarding the relationship between demand and price, developing an adequate demand model is a challenge. This is because it comprises more than just describing the sales quantity at the market, which is only the intersection of supply and demand. In fact, demand is the quantity the consumer is willing to buy at a certain price given the market situation and, therefore, reflects the consumer's preferences in this way. Consequently, a demand function with respect to price describes the relationship of required quantities and prices over the whole price region.

So far, the issue of analyzing and modeling demand has appeared in multiple research areas (e.g. microeconomics [MCWG95], operations research [KGvB+09, BC03], marketing [LKM92], or commodity pricing [BGS07, EW03]) and comprises different concepts.

The neoclassical consumer theory is a powerful tool for describing consumer behavior [DM80b, MCWG95, Var92, Var10] and provides the basis for multiple demand models in economics [DM80b, BS09, TC87, MCWG95]. Likewise, modeling the utility maximization problem of consumers is also used in many applications ranging from supply chain management [vRM99, LB08] to modeling demand for specific services or products [DM96, W+97, Pin79]. In contrast, numerous application-specific demand models are built on rather phenomenological assumptions [Jä08, NR03, HX08, KF07]. As for optimization models to determine optimal pricing and production quantities, demand is modeled as function with respect to price [Kan08, KGvB+09, Cha05] or as a stochastic random variable [GM03, BT06]. Equally, stochastic demand models are applied in revenue management [GvR94, BC03]. In particular, the aspects of substitution are included in demand models as part of assortment optimization in retail [vRM99, SA00, HX08, KF07].

This thesis focuses on analyzing and modeling the demand for commodities. As we are aiming to provide an explicit demand model for commodities that reflects the nonlinear demand-price relationship and includes all essential influencing factors, we provide a framework for demand models based on phenomenological assumptions. According to Kannegiesser et al. [KGvB+09], commodities display some specialities: they are products of standard quality that are produced and sold in large quantities and the most important influence factor is the price. Therefore, in commodity markets, the question is rather how much to buy than whether to buy at a certain price, which is often studied in discrete choice models [AdPT92, DM96, BC03].

In addition to the nonlinear relationship between demand of a commodity and its price,

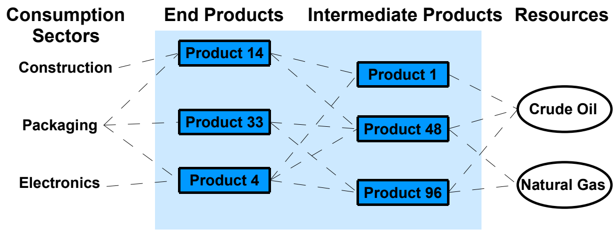

Figure 1.1: Exemplary connections of influencing factors of demand for petrochemical products

we also include model components reflecting the influences of substitutes and complements. Moreover, we investigate the impacts of the economic situation as well as characteristic variables of the consumer's side. Our description is suitable for business-to-business markets as well as for end-consumers which, for example, require heating oil.

Motivated by the development of a supply-demand trade network optimization model, a further objective of this thesis is to provide explicit demand functions in order to simulate prices and sales quantities of commodities. In doing so, finding the appropriate model is of high significance, because the profit maximization of the supply side goes according to the demand-price relationship. Hence, such market models based on explicit demand models are an important tool to investigate the complexity of the pricing mechanism. Moreover, they suitably reflect the common price development of commodities that share common features and are linked either by their production processes or identical purpose of use.

More precisely, since we aim to apply this network optimization model to the petrochemical industry, the purpose of modeling demand is the applicability to petrochemical products. The demand of these products is influenced by various influencing factors as shown in figure 1.1. In addition to the consumption caused by different industrial sectors on the right, demand of the respective products is also driven by other products. For example, the demand for product 1 is not only determined by the demand of product 14 and 4, but also on prices of its substitute products 48 and 96. On the supply side, the chemical products are connected by their production processes, where crude oil and natural gas are starting products of the production network so that their demand is also related to the demand of petrochemical products if only in a small part.

This thesis is part of the pioneering project *Modeling, Simulation, and Optimization of Price Dynamics* initiated by the Interdisciplinary Center for Scientific Computing Heidelberg, which combines methods from optimization and economics in order to model the price formation in the petrochemical industry. This results in an inequality constrained nonlinear optimization problem of a monopoly, where the constraints are given by the production capacities limits, the sales-production-transportation restrictions, and the market design (e.g., principle of no arbitrage). In addition to this modeling aspect of a supply-demand trade network optimization problem for multiple commodities, which is accomplished in cooperation with Kramer [Kra13], methods for network reduction are of utmost importance since information on all market components is hardly available. Therefore, Kramer [Kra13] presents a reduction method tailored to the multi-commodity production network. Her approach combines decomposition methods with concepts of graph theory. In doing so, subnetworks are identified that are suited to be approximated by an aggregated input/output-profit/cost relationship.

Contributions and Results

The main objective of this thesis is to develop a quantitative nonlinear demand model that reflects the influences of all products' prices in the market. This is in addition to other essential influencing factors such as, for example, the change in the economic situation. Therefore, we can summarize the contributions and results we have achieved as follows.

- We determine and analyze crucial influencing factors of demand for commodities to provide a basis for explicit demand models. Prices of all products in the market play a principal role in the demand formation of a specific product to a great extent. In addition to the price of the commodity under consideration, we investigate the dependencies that occur in terms of substitutes and complements. Moreover, we analyze the impacts of the economic situation and describe the influences of the consumer's characteristics.

- Notably, our approach to modeling demand for commodities comprises price-based substitution irrespective of their availabity, which represents a new approach in modeling demand for commodities. For this reason, we investigate in detail the various possibilities to switch production processes on behalf of the customer, which implicate substitution effects on the demand. To integrate this in our model, we aggregate all substitution possibilities and propose a demand model including substitution because of gradual switching.

- We develop an explicit demand model that can be applied to simulate the interactions of supply and demand, in order to determine optimal pricing and production strategies. Moreover, the parameterization chosen allows an easy interpretation. First simulation results of a small part of the petrochemical market show that our demand model integrated in the supply-demand trade network optimization model provides reasonable price and sales quantities results.

- In particular, our demand model for a specific product is a nonlinear decreasing function with respect to its price and includes the change in the economic situation specified by changes of macroeconomic indices. In addition, it reflects the influences of other products' prices on the demand under consideration.

- To identify parameters of our demand model including the influence of the product's own price and selected economic indices we investigate two approaches based on additional assumptions in order to cope with the incomplete data base. First, the heuristic approach takes information on the whole market into account in order to determine the demand parameters by simulating prices and sales quantities. The second approach results in a constrained weighted least-squares problem, where the constraints reflect additional assumptions on the shape of the demand model function.

Structure of the Thesis

The *second chapter* provides an overview of existing demand modeling approaches. In the first instance, we summarize the concept of neoclassical utility theory and present models for demand of households based on this concept. In addition, we summarize important issues with respect to demand that are considered in neoclassical production theory. Moreover, this summary comprises application-specific demand models in supply chain and revenue management. In particular, we review approaches to modeling the influence of substitution on demand in the context of assortment planning problems. Finally, we describe various approaches to modeling demand for specific services or products (e.g., urban traffic or energy).

In the *third chapter*, we give a general description of the characteristics of a demand model for commodities. In addition to the analysis of the relationship between demand and price, we consider the effects of economic indices quantifying the change in the economic situation. Moreover, we examine the effects of the specific consumer's characteristics and the influences of other products' prices. As a result, we transfer our assumptions concerning these factors influencing demand into a mathematical framework to provide a basis for explicit demand functions.

In the *fourth chapter*, we present a supply-demand trade network optimization model to simulate prices and sales quantities in a multi-commodity market. In this regard, we first review a selection of existing production and sales optimization models in the field of supply chain management or chemical engineering. Then, we outline our approach to determine the optimal pricing, production, and transport strategies by maximizing the overall profit in a multi-regional and multi-commodity market. Furthermore, we discuss the specialities of our optimization model with regard to the nonlinear demand-price relationship.

The *fifth chapter* comprises the theory of constrained optimization as well as algorithms to solve inequality constrained nonlinear optimization problems that are used throughout the thesis. In particular, it describes algorithms to solve least-squares problems such as the generalized Gauss-Newton method, which are applied to estimate parameters.

In the *sixth chapter*, we develop an explicit demand model that can be integrated in the supply-demand trade network optimization model applied to a product network of the petrochemical industry. In this context, we extend the basic model that reflects the relationship between demand and price, and include model components for the influence of changes in the economic situation, as well as the influence of substitutable and complementary products.

In the *seventh chapter*, we investigate methods to identify the demand parameters in the situation of incomplete data. In this context, the challenge is to tackle the problem that the presumed nonlinear structure is not evident from the available data. For this reason, we propose two different approaches. First, the heuristic method determines the parameters based on price and sales quantities simulations. Second, we establish a constrained parameter identification problem that can be solved by the generalized Gauss-Newton method.

2 Approaches to Modeling Demand in the Literature

This chapter encompasses a summary of distinct approaches to analyzing and modeling demand. Notably, publications on this subject arise out of different research areas ranging from neoclassical consumer theory to applications in supply chain and revenue management. In consequence of this variety, the contributions selected for this summary show the range of distinct possible applications and the different issues and requirements involved with regard to building appropriate quantitative demand models. Therefore, by summarizing their results we concentrate on describing the aspects of modeling demand and their influence on the respective problems under consideration.
In section 2.1, we summarize the theoretical concept of neoclassical consumer theory and outline important results provided by standard economics literature (e.g., [Var92, Var10, MCWG95]). Furthermore, we review a selection of approaches to modeling demand of households based on utility maximization and outline challenges regarding the empirical applicability of these models. Especially, the presence of aggregated data requires additional attention with regard to modeling demand. In addition to household theory, we survey a selection of papers dealing with the theoretical effects of uncertain demand on production theory based on utility theory.
Section 2.2 contains a review of different approaches to modeling demand in operations research or management science. In this research area, demand models are developed with the purpose to be incorporated in optimization problems of market participants (e.g., a firm, an industrial sector, a service company, or a retailer) to determine pricing and production strategies. Special focus of this summary is on approaches to include substitution in the demand model used to solve assortment planning problems.
In section 2.3, we review distinct demand models that are tailored for specific products (e.g., energy) or services (e.g., urban travel). The variety of these approaches once more display the distinct methods to build mathematical models for demand.

2.1 Modeling Demand in Economic Theory

In economics, analyzing and modeling demand is a central topic be it as independent research area or as part of others fields of research (e.g., equilibrium theory, welfare economics). The concept of neoclassical economics is a very powerful tool for describing consumer behavior. In section 2.1.1, we present the concept of rational choice and utility theory that provides the basis of neoclassical economic analysis. Section 2.1.2 comprises the various models for demand of a household. Furthermore, we discuss challenges with regard to empirical applications. The scope of section 2.1.3 is to give an overview of issues that are considered in neoclassical production theory with respect to demand.

2.1.1 Neoclassical Consumer Theory

In this section, we present the theoretical framework that provides the basis for establishing demand functions in neoclassical consumer theory. For this purpose, we follow the book of Deaton and Muellbauer [DM80b] and begin with listing the axioms of choice.
In doing so, we adopt their notation and denote the prices by $\boldsymbol{p} = (p_1, \ldots, p_n)'$, the quantities by $\boldsymbol{q} = (q_1, \ldots, q_n)'$, and the disposable budget by x. If two bundles $\boldsymbol{q^1}$ and $\boldsymbol{q^2}$ consisting of n products are compared and $\boldsymbol{q^1}$ is at least as good as $\boldsymbol{q^2}$, their notation is $\boldsymbol{q^1} \succsim \boldsymbol{q^2}$. Let the utility function $v(\boldsymbol{q})$ be a monotone increasing function that assigns a value to each bundle. Hence, it expresses the preferences of a consumer being faced with the set of available bundles.[1] For a detailed consideration of preferences, choice, and utility we refer to [MCWG95, Var92, Var10].

Axioms of choice.

1. *Reflexivity.* $\boldsymbol{q} \succsim \boldsymbol{q}$ *for each possible bundle* $\boldsymbol{q}$.
2. *Completeness. Any two bundles in the choice set* $\boldsymbol{q^1}$ *and* $\boldsymbol{q^2}$ *can be compared:* $\boldsymbol{q^1} \succsim \boldsymbol{q^2}$*, or* $\boldsymbol{q^2} \succsim \boldsymbol{q^1}$.
3. *Transitivity or consistency.* $\boldsymbol{q^1} \succsim \boldsymbol{q^2}$ *and* $\boldsymbol{q^2} \succsim \boldsymbol{q^3}$ *implies* $\boldsymbol{q^1} \succsim \boldsymbol{q^3}$.
4. *Continuity. Given bundle* $\boldsymbol{q_1}$*, let* $A(\boldsymbol{q_1}) = \{\boldsymbol{q} | \boldsymbol{q} \succsim \boldsymbol{q^1}\}$ *contain all bundles that are at least as good as* $\boldsymbol{q^1}$ *and let* $B(\boldsymbol{q_1}) = \{\boldsymbol{q} | \boldsymbol{q^1} \succsim \boldsymbol{q}\}$ *contain all bundles that are not better than* $\boldsymbol{q^1}$*. Then, both sets* $A(\boldsymbol{q_1})$ *and* $B(\boldsymbol{q_1})$*, for any* $\boldsymbol{q^1}$ *in the choice set, contain their own boundaries.*
5. *Nonsatiation. The utility function* $v(\boldsymbol{q})$ *is nondecreasing in each* q_i*,* $i = 1, \ldots, n$ *and increasing in at least one* q_i*,* $i = 1, \ldots, n,$*.*
6. *Convexity.* $\boldsymbol{q^1} \succsim \boldsymbol{q^0}$ *implies* $\lambda \boldsymbol{q^1} + (1 - \lambda)\boldsymbol{q^0} \succsim \boldsymbol{q^0}$ *for* $0 \leq \lambda \leq 1$*.*[2]

The first three axioms allow a preference ordering, but are not sufficient to establish a utility function. If, however, the first four axioms of choice hold, the preferences can be expressed by such a utility function. Finally, the fifth axiom ensures that the total budget is spent in order to maximize the utility. Hence, the theory outlined in the following is mainly based on these five axioms.
To begin with, we present the utility maximization problem of a consumer, where his expenses are constrained by his disposable income x. From now on, we assume strict convexity of preferences and smoothness of the utility function because, in this case, the optimization problem can be solved using differential calculus. Examples of nonconvex

[1] Note that utility functions are only defined up to the transformation by a monotone increasing function, i.e., their values have no meaning except the comparability.
[2] Preferences are convex if and only if the representing utility function is quasi-concave.

preferences are shown by Deaton and Muellbauer [DM80b].
Given prices $p_i,\ i = 1, \ldots, n$, and income x, the consumer's choice problem is

$$\max_{\boldsymbol{q}} v(\boldsymbol{q}) \text{ subject to } \sum_{i=1}^{n} p_i q_i = x, \tag{2.1}$$

where the equality constraint is due to the fifth axiom of choice and also known as *Walras' law* (cf. [MCWG95]). The solution functions with respect to prices $\boldsymbol{p}$ and income x of problem (2.1) are called *Marshallian* demand functions $q_i = g_i(x, \boldsymbol{p}),\ i = 1, \ldots, n$. In addition, if the prices are fixed, the relation $q_i = g_i^*(x),\ i = 1, \ldots, n$, is called *Engel curve*.
Problem (2.1) can be reformulated by its dual problem: here, the consumer minimizes his expenses $x = \boldsymbol{p} \cdot \boldsymbol{q}$ ensuring that a certain level of utility u is reached.[3] Hence,

$$\min_{\boldsymbol{q}} \boldsymbol{p} \cdot \boldsymbol{q} \text{ subject to } v(\boldsymbol{q}) = u. \tag{2.2}$$

This expenditure minimization problem results in demand functions with respect to u and $\boldsymbol{p}$, which are called *Hicksian* demand functions. Both solutions coincide, i.e.,

$$q_i = h_i(u, \boldsymbol{p}) = g_i(x, \boldsymbol{p}), \qquad i = 1, \ldots, n.$$

Substituting $g_i(x, \boldsymbol{p}),\ i = 1, \ldots, n$, into the optimization problem (2.1) results in the indirect utility function

$$u = v(q_1, \ldots, q_n) = v(g_1(x, \boldsymbol{p}), \ldots, g_n(x, \boldsymbol{p})) = \psi(x, \boldsymbol{p}). \tag{2.3}$$

Likewise, substituting $h_i(u, \boldsymbol{p}),\ i = 1, \ldots, n$, into optimization problem (2.2) leads to the cost function with respect to utility u and prices $\boldsymbol{p}$, i.e.,

$$x = \sum_{i=1}^{n} p_i h_i(u, \boldsymbol{p}) = c(u, \boldsymbol{p}), \tag{2.4}$$

which satisfies the following properties.

Properties of the cost function.

1. *Homogeneity of degree one in prices:* $c(u, \theta\boldsymbol{p}) = \theta c(u, \boldsymbol{p})$ *with* $\theta > 0$.

2. *The cost function increases if* u *increases.*

3. *The cost function is nondecreasing, concave, and continuous in* $\boldsymbol{p}$*. In addition, the first and the second derivatives with respect to* $\boldsymbol{p}$ *exist everywhere except at a set of measure zero. Moreover, the cost function increases if at least one price* $p_i,\ i = 1, \ldots, n$*, increases.*

[3] For more information on dual problems, we refer to standard optimization textbooks (e.g. [NW06] or [BV04] for convex optimization problems).

4. *The Hicksian demand function $q_i,\ i = 1, \ldots, n$, are equal to the partial derivatives of the cost function with respect to prices*

$$q_i = h_i(u, \boldsymbol{p}) \equiv \frac{\partial c(u, \boldsymbol{p})}{\partial p_i}$$

if they exist.

The fourth property is known as *Shephard's Lemma* and relates the cost function to the corresponding cost-minimizing demand function.
Furthermore, differentiation of the indirect utility function $\psi(c(u,p),p) = u$ with respect to p_i leads to *Roy's identity* (see [DM80b] for details)

$$q_i = g_i(x, \boldsymbol{p}) = -\frac{\partial \psi / \partial p_i}{\partial \psi / \partial x}, \quad i = 1, \ldots, n. \tag{2.5}$$

In the following, we list the properties of *Hicksian* and *Marshallian* demand functions (see again [DM80b] for more information).

Properties of utility-based demand functions.

1. *Adding Up. The sum of both Hicksian and Marshallian demands times prices is equal to total expenditure x*

$$\sum_{i=1}^{n} p_i h_i(u, \boldsymbol{p}) = \sum_{i=1}^{n} p_i g_i(x, \boldsymbol{p}) = x.$$

2. *Homogeneity. Both the Hicksian demand functions and the Marshallian demand function are homogeneous of degree zero: the former in prices and the latter in expenditure and prices*

$$h_i(u, \theta \boldsymbol{p}) = h_i(u, \boldsymbol{p}) = g_i(\theta x, \theta \boldsymbol{p}) = g_i(x, \boldsymbol{p}),$$

where $\theta > 0$.

3. *Symmetry. Differentiating the Hicksian demand functions $h_i(u, \boldsymbol{p}),\ i = 1, \ldots, n$, with respect to prices $p_j,\ j \neq i,\ j = 1, \ldots, n$, leads to*

$$\frac{\partial h_i(u, \boldsymbol{p})}{\partial p_j} = \frac{\partial h_j(u, \boldsymbol{p})}{\partial p_i}, \quad i \neq j,\ i, j = 1, \ldots, n.$$

.

4. *Negativity. The $n \times n$-matrix with elements $\frac{\partial h_i}{\partial p_j},\ i, j = 1, \ldots, n$, is negative semidefinite, i.e.,*

$$\sum_{i=1}^{n} \sum_{j=1}^{n} \xi_i \xi_j \frac{\partial h_i}{\partial p_j} \leq 0 \tag{2.6}$$

for any n-vector $\boldsymbol{\xi}$.

Moreover, the symmetric and negative semidefinite matrix with entries $s_{ij} = \frac{\partial h_i}{\partial p_j}$ is known as *substitution matrix* or *Slutsky matrix* of compensated price responses. Equation (2.6) implies for all i

$$s_{ii} \leq 0, \quad i = 1, \dots, n,$$

so that we can infer that the demand of good $i,\ i = 1, \dots, n$ falls or remain unchanged if the respective price $p_i,\ i = 1, \dots, n$ rises. This result is also known as *law of demand.*

Remark 2.1. Mas-Colell [MCWG95] distinguishes between the property of *compensated law of demand* if

$$(\boldsymbol{p}^1 - \boldsymbol{p}^2) \cdot (h_i(u, \boldsymbol{p}^1) - h_i(u, \boldsymbol{p}^2)) \leq 0, \quad i = 1, \dots, n, \tag{2.7}$$

and the property of *uncompensated law of demand* if

$$(\boldsymbol{p}^1 - \boldsymbol{p}^2) \cdot (g_i(x, \boldsymbol{p}^1) - g_i(x, \boldsymbol{p}^2)) \leq 0, \quad i = 1, \dots, n. \tag{2.8}$$

More generally, this law implies that if one thinks of the product as a collection of goods in a fixed ratio and its price is equal to the prices of its parts, the demand of this product also decreases if the respective price increases. This implication is known as the *law of demand* in the multi-commodity case. We refer to [JQ08] for a survey of the *law of demand* in different contexts. Likewise, they underline that the *law of demand* in its different versions also plays an important role in equilibrium theory, because strict monotonicity of excess demand implies uniqueness and stability of an equilibrium.
So far, the *substitution matrix* is written in terms of the *Hicksian demand.* Through the *Slutsky equation*

$$s_{ij} = \frac{\partial h_i}{\partial p_j} = \frac{\partial g_i}{\partial x} \cdot q_j + \frac{\partial g_i}{\partial p_j}, \quad i, j = 1, \dots, n, \tag{2.9}$$

the elements $s_{ij},\ i, j = 1, \dots, n$ can be expressed using the *Marshallian demand* functions. This notation provides some advantages: since the right-hand site of equation (2.9) is in principle observable, the substitution matrix can be calculated empirically and, hence, symmetry and negativity are testable. Furthermore, equation (2.9) reveals that the effects of a price change on *Marshallian* demand functions $\frac{\partial g_i}{\partial p_j},\ i, j = 1, \dots, n$, can be decomposed into a substitution effect $\frac{\partial h_i}{\partial p_j},\ i, j = 1, \dots, n$, and an income effect $\frac{\partial g_i}{\partial x} \cdot q_j,\ i, j = 1, \dots, n$. This means, changes in the price of a good implies that the exchange rate, for which two goods are substituted, varies, and also that the purchasing power of income changes (cf. [Var10]). Likewise, this notation allows for new information regarding the *Marshallian* demand functions. For example, the *law of demand* is not necessarily valid: a good $i,\ i = 1, \dots, n$, can exhibit a positive price derivative, because the negative price compensated response is outweighted by a positive income effect (cf. [DM80b]), which is a phenomenon that is, however, quite rare.[4] The connections of the terminology explained so far is illustrated in figure 2.1.

[4] A popular example for these *Giffen* goods are potatoes in the 19th century. People spending their total income for food purchase more potatoes than meat if the price of potatoes rises. In comparison, *inferior goods* are products for which the demand increases if income decreases.

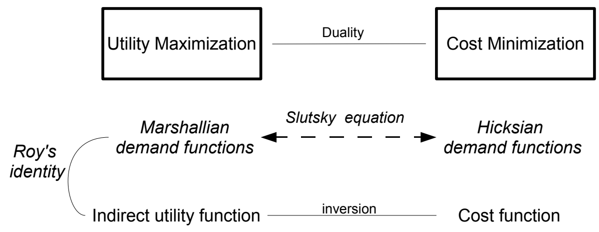

Figure 2.1: Connections of utility maximization and cost minimization in neoclassical consumer theory

We are now in the position to present a very important result of the neoclassical consumer theory, which is known as the *integrability problem*: given a set of goods, their demand functions are the result of the consumer's utility maximization and hence, there is a preference ordering if and only if the demand functions add up, are homogeneous of degree zero, and the substitution matrix is symmetric and negative semidefinite.
Subsequently, for the sake of completeness, we present additional useful terminology in the context of demand analysis: we start with presenting the *weak axiom of revealed preferences* according to the definition of Mas-Colell [MCWG95].

Definition 2.1. *Weak Axiom of Revealed Preferences*
Given two pairs of prices and income $(\boldsymbol{p}^1, x^1)$ *and* $(\boldsymbol{p}^2, x^2)$

$$\boldsymbol{p}^1 \cdot \boldsymbol{q}(x^2, \boldsymbol{p}^2) \leq x^1 \quad \textit{implies} \quad \boldsymbol{p^2} \cdot \boldsymbol{q}(x^1, \boldsymbol{p}^1) > x_2.$$

In words, under the assumption of unchanged preferences, if $\boldsymbol{q}(x^1, \boldsymbol{p}^1)$ is chosen over $\boldsymbol{q}(x^2, \boldsymbol{p}^2)$, although $\boldsymbol{q}(x^2, \boldsymbol{p}^2)$ is also affordable, then under no conditions $\boldsymbol{q}(x^2, \boldsymbol{p}^2)$ is preferred to $\boldsymbol{q}(x^1, \boldsymbol{p}^1)$. That means, if $\boldsymbol{q}(x^2, \boldsymbol{p}^2)$ is chosen, $\boldsymbol{q}(x^1, \boldsymbol{p^1})$ is not affordable. Note that this property is an implication of utility maximization. The strong axiom of revealed preferences implies that, for a given set $(\boldsymbol{p}^1, x^1), \ldots, (\boldsymbol{p}^n, x^n)$, if $\boldsymbol{q}(x^1, \boldsymbol{p}^1)$ is either directly or indirectly preferred to $\boldsymbol{q}(x^n, \boldsymbol{p}^n)$, $\boldsymbol{q}(x^n, \boldsymbol{p}^n)$ cannot be chosen over $\boldsymbol{q}(x^1, \boldsymbol{p}^1)$. Choices for which the strong axiom holds are consistent with the utility maximization model. We refer to [Var92, Var10, MCWG95] for a more detailed discussion of revealed preferences. Lastly, before passing on to the modeling approaches, there remain the elasticities to be defined (cf. [MCWG95, Var92, Var10]).

Definition 2.2. *Total Expenditure Elasticity*

$$e_i = \frac{\partial g_i(x, \boldsymbol{p})}{\partial x} \cdot \frac{x}{g_i(x, \boldsymbol{p})} = \frac{\partial \log(g_i(x, \boldsymbol{p}))}{\partial \log(x)}, \quad i, j = 1, \ldots, n. \tag{2.10}$$

If $e_i > 0, \ i = 1, \ldots, n$, good i is classified to be a *normal* good, whereas, if $e_i < 0, \ i = 1, \ldots, n$, good i is termed *inferior* good. If $e_i > 1, \ i = 1, \ldots, n$, good i is a luxury good, and if $e_i < 1, \ i = 1, \ldots, n$, it is classified as a necessity.

Definition 2.3. *Price Elasticity*

$$e_{ij} = \frac{\partial g_i(x, \boldsymbol{p})}{\partial p_j} \cdot \frac{p_j}{g_i(x, \boldsymbol{p})} = \frac{\partial \log(g_i(x, \boldsymbol{p}))}{\partial \log(p_j)}, \quad i, j = 1, \ldots, n. \tag{2.11}$$

If $e_{ij} > 0,\ i, j = 1, \ldots, n$, the goods are classified as gross substitutes, and if $e_{ij} < 0,\ i, j = 1, \ldots, n$, the goods under consideration are gross complements. This definition is mostly frequently applied in economics text books although there are alternative definitions which additionally include further aspects (see [BS09] for other elasticity definitions). For example, Hicks [Hic46] suggested to make use of the *Slutsky equation* (2.9) to classify goods, since the classification above ignores the income effect. Consequently, according to this definition good i and good j are complements if $s_{ij},\ i, j = 1, \ldots, n$, is negative, and they are substitutes if s_{ij} is positive.
In contrast to derivatives, these measures capturing the demand responsiveness are unit-free. To conclude, the elasticity of substitution indicates how easy a good can be substituted by another ensuring that the utility level remains unchanged. Subsequently, we adopt the definition of Varian [Var92].[5]

Definition 2.4. *Elasticity of Substitution*
Given two goods q_i and q_j

$$e_{ij}^{sub} = \frac{MRS}{q_j/q_i} \frac{d(q_j/q_i)}{d(MRS)} = \frac{d(\ln(q_j/q_i)}{d(\ln(MRS))}, \quad i, j = 1, \ldots, n, \tag{2.12}$$

where the marginal rate of substitution for sustaining the utility level is given by $MRS = -\frac{\partial U(\boldsymbol{q})/\partial q_i}{\partial U(\boldsymbol{q})/\partial q_j}$.

2.1.2 Demand of Households

In this section, we summarize the properties of selected approaches to modeling demand that are presented in established theory books. Likewise, we give a short overview of empirical results and list shortcomings, since not all of these models, for example, fulfill the integrability conditions. Concerning the chronology we orientate ourselves by that of Deaton and Muellbauer [DM80b] supplemented by examples of Barnett [BS09]. Similarly, Theil [TC87] present certain models of consumption theory.
In doing so, the first two models presented in this section are not established with reference to the utility theory and hence, do not exhibit the properties described above. Their presentation starts with the *log-log Demand System* that models the logarithm of demand as function of income and prices of the goods under consideration

$$\log q_i = \alpha_i + \eta_i \log x + \sum_{j=1}^{n} \eta_{ij} \log p_j, \quad i = 1, \ldots, n. \tag{2.13}$$

[5] The elasticity of substitution is also an important index in production theory. We refer to [Var92, Hic63] for more information.

Here, the coefficients α_i, η_i and η_{ij} are constant. In accordance with the definitions 2.2 and 2.3, η_i is the income elasticities of demand and η_{ij} is the price elasticity of good i. For this reason, this approach has often been estimated on time series to measure the elasticities. However, Deaton and Muellbauer [DM80b] show that equation (2.13) does not satisfy adding up.
Under the *Working model*, the budget share w_i for good i, $i = 1, \dots, n$, is specified as function of the logarithm of income x

$$w_i = \frac{p_i \cdot q_i}{x} = \alpha_i + \beta_i \log x, \quad i = 1, \dots, n. \tag{2.14}$$

The fact that the sum of the budget shares is equal to 1 implies $\sum_{i=1}^n \alpha_i = 1$ and $\sum_{i=1}^n \beta_i = 0$. Hence, this model approach is consistent with adding up.
Stone [Sto54b] starts to combine the theory of preferences with the traditional approaches to modeling demand as function of prices and income. By proposing to individually model the demand for each commodity based on utility maximization, he offers flexibility. Deaton and Muellbauer [DM80b] present his methods and results using the example of model (2.13). Substituting the *Slutsky equation* (2.9) in elasticity form $e_{ik} = e^*_{ij} - e_i w_j$, where e^*_{ij} is the compensated cross-price elasticity $\frac{\partial h_i}{\partial p_j}$, they derive

$$\log q_i = \alpha_i + e_i \log(x/P) + \sum_{j=1}^{n} e^*_{ij} \log p_j, \quad i = 1, \dots, n, \tag{2.15}$$

where $\sum_{j=1}^n w_j \log p_j = \log(P)$. If $\sum_{j=1}^n e^*_{ij} = 0$, homogeneity is fulfilled. Therefore, all prices can be deflated by the index P and equation (2.15) is approximately equivalent to

$$\log q_i = \alpha_i + e_i \log(x/P) + \sum_{j=1}^{n} e^*_{ij} \log(p_j/P), \quad i = 1, \dots, n. \tag{2.16}$$

Since $e^*_{ij} = 0$ for unrelated good i and j, the sum in the last term of equation (2.16) is reduced to a set K of substitutes and complements of good i, $i = 1, \dots, n$.
Following the chronology of Deaton and Muellbauer [DM80b], an alternative modeling approach is the *Linear Expenditure System* that is also studied by Stone [Sto54a]. Imposing the restrictions of adding up, homogeneity, and symmetry on the general linear demand model

$$p_i q_i = \beta_i x + \sum_{j=1}^{n} \beta_{ij} p_j, \quad i = 1, \dots, n, \tag{2.17}$$

leads to

$$p_i q_i = p_i \gamma_i + \beta_i (x - \sum_j p_j \gamma_j), \quad i = 1, \dots, n, \tag{2.18}$$

where $\sum_{j=1}^n \beta_j = 1$. This is the only valid form of equation (2.17) satisfying the above restrictions. If $\beta_i \geq 0$ for $i = 1, \dots, n$ and $x \geq \sum_{i=1}^n p_i \gamma_i$ implies $q_i \geq \gamma_i$ for $i = 1, \dots, n$, the corresponding cost function $c(u, \boldsymbol{p}) = \sum_{i=1}^n p_i \gamma_i + u \prod_{i=1}^n p_i^{\beta_i}$ is concave and hence,

equation (2.18) is consistent with utility maximization.[6] The *linear expenditure system* provides the following interpretation: if γ_i $\forall i = 1, \ldots, n$, are positive, they can be seen as minimum required quantities that are bought first. The remaining disposable income is then split up between the goods.
Nevertheless, their analyses and the estimation results of Stone show that the *linear expenditure system* is also too restrictive. Among other results, the estimation results, for example, indicate that price and income elasticities are proportional.
According to Barnett and Serletis [BS09], the *Rotterdam model* studied by Theil [The65] and Barten [Bar67] is a mile stone in empirical demand analysis. Having totally differentiated equation (2.13), they derive

$$d \log q_i = e_i d \log x + \sum_{j=1}^{n} e_{ij} d \log p_j, \quad i = 1, \ldots, n, \tag{2.19}$$

where they assume that e_i and e_{ij} are not necessarily constant. Using again the Slutsky decomposition leads to

$$w_i d \log q_i = b_i d \log \bar{x} + \sum_{j=1}^{n} c_{ij} d \log p_j, \quad i = 1, \ldots, n, \tag{2.20}$$

where

$$\begin{aligned} d \log \bar{x} &= d \log x - \sum_{k=1}^{n} w_k d \log p_k = \sum_{k=1}^{n} w_k d \log q_k, \\ b_j &= w_i e_i, \\ c_{ij} &= w_i e_{ij}^{*} = \frac{p_i \cdot p_j \cdot s_{ij}}{x}. \end{aligned}$$

If the differentials are replaced with finite approximations and under the assumptions that b_i and c_{ij} are constant, an estimation of the parameters is possible. The adding-up restrictions $\sum_{k=1}^{n} b_k = 1$ and $\sum_{k=1}^{n} c_{kj} = 0$ for all j, are already included in the data and hence are no further constraint (cf. [DM80b]). Homogeneity (i.e., $\sum_{i=1}^{n} c_{ji} = 0$ for all j) and symmetry (i.e., $c_{ij} = c_{ji}$ since symmetry of the substitution matrix implies symmetry of C), however, can be tested. Among others, Deaton [Dea74] estimates different versions of this model using British household consumption data from the twentieth century. His tests, as others before, reveals that homogeneity is rejected, while symmetry as an additional restriction is not very strict and decisive. As for him, he emphasizes the advantage that the symmetric version of the Rotterdam model provides for the first time a symmetric substitution and, hence, allows for an identification of substitutes and complements (see [DM80b] or [Dea74] for a detailed discussion of the estimation results).
In contrast, there is a variety of contributions that use a particular functional form for the utility function, the indirect utility, or the cost function following the approach developed

[6]See [TC87, Var92] for the derivation of the *linear expenditure system* on the basis of a specific utility function.

by Diewert [Die71]. However, functional forms that are consistent with the theoretical restrictions prove to be too stringent. For example, the *CES (Constant Elasticity of Substitution)* functional form

$$U(\boldsymbol{q}) = \sum_{j=1}^{n} (\alpha_j q_j^r)^{(1/r)}, \quad 0 < \alpha_j < 1, \ -\infty < r < 1, \tag{2.21}$$

results in constant elasticities $1/(1-r)$ between any two pairs of goods (cf. [BS09]). Alternatively, *(locally) flexible functional forms* represent approximations to a (indirect) utility function or a cost function that provide enough parameters in order to derive the corresponding demand system. However, although these flexible demand systems allows for the inclusion of neoclassical microeconomic theory in econometric applications, the theory does not hold for all prices and income and, thus, global integrability is not possible (see also [BS09] for further information). An example for *flexible functional forms* is the *translog indirect utility function* studied by Christensen et al. [CJL75]

$$\psi(\boldsymbol{p}, x) = \alpha_0 + \sum_{i=1}^{n} \alpha_i \log\left(\frac{p_i}{x}\right) + \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} \beta_{ij} \log\left(\frac{p_i}{x}\right) \log\left(\frac{p_j}{x}\right) \tag{2.22}$$

that approximates the indirect utility function for appropriate parameters α_0, α_i, $i = 1, \ldots, n$, and β_{ij}, $i, j = 1, \ldots, n$ (see [CJL75, BS09] for more details). Another example is the *AIDS - Almost ideal demand system* developed by Deaton and Muellbauer [DM80a, DM80b]. Their choice of the specific cost function

$$\log c(u, \boldsymbol{p}) = a(\boldsymbol{p}) + u b(\boldsymbol{p}), \tag{2.23}$$

where (see also [DM80b])

$$\begin{aligned} a(\boldsymbol{p}) &= \alpha_0 + \sum_i \alpha_i \log p_i + \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} \gamma_{ij}^* \log p_i \log p_j, \\ b(\boldsymbol{p}) &= \beta_0 \prod_{i=1}^{n} p_i^{\beta_i}, \end{aligned}$$

ensures that the resulting demand functions are first-order approximations to any demand function that is consistent with utility theory. Moreover, $c(u, \boldsymbol{p})$ is homogeneous in $\boldsymbol{p}$ if $\sum_{i=1}^{n} \alpha_i = 1$, $\sum_{i=1}^{n} \gamma_{ij}^* = \sum_{j=1}^{n} \gamma_{ij}^* = \sum_{i=1}^{n} \beta_i = 0$, and represents a special class of preferences called *PIGLOG*, which allows exact aggregation of all consumers' demand.[7] Given

$$\frac{\partial \log c(u, \boldsymbol{p})}{\partial \log p_i} = \frac{p_i q_i}{c(u, \boldsymbol{p})} = w_i \tag{2.24}$$

[7] A representative consumer exists if the average budget share can be expressed as a function of prices and a scalar, which is again a function of all prices and all incomes. This is, for example, the case if the budget shares of the households result from a cost function with a "price-independent generalized linearity - logarithm (PIGLOG)" form (see [DM80a, DM80b] for more information). Hence, the market demand can be seen as the demand of a rational representative consumer. In section 2.1.2.1 we summarize important results in the field of aggregation.

and $x = c(u, \boldsymbol{p})$ they substituted for u and derived

$$w_i = \alpha_i + \sum_j \gamma_{ij} \log p_j + \beta_i \log(x/P), \tag{2.25}$$

where P is defined by

$$\log P = \alpha_0 + \sum_{k=1}^{n} \alpha_k \log p_k + \frac{1}{2} \sum_{k=1}^{n} \sum_{l=1}^{n} \gamma_{kl} \log p_k \log p_l \tag{2.26}$$

and $\gamma_{ij} = \frac{1}{2}(\gamma_{ij}^* + \gamma_{ji}^*) = \gamma_{ji}$. The theoretical restrictions are satisfied if

$$\begin{array}{ll} \sum_{i=1}^{n} \alpha_i = 1,\ \sum_{i=1}^{n} \beta_i = 0,\ \sum_{i=1}^{n} \gamma_{ij} = 0 & \text{(Adding up)} \\ \sum_{i=1}^{n} \gamma_{ji} = 0,\ j = 1, \ldots, n & \text{(Homogeneity)} \\ \gamma_{ij} = \gamma_{ji},\ i = 1, \ldots, n,\ j = 1, \ldots, n & \text{(Symmetry).} \end{array}$$

The change of expenditures are influenced by β_i, where the sign of β_i indicates whether goods are luxuries or necessities. Having set up the system of demand functions for aggregated demand of households, parameter estimation is realized with aggregate time series data to test the model. Once more, tests of homogeneity show conflict with the theory. Deaton and Muellbauer [DM80b] note that the imposition of homogeneity provokes correlation in the errors, which is, among others, caused by the fact that the dynamical behavior of demand is insufficiently modeled. Furthermore, the test for symmetry provides an indication for a further rejection. However, as in the *Rotterdam model*, they state that it is not possible to have a unique statement about the rejection of symmetry beyond homogeneity (cf. [DM80b]). Nevertheless, they emphasize that their model possesses considerable advantages compared to others, and serves as a tool for testing, extending, and improving demand analysis (cf. [DM80a]).
To conclude, we aim to summarize the remarks of Deaton and Muellbauer [DM80b] with respect to arising problems in the application of these theoretical models. They state that a more detailed theoretical analysis is necessary to obtain better illustrative models. Hence, there are a range of further aspects that are fundamental for better comprehending the customer's decision-making.

- Aggregation over commodities: otherwise detailed analysis of a large number of commodities is too complex.[8]
- Aggregation over consumers: so far, many studies have neglected the emerging problems and have treated aggregated demand as if there was exact one single representative consumer, but this did not necessarily hold.[9]
- Relation and influence of labor supply, savings, and total expenditure, which is not necessarily given exogenously and to be spent.

[8] We refer to [Hil94] who distinguishes between elementary commodities and commodities aggregates and establishes a relation between them prior to his empirical studies.
[9] We will further consider important aspects of aggregation theory in section 2.1.2.1.

- Inclusion of durable commodities, product availability, or rationing of products is essential.
- There is uncertainty regarding the consumer's behavior in the short and long run. For example, they do not have full information about the quality or the durability of their purchases. Likewise, they do not know all current prices when they decide to purchase.

In the course of their book, Deaton and Muellbauer [DM80b] investigate the theoretical impacts of the issues mentioned above. In section 2.1.2.1, we take up the question of appropriate aggregation and give a summary of research topics. In this context, Barnett [BS09] state that extensions of the basic demand models include household-production/labor-combinations and intertemporal utility models for dynamic household-production models. For more information about intertemporal models, we refer to [MCWG95, Var10, DM80b]. In section 2.1.3, we give an overview of questions concerning effects of demand in production theory.

2.1.2.1 Aggregation Theory

In the context of modeling demand, aggregation over consumers is an important issue because of several reasons. Predominantly, only aggregated data is available for case studies. A survey of research questions regarding aggregated demand is provided by Mas-Colell [MCWG95]. Among others, these comprise the functional form and general properties of the aggregated demand function. Likewise, Deaton and Muellbauer [DM80b] investigated under which conditions the aggregated behavior can be expressed as function of prices and aggregated income, i.e., as the demand of a single representative consumer. Hildenbrand [Hil94, Hil08] studies under which conditions the aggregated demand fulfills the *law of demand*.

In the following, we will consider these topics in more detail. Concerning the former question, we again adopt the notation of Deaton and Muellbauer [DM80b] (cf. also [MCWG95]). Exact linear aggregation, i.e., writing aggregate or market demand of good $q_i,\ i = 1, \dots, n$ as function of prices $p_i,\ i = 1, \dots, n$ and aggregated expenditure $\bar{x}$

$$\bar{q}_i = \frac{1}{H} \sum_h q_i^h(x^h, \boldsymbol{p}) = q_i(\bar{x}, \boldsymbol{p}), \quad i = 1, \dots, n, \tag{2.27}$$

necessitates that the marginal propensities to spend $\partial q_i^h / \partial x^h,\ i = 1, \dots, n$, are identical for all households, which implies that

$$q_i^h = \alpha_i^h(\boldsymbol{p}) + \beta_i(\boldsymbol{p}) x^h, \quad i = 1, \dots n,\ h = 1, \dots, H, \tag{2.28}$$

where $\beta_i(\boldsymbol{p})$ is identical for all households $h = 1, \dots, H$. Hence, $\bar{q}_i = \alpha_i(\boldsymbol{p}) + \beta_i(\boldsymbol{p})\bar{x}$. If this holds for all $\bar{x}$, $\alpha_i^h(\boldsymbol{p}) = \alpha_i(\boldsymbol{p}) = 0$ so that q_i^h and $\bar{q}_i$ are proportional to x^h and $\bar{x}$.
If, in addition, consistence with utility maximization is required, the corresponding cost function must be of the form

$$c^h(u^h, \boldsymbol{p}) = a^h(\boldsymbol{p}) + u^h \cdot b(\boldsymbol{p}) \tag{2.29}$$

(see [DM80b] for the proof and the connection of the coefficients of q_i^h and $c^h(u^h, \boldsymbol{p})$).[10] This, however, is quite stringent, because commodities that are only consumed at higher budget are not included at all. Consequently, linear aggregation is rather reasonable for broadly defined groups of commodities.
Alternatively, nonlinear aggregation also allows for new consumers entering the market. By aggregating over expenditure patterns instead of quantities

$$\bar{w}_i = \frac{p_i \sum_h q_i^h}{\sum_h x^h} = \sum_{h=1}^{H} \frac{x^h}{\sum x^h} \cdot w_i^h \tag{2.30}$$

they consider the average aggregate budget share $\bar{w}_i$ which is the weighted average of individual household patterns. Basically, $\bar{w}_i$ depends on all prices $p_i,\ i = 1, \ldots, n$, and each household's expenditure $x^h,\ h = 1, \ldots, H$. Requiring that $\bar{w}_i$ can be written as function of prices and a representative level of total expenditure x_0, it can be assumed to represent a single representative consumer. Therefore,

$$\bar{w}_i = \frac{\partial \log c(u_0, \boldsymbol{p})}{\partial \log p_i} = \sum_{h=1}^{H} \frac{x^h}{\sum x^h} \frac{\partial \log c^h(u_0^h, \boldsymbol{p})}{\partial \log p_i}, \tag{2.31}$$

where $c(u_0, \boldsymbol{p})$ is the cost function of the representative consumer and $c^h(u_0^h, \boldsymbol{p})$ is the cost function of household h. The conditions for the cost functions $c^h(u_0^h, \boldsymbol{p})$ so that a representative consumer exists and exact nonlinear aggregation is possible are provided by Deaton and Muellbauer [DM80b] and are called "generalized linearity (GL)"-conditions.[11] For more details, we refer to [DM80b]. Alternative contributions considering the aggregated demand as function of characteristics of the wealth/income distribution are presented by [MCWG95, Hil08].
Concerning the properties of the aggregated demand function, Hildenbrand [Hil94, Hil08] identifies under which conditions the *law of demand* is satisfied by market demand.[12] In doing so, he does not require that the individual demand function satisfies the *law of demand* but investigates necessary and sufficient characteristics of the distribution of single demand of all households with fixed income in case of a very large and heterogenous population so that the mean demand is strictly decreasing, i.e.,

$$(\boldsymbol{p^1} - \boldsymbol{p^2}) \cdot (D(\boldsymbol{p^1}) - D(\boldsymbol{p^2})) < 0, \quad \boldsymbol{p^1}, \boldsymbol{p^2} \in \mathbb{R}^L_{++}. \tag{2.32}$$

In general, he assumes that the demand of each household depends on the price system, the expected future prices, the present and the expected future income, the past consumption, and the household characteristics. At this point, we don't pursue this topic further and refer to [Hil94] for a detailed presentation of his research results.

[10] The corresponding preferences of this cost function are called quasi-homothetic preferences.
[11] Special cases are called PIGL (*price independent generalized linearity*) and PIGLOG. For example, the cost function of *AIDS* model described in section 2.1.2 satisfies the conditions of PIGLOG.
[12] Note that the law of demand refers to a hypothetical situation and, hence, cannot be tested empirically.

2.1.3 Effects of Demand in the Context of Production Theory

In the following section, we will proceed with focusing on the profit maximization, respectively expenditure minimization of firms. For a general comparison of firms and households, we refer to [Spu09]. The concepts of utility maximization in the *neoclassical theory* can also be applied to describe behavior of a firm. Mas-Colell [MCWG95] and Spulber [Spu09] state that the firm's objective is profit maximization (cf. "Fisher-separation theorem" discussed in [Spu09]). Given a vector of prices for inputs and outputs the firm aims to maximize profit, i.e.,

$$\max_{\boldsymbol{y}} \boldsymbol{p} \cdot \boldsymbol{y} \quad \text{subject to } \boldsymbol{y} \in Y, \tag{2.33}$$

where X is the set of all production possibilities, or, alternatively, to minimize costs

$$\min_{\boldsymbol{y}} \boldsymbol{w} \cdot \boldsymbol{y} \quad \text{subject to } \boldsymbol{y} \in Y. \tag{2.34}$$

If the firm only produces one good $y = f(\boldsymbol{z})$, where $f(\cdot)$ is the production function dependent on the input quantities $\boldsymbol{z}$, the profit maximization problem can be written as

$$\max p \cdot f(\boldsymbol{z}) - \boldsymbol{w} \cdot \boldsymbol{z}, \tag{2.35}$$

where the scalar p is the price for output $f(\boldsymbol{z})$. Then, the optimal input quantity function $z_i(p, \boldsymbol{w})$ for input product i with respect to a vector of prices $(p, \boldsymbol{w})'$ is called factor demand function. In parallel to the demand function in section 2.1.1, $x_i(p, \boldsymbol{w})$ is homogeneous of degree zero, has a negative slope and its substitution matrix is symmetric (see [Var92]). For further results regarding the firm's behavior (weak axiom of profit maximization, properties of profit function), we refer the interested reader to [Var92, MCWG95].

In general, if the firm operates under imperfect competition, the output prices also become decision variables, i.e., the price depends on the quantity in the market $\boldsymbol{y^M}$, or the output, respectively $\boldsymbol{p}(\boldsymbol{y^M})$ (cf. [Var10]).

In the following, we summarize a selection of publications dealing with theoretical impacts of demand uncertainty on production and pricing decisions of firms. In this context, neoclassical models of both competitive and monopolistic firms are extended with stochastic components to analyze optimal output and input decisions while keeping the demand models very general. With regard to demand analysis the results are interesting from two points of view: the influence of uncertainty in general or random demand in particular on their output as well as on their demand for input products.

To begin with, Mills [Mil62] investigates a firm's decision problem to determine optimal prices and output quantities in the situation of imperfect competition.He assumes that demand can be modeled as the sum of deterministic demand function dependent on price and a random variable. Therefore, he shows that the optimal price and output decisions differ from the results in a deterministic setting, and gives conditions under which the price is lower in the uncertain case than the resulting price of the static model. Dhrymes [Dhr64] analyzes the effects of uncertainty on optimal output mix of a monopolistic firm

producing multiple products, where the price is modeled as a function of output quantities and a random variable. He splits the decision-making problem: first optimal output is determined by maximizing expected utility, then optimal input quantities are the solution of the cost minimization problem with given output. He concludes that determining the influence of uncertainty on output quantities is more complex than in the single product case.
Whereas Baron [Bar70] investigates the firm's decisions in a purely competitive setting and emphasizes the impact of the attitude towards risk on the decision-making, Leland [Lel72] considers the influences on decision-making of a monopolistic firm assuming that demand is downward sloping and stochastic. He shows that, in addition to the attitude towards risk, the behavioral mode of the firm plays a prevalent role.
Moreover, Batra et al. [BU74] provide theoretical results for optimal output and input demand for labor and capital of a purely competitive firm that maximizes expected utility of profit given an uncertain market price. Likewise, they noted that the attitude towards risk is crucial for determining the changes of output decisions and the behavior of the production function is decisive to the input demand functions. On the basis of Leland's approach for modeling demand [Lel72], Holthausen [Hol76] studies the influence of uncertain demand on input decisions of a competitive firm as well as a firm in imperfect competition with quantity-setting decisions and price-setting decisions. Whereas output and input decisions are made simultaneously in the first two situations, input choices of a price-setting firm has to be made before the output decision is made and, hence, they are also influenced by the attitude towards risk.

2.2 Modeling Demand in Operations Research and Management Science

In this section, we review a selection of publications dealing with approaches to modeling demand in the field of supply chain management, assortment planning, or revenue management. Setting up distinctive optimization problems tailored to the specific features of the respective sector (e.g., industry, service, or retail), they aim to determine optimal strategies in procurement, production, distribution, assortment, or pricing. As these optimization models display very different modeling concepts ranging from mixed integer nonlinear to stochastic optimization problems, the approaches to modeling demand also vary in many aspects.
In the field of production optimization along a value chain (e.g., in chemical engineering), demand is often assumed to be price-insensitive and stochastic. Here, a common approach is to model the uncertain demand as random variable (cf. [BT06, GM03, GMB+05, CL04]). If, additionally, pricing decisions are included, demand models with respect to prices are incorporated in the optimization model. These comprise linear models (cf. [KGvB+09]) and nonlinear models (cf. [Cha05, LB08]).[13] The arising optimization problems are mainly solved by means of two-stage stochastic programs. More details of these optimization models are provided in section 4.1.

[13] Such models are also used to analyze demand in the research area of marketing (cf. [LKM92]).

In addition, some publications deal with specific situations focusing on few products. Regarding distribution, for example, Bernstein and Federgruen [BF03] investigate optimal strategies of a supplier being faced with multiple retailers in the case of both a centralized and a decentralized setting. The demand rate of one retailer i also depends on all others retailers' prices $p_j,\ j \neq i,\ j = 1, \ldots, n$, i.e., their demand model is given by

$$d_i(p) = a_i - b_i p_i + \sum_{j \neq i} \beta_{ij} p_j, \quad i = 1, \ldots, n, \tag{2.36}$$

where $a_i > 0,\ b_i > 0$, and $\beta_{ij} > 0$ so that the retailer's prices represent substitutes. Moreover, $b_i > \sum_{j \neq i} \beta_{ij}$ for all $i \neq j,\ i = 1, \ldots, N$, implies that the products are also substitutes with regard to the inverse demand function. In particular, in the decentralized system, in which the retailers select sales quantities and replenishment strategies, the coordination mechanism is based on discount schemes. For further detailes about contracts in supply chain management we refer to [CL05].

Goyal and Netessine [GN11] study the benefits of volume and product flexibility of a single firm that produces two products $i = 1, 2$. They assume that the demand-price relationship is given by

$$p_i(q_i, q_{3-i}) = A_i - q_i - \beta q_{3-i},\ i = 1, 2, \tag{2.37}$$

where $\beta \in (-1, 1)$. If $\beta > 0$, the products are substitutes, and if $\beta < 0$, the products are complements. Moreover, the demand for both product is correlated by assuming that the intercepts $A_i \in \mathbb{R}_+,\ i = 1, 2$ follow a bivariate continuous distribution with covariance factors $\sigma_{12} = \rho\sigma_1\sigma_2$. Their analyses highlight the impacts of demand correlation ρ and the product substitutability parameter β on the decisions, and show the importance of managing the production together.

As already stated, modeling demand also plays an important role in revenue management. Here, the objective is to determine optimal pricing strategies and to ensure product availability in order to maximize profit of retail or service companies (e.g., airline industry, car rental agencies). In this context, the concept of dynamic pricing plays a dominant role. We refer to [BC03] for an overview of pricing models in the field of revenue management. Concerning the modeling for demand, cumulative potential demand is often described by a stochastic process dependent on the information available for the customer. The decision whether to purchase or not depends largely on prices. For example, given an initial assortment Gallego and van Ryzin [GvR94] investigate optimal pricing strategies modeling realized demand as Poisson process with intensity $\lambda(p)$ dependent on the price p.

The effects of substitution are of importance in order to determine optimal strategies in assortment planning problems of a retailer. Substitution effects occur if a product is out of stock or is, generally, not available at the store under consideration. In general, there are two common possibilities to model demand substitution: substitution models associating a utility with each product and exogenous models of substitution which allow for choosing an available variant if the first choice is out of stock. As an example for the utility-based approach, van Ryzin and Mahajan [vRM99] employ the *multinominal* *logit* model in order to model consumer choice: given a set of available products S, each consumer associates a utility with each product $i \in S$, and prefers the one for which his utility is at the maximum. The *multinominal logit* approach defines the utility of buying product j as $U_j = u_j + \zeta_j$, where u_j is deterministic and ζ_j follows a Gumbel distribution with mean zero and variance $\mu^2\pi^2/6$.[14] Then,

$$P(U_j = \max[U_i,\ i \in S \cup \{0\}]) = \frac{e^{u_j/\mu}}{\sum_{i \in S} e^{u_i/\mu} + e^{u_0/\mu}}, \tag{2.39}$$

where 0 represents the case of no purchase. Moreover, the consumer has only one choice. If his preferred product is out of stock, the sale is not realized. This model satisfies the “independence from irrelevant alternatives (IAA)”-property, which claims that the ratio of choice probability for two products i and j is independent of the alternatives. In their approach, they also distinguish between aggregation of independent consumers and aggregation of consumers following trends.[15]

Regarding exogenous models of substitution, a customer has a first choice and if the preferred product is not available, he chooses another product with given substitution probability. Smith and Agrawal [SA00] present a probabilistic demand model: let $x_i,\ i = 1, \ldots, n$, indicate whether a product i is available ($x_i = 1$) in the assortment or not ($x_i = 0$). Given the substitution probability α_{ji} of two items $j \neq i$, the probability that item i with $x_i = 1$ is required by the m-th customer is given by

$$P_i(\boldsymbol{x}, m) = f_i + \sum_{j \neq i} (f_j - x_j A_j(\boldsymbol{x}, m))\alpha_{ji}, \quad i = 1, \ldots, n, \tag{2.40}$$

where $f_k,\ k = i, j$, is the probability that the customers initially prefers $k,\ k = i, j$. On this basis, they determine the effects of substitution on demand distributions given that the number of arriving customers follows a negative binomial distribution. Moreover, they propose a method to determine optimal inventory levels.

The work of Netessine and Rudi [NR03] is another example for determining optimal stocking strategies for multiple products if substitution is possible. They assume that demand $\boldsymbol{D} = (D_1, \ldots, D_n)$ for the products $1, \ldots, n$ follows a continuous multivariate distribution. If the product required is out of stock, a deterministic fraction of the demand is satisfied by other products. Thus, the total demand of product $i,\ i = 1, \ldots, n$, is given by

$$D_i^s = D_i + \sum_{j \neq i} a_{ji}(D_j - Q_j)^+,\ i = 1, \ldots, n, \tag{2.41}$$

[14]The corresponding distribution function is given by

$$P(\zeta_i \leq x) = \exp(-\exp(-(x/\mu) + \gamma)), \tag{2.38}$$

where $\gamma = 0.5772$ is Euler's constant.

[15]In general, discrete choice models as introduced above often appear in revenue management and assortment optimization but also for modeling travel demand. For more information, we refer to [AdPT92]. Moreover, the book of Domencich and McFadden [DM96] provides a comprehensive survey of various modeling approaches for urban travel demand (see also section 2.3).

where $D_i,\ i = 1, \dots, n$, is the initial demand of product i, $Q_i,\ i = 1, \dots, n$, are the units of product i stocked at the beginning of the sales period, and a_{ji} is the deterministic fraction of the excess demand for product j that will be substituted by product i. They determine optimal inventory levels for both centralized and decentralized inventory management. For the former case, they show that profit decreases if demand correlation increases.
Kök and Fisher [KF07] also consider an assortment optimization problem of a retailer in which substitution can take place in subcategories of the product range containing, in total, n products. Let S be the set of products available at the retail. If the preferred one is not available, the consumer selects a substitute product with probability δ. Then, the effective demand rate for product i

$$D_i(\boldsymbol{f}, \boldsymbol{d}) = d_i + (\sum_{k \notin S} \alpha_{ki} d_k + \sum_{k \in S} \alpha_{ki} L_k(f_k, d_k)),\ i = 1, \dots, n, \tag{2.42}$$

is composed of the original demand rate d_i for product i, the supplementary demand $\alpha_{ki} d_k$ because of assortment-based substitution, and the incremental demand because of the stockout-based substitution $\alpha_{ki} L_k(f_k, d_k)$. In this case, $L_k(f_k, d_k)$ denotes the lost sales of product k. The probability that product i substitutes product k is denoted by α_{ki} and depends on the general probability to substitute δ. In addition, they develop a method to estimate the demand and substitution parameters given varying data availability. The resulting optimization problem is a knapsack problem, where the objective function is nonlinear and nonseparable. Applying the model to the assortment of a supermarket chain, their iterative heuristic algorithm reveals the optimal assortment to increase profit.
Hopp and Xu [HX08] present a static approximation of dynamic demand substitution by using a memoryless flow network in order to model the substitution process. Let $r_i,\ i = 1, \dots, n$, be the attraction factor for product $i,\ i = 1, \dots, n$, dependent on price and quality, and $s_i,\ i = 1, \dots, n$, represents the constant service rate for product $i,\ i = 1, \dots, n$. The number N of customers arriving is a continuous random variable. Then, the expected effective demand for product i is given by

$$\mathbb{E}(D_i^e) = \mathbb{E}(N) \frac{r_i s_i}{r_0 + \sum_{j=1}^{L} r_j s_j},\ i = 1, \dots, n.$$

Their model is applied to determine optimal prices, service, and product assortment strategies in competitive and noncompetitive markets.
So far, the models presented do not explicitly include the effect of prices on the substitution. In contrast, price-dependent substitution in a two vertically differentiated product setting is studied by Transchel [Tra11]. Here, the customers are willing to buy the high-quality product, if the low-quality product is out of stock. The demand for the low-quality product L is modeled as a price-insensitive random variable and the demand for the high-quality product H as a function dependent on price r_H and a random variable. The substitution rate depends on the price difference and is defined as

$$\gamma(r_H) = \begin{cases} 1 & \text{if } r_H \leq r_L, \\ (0, 1) & \text{if } r_H \in (r_L, r_{s0}), \\ 0 & \text{if } r_H \geq r_{s0}, \end{cases}$$

where r_{s0} is the minimum price of the high-quality product H if the substitution rate is zero, and r_L is the price of the low-quality product. Her studies reveal that the price-sensitivity of substitution is a critical factor because of its influence on revenue and price effects. Alternatively, an example of demand learning in assortment planning is provided by Talebian et al. [TBS12]. They solve the assortment and pricing decision problem of a retailer with stochastic dynamic programming, where new insights about demand are obtained using Bayesian updating, and are incorporated in the optimization problem.

2.3 Miscellaneous Demand Models for Specific Products

This section summarizes demand models that are tailored to specific services (transportation), products (e.g. automobiles or electric appliance) or commodities (e.g. energy). These models are based on different concepts: whereas some contributions select approaches to modeling the utility, others are rather phenomenological.

In the range of travel demand, Domencich and McFadden [DM96] present a behavioral model based on the concept of discrete choice theory that is also used in the context of revenue management and assortment planning (see section 2.2). They start with a rather general framework before passing on to develop concrete models with a sufficiently simple structure to facilitate the usage of estimation methods. For instance, separability of the decisions is required to simplify data analysis. In general, decisions of the passengers related to transportation include location of residence and job, sales of labor and purchase of commodities, frequency of work and leisure activities, destination of trips, time and mode of travel.

On the basis of consumer choice theory, the utility function $U(\boldsymbol{x}^i, \boldsymbol{s}) = V(\boldsymbol{x}^i, \boldsymbol{s}) + \eta(\boldsymbol{x}^i, \boldsymbol{s})$ of each passenger for option $i,\ i = 1, \dots, J$, is a function of a deterministic part $V(\boldsymbol{x}^i, \boldsymbol{s})$, which is assumed to be representative for the population under consideration, and a random term $\eta(\boldsymbol{x}^i, \boldsymbol{s})$, where both depend on the observable attributes $\boldsymbol{x}^i$ of option i and on the socioeconomic characteristics $\boldsymbol{s}$. Let $\eta(\boldsymbol{x}^i, \boldsymbol{s}),\ i = 1, \dots, J$, be a random variable with

$$P(\eta(\boldsymbol{x}^i, \boldsymbol{s}) \leq \eta) = \exp(-\exp(-(\eta + \alpha)),\ i = 1, \dots, J,$$

where α is a parameter of the respective distribution. Then, the probability of choosing option i can be written as

$$P_i = P(U(\boldsymbol{x^i}, \boldsymbol{s}) > U(\boldsymbol{x^j}, \boldsymbol{s}) \text{ for } j \neq i,\ j = 1, \dots, J) \tag{2.43}$$

$$= \frac{e^{V(\boldsymbol{x^i}, \boldsymbol{s})}}{\sum_{j=1}^{J} e^{V(\boldsymbol{x^j}, \boldsymbol{s})}}, \tag{2.44}$$

where α is absorbed into $V(\boldsymbol{x}^i, \boldsymbol{s})$, which means that option i optimizes the passengers' utility, This result is known as *multinominal logit model* (cf. model equation (2.39)). Likewise, they study alternative probability distributions for $\eta(\cdot,\cdot)$ and establish probability models that are consistent with the theory of individual utility maximization.

Now, we turn our attention to demand models for energy. To identify the demand of energy in Baden-Wuerttemberg, Weber et al. [W$^+$97] analyze consumer behavior with

regard to energy and energy-consuming goods in households. In this context, they model the demand for habitation, automobiles, electric appliance, and other household's needs by means of household production theory and develop a hierarchical decision model, in which the decision parameter of lower level influence the superior decisions in a aggregated way. At each level, the most important influencing factor is the remaining budget. Among others, they propose to model the budget shares for automobile purchase and maintenance in the framework of the *Almost Ideal Expenditure System.* Concerning the intensity of automobile utilization, they use a generalized *CES* utility function. Additionally, to determine energy demand in the production and service sector and its change because of technological changes, they apply input-output analysis.
Likewise, Pindyck [Pin79] uses the concept of neoclassical consumer theory to model energy demand for different sectors. In particular, he investigates different formulas to describe the demand formation: the *indirect translog utility function* in order to model energy demand for households, an analogous second-order approximation for the cost function in order to model industrial energy demand and a "simultaneous equation model" for the transportation sector for which the required quantity is a function of stock, fuel efficiency, and distance gone by car.
Different world oil models are studied and compared by Huntington [Hun93]. In general, the main influencing factors for most of these models under consideration are crude oil price, gross domestic product (GDP), prices of substitutes, and time trend for improvements. To estimate and compare the response of each model to important factors, he specifies oil demand q as loglinear form of

$$\frac{q_t}{q_{t-1}} = \alpha^{\lambda} p^{\lambda\beta} \frac{y_t}{y_{t-1}}^{a} y_{t-1}^{\lambda a} q_{t-1}^{-\lambda} e^{-\lambda g(t-1)}, \quad g < 0, a > 0, \tag{2.45}$$

which is function of price p, the constant rate of improvements in efficiency g and the GDP y. According to him, this corresponds to the structure of most demand models in his study. That means, his procedure is as follows: on the basis of multiple scenarios reflecting different price trends and different growth rates of GDP, each model generates demand data. On the basis of this data base, he estimates the coefficients of his specification using the method of least-squares in order to compare the econometric response of these models.
Another model for oil demand is developed by Jäger [Jä08] with the intention to analyze the dynamics in the oil market. In addition to the oil price, he assumes that the general level of income or economic activity determines the demand for oil. Since he emphasizes that demand need to be distinguished from the sum purchased in the market, which is less or equal to the supply, he structures the demand as follows. Firstly, he defines potential demand $D^*(t)$ to be the overall quantity that can be applied in the market. Assuming that this quantity is influenced by economic or technological factors, he uses a log-linear demand approach

$$D^*(t) = c \prod_{i=1}^{n} Z_i(t)^{\theta_i}, \tag{2.46}$$

where $Z_i,\ i = 1, \ldots, n$, represent the influencing factors such as gross domestic product, population size, number of vehicles, or indices quantifying technological change, and seasonality.[16] Secondly, the budget conditioned demand $D^B(t)$ depends on the oil price $P(t)$, the gross domestic product $Z_1(t)$, and the potential demand $D^*(t)$.

$$D^B(t) = \min[\epsilon(P(t))Z_1(t), D^*(t)] \tag{2.47}$$

where

$$\epsilon(P(t)) = \xi_0 + \frac{\xi_1}{\xi_2 + \xi_3 P(t)}. \tag{2.48}$$

Thus, he proposes to state the strategy of the consumer, i.e., the actual demand, as follows

$$D(t) = D^0(t) + \gamma(X(t))[D^B(t) - D^0(t)]^+ \tag{2.49}$$

where $D^0(t)$ is the minimum demand and

$$\gamma(P) = \phi(1 + \theta(P^* - P)). \tag{2.50}$$

In words, if demand exceeds supply, customers accept price increases as long as the price is below a certain threshold P^*.
Modeling demand for electricity represents a special case, since demand is predominantly modeled price-insensitive and depends on the season, the day of the week, the hour of the day as well as the weather (cf. [BGS07, EW03] for a more detailed discussion). Another possibility is provided by Barlow [Bar02], who determines electricity spot prices by means of a fundamental market model, for which electricity demand is modeled as stochastic differential equation

$$D_t = a_1 - \sigma_1 Y_t, \quad \text{where } dY_t = -\lambda Y_t dt + dW_t, \tag{2.51}$$

an Ornstein-Uhlenbeck process.
So far, the models presented in this section are applicable to commodities, which are products of standard quality and required in large quantities. In contrast, Huschto et al. [HFH$^+$11] develops a pricing model for conspicuous products, i.e., luxuries that are bought because of their reputation, which is supposed to increase if prices increase.

[16] In general, his modeling approach allows to distinguish between developed regions and emerging regions, whereas he simply considers the sum of potential demand for both regions.

3 General Approach to Modeling Demand for Commodities

In this chapter, we state our basic assumptions concerning modeling demand, i.e., we give a general market description and we collect fundamental characteristics and dependencies of demand. In doing so, we prefer a phenomenological approach to establishing a utility function of a customer. This basically means that we directly model the dependencies of demand without quantifying the consumer's preferences, which would require an elaborate structuring of their decision-making.[1]

The distinct approaches to modeling demand reviewed in chapter 2 reveal that the relationship between demand and prices plays a predominant role. In addition, numerous models include more influencing factors on demand, be it income of households, prices of other products, assortment, or economic factors. The focus of our approach is on the dependencies of prices and economic factors, but we also take characteristics of the consumer into account. Moreover, we aim to retain fundamental characteristics of a demand function such as negativity of its derivative with respect to the price or symmetry of the cross-price derivatives (cf. section 2.1.1).

Thus, we provide the framework for a general demand model within which we will be able to present a quantitative demand function for various applications in different markets. In doing so, we propose model components that can be added to the model whenever corresponding market data is available. At this stage, we restrict our general approach to be deterministic and keep it simple by aggregating all consumers unless more information becomes available. In doing so, our basic framework is supposed to serve as a manageable tool for establishing explicit demand models that are also integrable in production optimization and pricing models.

This chapter is structured as follows: In section 3.1, we draft our concept to model demand and list our basic assumptions concerning the market under consideration, the dependencies of demand, and the properties of a respective demand model function. Section 3.2 addresses the relationship between the demand of a product and its price. In section 3.3, we explain our approach to integrate the influences of changes in the economic situation of the market through economic indices. Section 3.4 considers the impacts of the consumer's characteristics on his demand. In section 3.5, we examine the occurrences of price-based substitution. To cope with the arising complexity, we aggregate all substitution possibilities and consider the effects of substitution on demand as if it is based on gradual switching. Finally, section 3.6 proposes a model enhancement to include the effects of complementary products.

[1] To compare, the profit maximization problems described in section 2.1.3 display the theoretical structure of such a decision process of an industrial consumer.

3.1 General Market Description and Approach to Modeling Demand

In this section, we restrict our description to one region. Hence, we consider from now on a general market in a region r with the following properties, where P^M is the set of products produced and sold in the market.

Assumptions 3.1. *Demand-related characteristics of the market*

1. *All consumers act independently, but have the same demand behavior and can be seen as just one consumer by aggregating their demand. Consequently, by referring to the consumer, we explicitly bear the whole economy, i.e., all sectors, in mind.*

2. *The products $p \in P^M$ are connected by their production processes and possibly by their subsequent processing or by their end consumption.*

3. *The products $p \in P^M$ are of standard quality and are in demand of large quantities with the price as main influencing factor for demand (cf. [KGvB+09, Kan08]).*

Example 3.1. *This market description corresponds to most commodity markets. Among others, the market for agricultural products, the petrochemical market or energy markets (e.g., fuel oil or natural gas) satisfy these characteristics.*[2] *For instance, the dependency on crude oil of natural gas, which arises because of identical purposes of use, is studied in [Kel09].*

In addition to the price, there are more influencing factors on demand summarized in the following.

Assumptions 3.2. *Dependencies of demand*
In a market that satisfies the assumptions 3.1, we assume that the demand $\phi_{p,r,t}$ of a certain product $p \in P^M$ in region r at time t can be specified as a function of the following factors:

1. ***time*** *t,*

2. ***prices*** *$x^{\pi}_{p_i,r,t}$ of products $p_i \in P \subseteq P^M$,*[3]

3. ***present economic situation*** *$\boldsymbol{a^{\zeta}}_{r,t}$ in region r at time t or rather the* ***change in the economic situation*** *$\boldsymbol{\Delta a^{\zeta}}_{r,t}$ from previous times to t,*[4]

[2]The electricity market is a counterexample, since the demand for electricity is often price-insensitive in the short-run (see also [Kra09] for a detailed discussion of demand for electricity).

[3]Note that we consider a unique price for all products. In contrast, Kannegiesser [KGvB+09, Kan08] assumed that the products can be sold at diverse prices at the spot market. In addition, his model also includes contract prices. For more information on price discrimination see also [LKM92].

[4]Among others, the current economic situation, e.g., in terms of GDP growth, influences demand for energy according to [Jä08, Hun93, Pin79].

4. ***forecast of future economic situation*** $\boldsymbol{a}^{E\boldsymbol{\zeta}}_{r,t,t+1}$ *in region r for time* $t+1$ *at time t, respectively the* ***forecast of the economic development*** $\boldsymbol{\Delta a}^{E\boldsymbol{\zeta}}_{r,t,t+1}$ *given* $\boldsymbol{a}^{E\boldsymbol{\zeta}}_{r,t-1,t}$ *or* $\boldsymbol{a}^{\boldsymbol{\zeta}}{}_{r,t}$*, and*

5. ***characteristics of the consumer*** *summarized in the vector* $\boldsymbol{\alpha}^{consumer}_{r,t}$*. For example, his budget* $\alpha^{budget}_{r,t}$*, his maximum capacity* $\alpha^{\max\_\text{quant}}_{p,r,t}$*, or his expectation on the price development* $\alpha^{E\pi}_{p,r,t}$ *are included.*[5]

In this modeling approach, we concentrate on influencing factors that are straightforwardly determinable and preferably even observable. For example, we decide to omit further influencing factors such as technological progress of the industry, because its influence cannot easily be quantified. Moreover, we suggest that it is for the most part covered by other influencing factors. To summarize, we define the demand function as follows.[6]

Definition 3.1. *The demand of a single product p in region r at time t is given by* $\phi_{p,r,t}\colon (\mathbb{R}^+_0)^{|P|} \times \mathbb{R} \times \mathbb{R}^I \times \mathbb{R}^I \times \mathbb{R}^C \to \mathbb{R}^+_0$*,*

$$\phi_{p,r,t}(\boldsymbol{x}^{\pi}_{r,t}; t, \boldsymbol{\Delta a}^{\boldsymbol{\zeta}}{}_{r,t}, \boldsymbol{\Delta a}^{E\boldsymbol{\zeta}}_{r,t,t+1}, \boldsymbol{\alpha}^{consumer}_{r,t}),$$

where $\boldsymbol{x}^{\pi}_{r,t} = (x^{\pi}_{p_1,r,t}, \ldots, x^{\pi}_{p_{|P|},r,t})'$*, I is the number of the economic indices, and C is the number of the consumer's characteristics included. More generally, the demand of all products at time t is given by* $\boldsymbol{\phi}_{r,t}\colon (\mathbb{R}^+_0)^{|P|} \times \mathbb{R} \times \mathbb{R}^I \times \mathbb{R}^I \times \mathbb{R}^C \to (\mathbb{R}^+_0)^{|P|}$

$$\boldsymbol{\phi}_{r,t}(\boldsymbol{x}^{\pi}_{r,t}; t, \boldsymbol{\Delta a}^{\boldsymbol{\zeta}}{}_{r,t}, \boldsymbol{\Delta a}^{E\boldsymbol{\zeta}}_{r,t,t+1}, \boldsymbol{\alpha}^{consumer}_{r,t}) = \begin{pmatrix} \phi_{p_1,r,t}(\boldsymbol{x}^{\pi}_{r,t}; t, \boldsymbol{\Delta a}^{\boldsymbol{\zeta}}{}_{r,t}, \boldsymbol{\Delta a}^{E\boldsymbol{\zeta}}_{r,t,t+1}, \boldsymbol{\alpha}^{consumer}_{r,t}) \\ \vdots \\ \phi_{p_{|P|},r,t}(\boldsymbol{x}^{\pi}_{r,t}; t, \boldsymbol{\Delta a}^{\boldsymbol{\zeta}}{}_{r,t}, \boldsymbol{\Delta a}^{E\boldsymbol{\zeta}}_{r,t,t+1}, \boldsymbol{\alpha}^{consumer}_{r,t}) \end{pmatrix}.$$

For the sake of simplicity, we omit the parameters in the following and write $\phi_{p,r,t}(\boldsymbol{x}^{\pi}_{r,t})$ instead of $\phi_{p,r,t}(\boldsymbol{x}^{\pi}_{r,t}; t, \boldsymbol{\Delta a}^{\boldsymbol{\zeta}}{}_{r,t}, \boldsymbol{\Delta a}^{E\boldsymbol{\zeta}}_{r,t,t+1}, \boldsymbol{\alpha}^{consumer}_{r,t})$, as we will do for all extended demand functions in the course of this chapter.
Before we start analyzing these dependencies and further characteristics of demand, we have to make further assumptions. To begin with, we suggest the following regarding the customer's behavior.

Assumptions 3.3. *The customer's decisions are rational. That means he acts to optimize his personal benefit.*

[5]Most models in economic theory include the budget as influencing factor, whereas the others factor mentioned above are mostly neglected. Therefore, if the customer is confronted with uncertainty, they investigate the attitude towards risk which is supposed to influence the decision process (see section 2.1.3 or [Hol76]). Regarding demand models for energy, Jäger [Jä08] included the maximum potential demand and the minimum demand in his model.

[6]By way of comparison, Hildenbrand [Hil94] assumed that demand is influenced by the price system, expected future prices, present and expected future income, past consumption, and household characteristics.

The influencing factor that is considered most frequently in demand theory is the own price $x^{\pi}_{p,r,t}$ of product p. In general, we assume that demand can be modeled as a nonlinear, strictly decreasing function of $x^{\pi}_{p,r,t}$. Regarding the prices of other products, we suppose that there are two reasons why prices influence each other. First, the products under consideration are substitutes and can be interchanged in their further processing or in their end consumption. Second, the products are complements and can only be processed in a fixed ratio. Prices of products that are neither substitutes nor complements have no impact on the demand under consideration.
We will analyze these demand-price relations in more detail in the following sections. For this purpose, the following assumptions are crucial.

Assumptions 3.4. *Characteristics of demand function*

- *Demand and price are always non-negative as defined in definition 3.1.*
- *The demand function $\phi_{p,r,t}$ is differentiable with respect to $x^{\pi}_{p_i,r,t}$ $\forall p_i \in P$.*

Although, we model the demand function for a fixed time and not dynamically, we explicitly want to include temporal aspects in the modeling expressed by the parameter t in the definition above. Namely, among others, intertemporal considerations occur in modeling substitution or modeling the influence of the customer's expectation on the future price development. Moreover, we make the following assumption concerning past consumption and price data.[7]

Assumptions 3.5. *Influence of historical data on demand's parameters*
Instead of modeling the time-dependency explicitly, we assume that the remaining demand parameters of time t are influenced by historical data such as the sales quantities and the prices at previous times $t-1,\ t-2,\ldots$.

In the following sections, we specify the dependencies of demand defined in assumptions 3.2. In section 3.2, we focus on the influence of the products' price. The impacts of the market's economic situation are analyzed in section 3.3. Section 3.4 comprises the studies on the influence of the consumer's characteristics. Regarding the influences of others products' prices, the impacts of substitutes are considered in section 3.5 and the impacts of complements in section 3.6.

3.2 Influence of the Product's Price

Obviously, the price of the product under consideration plays a crucial role of demand. In general, we assume that demand of a product rises if the price of this product decreases and hence, we state monotonicity of the demand function. In doing so, our modeling satisfies the *law of demand*, an attribute which is also required in the model contributions presented in section 2.1 (cf. [JQ08]).

[7] We return to this assumption in chapter 7, in which we discuss methods to identify parameters of explicit modeling approaches.

Characteristics of demand 3.1. *Dependency on the product's price*
Under the assumption that there are neither substitutes nor complements in the market, we state the following property of $\phi_{p,r,t}$

$$\frac{\partial \phi_{p_l,r,t}}{\partial x^{\pi}_{p_l,r,t}} \left(\boldsymbol{x}^{\pi}_{r,t}\right) \leq 0 \quad \text{for all } l = 1, \ldots, |P| \tag{3.1}$$

and

$$\frac{\partial \phi_{p_l,r,t}}{\partial x^{\pi}_{p_m,r,t}} \left(\boldsymbol{x}^{\pi}_{r,t}\right) = 0 \quad \text{for all } l,\ m = 1, \ldots, |P|, \quad l \neq m. \tag{3.2}$$

Consequently, there are no Giffen goods in the market under consideration because the derivative of the demand function with respect to the price is negative.
Note that other influencing factors can counteract these characteristic. For example, incorporating the consumer's expectation on the future price development causes scenarios, in which price and demand rise in common because the consumer expects even higher prices in the future. Another example is the effect of changes in the economic situation, which are covered in the next section.

3.3 Influence of Economic Development

In general, we suppose that, compared to the economic state in region r at previous dates, a better, i.e., auspicious, economic situation or a boom phase boosts the demand of products reprocessed in the industry as well as end products. In other words, the consumer is willing to pay a higher price for the same quantity if he believes that the economy is stipulated. In addition, his financial situation is favorable. Otherwise, a negative economic development or a downturn causes the demand to decrease.
To include this effect in our modeling, we assume that the rating of the economic situation at time t can be described by the change of economic statistics or indices such as the gross domestic product (GDP) from previous times to t.[8]
Hence, we refer to an economic index as ζ_i, $i = 1, \ldots, I$, where I is the number of the economic statistics, and denote its absolute value in region r at time t by $a^{\zeta_i}_{r,t}$. For instance, ζ_i can be the gross domestic product, the industrial production index, or a specific product-related index. Consequently, we write

$$\boldsymbol{a}^{\boldsymbol{\zeta}}{}_{r,t} = \left(a^{\zeta_1}_{r,t}, \ldots, a^{\zeta_I}_{r,t}\right)'$$

for the vector representing the economic situation in region r at time t. Accordingly, the vector

$$\boldsymbol{\Delta a}^{\boldsymbol{\zeta}}{}_{r,t} = \left(\Delta a^{\zeta_1}_{r,t}, \ldots, \Delta a^{\zeta_I}_{r,t}\right)'.$$

[8]The GDP is the sum of all output in an economy (cf. [BFD08], page 742). For example, Belke et al. [BDdH10] employ the gross national product (GNP) per capita to approximate the economic growth in their study about energy consumption. Likewise, Jäger [Jä08] and Huntington [Hun93] include this economic indicator in their models, where Huntington considers the GDP as measure for the income of the whole economy.

describes the economic development from previous times to time t. To define $\Delta a^{\zeta_i}_{r,t}$ for all available statistics, we make the following assumption.

Assumptions 3.6. Rating of the economic situation
The consumer considers the economic situation at time t as positive if the change of the economic indices from the previous time points to time t is positive.

Therefore, we add a further index to $\Delta a^{\zeta_i}_{r,t}$ representing the number of past years that will be included in the calculation of our approach and write

Definition 3.2. Definition of $\boldsymbol{\Delta a^{\zeta}}_{r,t,J}$

We define $\Delta a^{\zeta_i}_{r,t,J}$ for an economic index ζ_i as follows

$$\Delta a^{\zeta_i}_{r,t,J} := \sum_{j=1}^{J} w_j \cdot (a^{\zeta_i}_{r,t} - a^{\zeta_i}_{r,t-j}), \tag{3.3}$$

where J is the number of data for which we assume that they influence the economic situation. Consequently,

$$\boldsymbol{\Delta a^{\zeta}}_{r,t,J} := (\Delta a^{\zeta_1}_{r,t,J}, \ldots, \Delta a^{\zeta_I}_{r,t,J})'. \tag{3.4}$$

Note that we include weighting factors, since we assume that older data has less influence than current data. In the following, we give some examples how to weight historical data.

Example 3.2. Weighting factors of historical data
Given J we propose two possibilities for weighting factors w_j, $j = 1, \ldots, J$:

- *exponentially weighting*

$$w_j = \lambda \cdot (1-\lambda)^{j-1} \quad j = 1, \ldots, J, \tag{3.5}$$

  where $\lim_{J\to\infty} \sum_{j=1}^{J} w_j = 1$ and $0 < \lambda < 1$,

- *and linear weighting*

$$w_j = \frac{2(J+1-j)}{J(J+1)} \quad j = 1, \ldots, J, \tag{3.6}$$

  where $\sum_{j=1}^{J} w_j = 1$.

These weighting techniques are known as weighted moving averages techniques, which are often applied to time series in finance (e.g., to calculate the volatility of energy prices (see [EW03, BGS07])). In this context, J denotes the length of the moving window of data included.

Accordingly, we denote the forecast of the future economic situation by

$$\boldsymbol{a}^{E\boldsymbol{\zeta}}_{r,t,t+1} = (a^{E\zeta_1}_{r,t,t+1}, \dots, a^{E\zeta_I}_{r,t,t+1})'$$

and the corresponding forecast for the future development with

$$\boldsymbol{\Delta a}^{E\boldsymbol{\zeta}}_{r,t,t+1,J} = (\Delta a^{E\zeta_1}_{r,t,t+1,J}, \dots, \Delta a^{E\zeta_I}_{r,t,t+1,J})'.$$

Note that both parameters $\boldsymbol{a}^{E\boldsymbol{\zeta}}_{r,t,t+1}$ and $\boldsymbol{\Delta a}^{E\boldsymbol{\zeta}}_{r,t,t+1,J}$ display the prediction for time $t+1$ given all information available at time t. In analogy with definition 3.2, we specify the entries as follows.

Definition 3.3. *Definition of* $\boldsymbol{\Delta a}^{E\boldsymbol{\zeta}}_{r,t,t+1,J}$
The entries $\Delta a^{E\zeta_i}_{r,t,t+1,J}$ *of* $\boldsymbol{\Delta a}^{E\boldsymbol{\zeta}}_{r,t,t+1,J}$ *are defined as*

$$\Delta a^{E\zeta_i}_{r,t,t+1,J} := \sum_{j=1}^{J+1} w_j \cdot (a^{E\zeta_i}_{r,t,t+1} - a^{\zeta_i}_{r,t+1-j}). \tag{3.7}$$

Since we assume that demand rises if the change in the economic situation is positive, we conclude, that demand rises if $\Delta a^{\zeta_i}_{r,t,J}$ rises. Hence, we obtain

Characteristics of demand 3.2. *Influence of economic development on demand*
Let $\phi_{p,r,t}$ be differentiable with respect to $\Delta a^{\zeta_i}_{r,t,J}$ and $\Delta a^{E\zeta_i}_{r,t,t+1,J}$. Then, the demand function for product p in region r at time t satisfies

$$\frac{\partial \phi_{p,r,t}}{\partial \Delta a^{\zeta_i}_{r,t,J}} \left(\boldsymbol{x}^{\pi}_{r,t}\right) \geq 0 \quad \textit{for all } i = 1, \dots, I,$$

and accordingly

$$\frac{\partial \phi_{p,r,t}}{\partial \Delta a^{E\zeta_i}_{r,t,t+1,J}} \left(\boldsymbol{x}^{\pi}_{r,t}\right) \geq 0 \quad \textit{for all } i = 1, \cdots, I.$$

This implies that consumption rises if the forecasted change of economic indices rises. In the following, the focus is on characteristics of the consumer that affect his buying decisions.

3.4 Influence of Specific Consumer's Characteristics

In addition to effects from market parameters, characteristics of the consumer such as the availability of facilities or production settings considerably influence the formation of demand. Moreover, financial aspects play a crucial role regarding his purchase decisions because, for instance, the expenses of the customer are limited by his budget.
In this section, we list the most important influencing factors on behalf of the consumer. Note that, whereas a stands as a symbol for parameters with respect to the economic situation, we refer to the characteristics of the consumer as α.

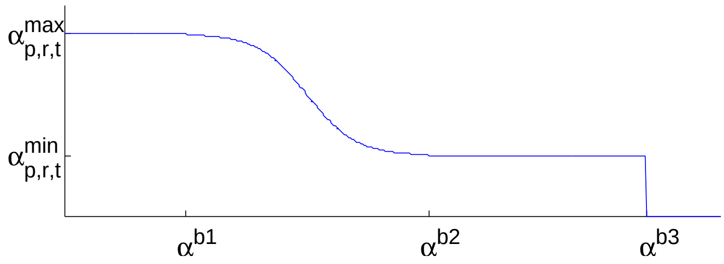

Figure 3.1: Illustration of the nonlinear relationship between demand and price according to the assumptions on the customer's behavior in different price ranges

To begin with, we distinguish several price ranges in which we assume that the consumer behaves differently.[9] Figure 3.1 illustrates the shape of such a demand behavior. To be more precise,

- In lower price regions $[0, \alpha^{b1}_{p,r,t})$, the consumer buys/consumes/invests according to his possible production and inventory capacities. Consequently, since prices are low, the consumer completely utilizes his (production and inventory) capacity $\alpha^{\text{max\_quant}}_{p,r,t}$.[10]. This quantity is also called possible demand or potential demand.

- In the second price range $[\alpha^{b1}_{p,r,t}, \alpha^{b2}_{p,r,t})$, the demand is strictly decreasing if prices rise.

- In the third price range $[\alpha^{b2}_{p,r,t}, \alpha^{b3}_{p,r,t})$, demand is on a minimum level. In other words, if prices exceed a certain price level $\alpha^{b2}_{p,r,t}$, the consumer reduces his production. Since prices are high, he buys as little as necessary $\alpha^{\text{min\_quant}}_{p,r,t}$, but still enough to satisfy existing contracts or to meet his basic needs.

- If $\alpha^{b3}_{p,r,t} \leq x^{\pi}_{p,r,t}$, demand is equal to zero. The consumer cannot afford to purchase anything.

In addition to the arrangement of price intervals to describe consumer behavior, we also insert the notion of the consumer's maximum price $\alpha^{\text{max\_price}}_{p,r,t}$, which is characterized by the following pattern: the demand is positive for all prices $x^{\pi}_{p,r,t} < \alpha^{\text{max\_price}}_{p,r,t}$ and it is zero at $\alpha^{\text{max\_price}}_{p,r,t}$. The description above induces that $\alpha^{\text{max\_price}}_{p,r,t} = \alpha^{b3}_{p,r,t}$ for $\alpha^{\text{min\_quant}}_{p,r,t} > 0$. In case $\alpha^{\text{min\_quant}}_{p,r,t} = 0$, there is no maximum price included in the model. For some commodities, there is $\alpha^{\text{max\_price}}_{p,r,t} < \alpha^{b2}_{p,r,t}$ such that $\phi_{p,r,t}(\boldsymbol{x}^{\pi}_{r,t}) = 0$. The effects of these distinctions on modeling the demand function are summarized in the following.

[9] Jäger [Jä08] also distinguishes between different kinds of consumption behavior (see also section 2.3).

[10] This capacity also includes storage capacities of the consumer. This aspect needs also to be taken into account by modeling demand for multiple time points because the surplus stored at time t reduces the maximal capacities at time $t + 1$.

Characteristics of demand 3.3. <u>*Influence of consumer's characteristics on demand*</u> *To reflect the varying demand-price relationship described above, we define the demand function as follows*

$$\phi_{p,r,t}(\boldsymbol{x}^{\pi}_{r,t}) = \alpha^{\text{max\_quant}}_{p,r,t} \cdot \mathbb{1}_{[0,\alpha^{b1}_{p,r,t})}(x^{\pi}_{p,r,t}) + \varphi_{p,r,t}(\boldsymbol{x}^{\pi}_{r,t}) \cdot \mathbb{1}_{[\alpha^{b1}_{p,r,t},\alpha^{b2}_{p,r,t})}(x^{\pi}_{p,r,t}) \\ + \alpha^{\text{min\_quant}}_{p,r,t} \cdot \mathbb{1}_{[\alpha^{b2}_{p,r,t},\alpha^{b3}_{p,r,t})}(x^{\pi}_{p,r,t}) + 0 \cdot \mathbb{1}_{[\alpha^{b3}_{p,r,t},\infty)}(x^{\pi}_{p,r,t}), \quad (3.8)$$

where $\varphi_{p,r,t}$ *w.r.t.* $x^{\pi}_{p,r,t}$ *is differentiable and strictly decreasing, i.e.,*

$$\frac{\partial \varphi_{p,r,t}}{\partial x^{\pi}_{p,r,t}}(\boldsymbol{x}^{\pi}_{r,t}) < 0 \qquad \textit{if } x^{\pi}_{p,r,t} \in \left[\alpha^{b1}_{p,r,t}, \alpha^{b2}_{p,r,t}\right).$$

In general, $\phi_{p,r,t}$ *w.r.t.* $x^{\pi}_{p,r,t}$ *is continuous on the price interval* $[0, \alpha^{b3}_{p,r,t})$ *if*

$$\varphi(\boldsymbol{x}^{\pi}_{r,t}) = \alpha^{\text{max\_quant}}_{p,r,t} \quad \textit{for } \{\boldsymbol{x}^{\pi}_{r,t} | x^{\pi}_{p,r,t} = \alpha^{b1}_{p,r,t}\} \quad (3.9)$$

$$\textit{and} \qquad \lim_{x^{\pi}_{p,r,t} \to \alpha^{b2}_{p,r,t}} \varphi(\boldsymbol{x}^{\pi}_{r,t}) = \alpha^{\text{min\_quant}}_{p,r,t}, \quad (3.10)$$

and differentiable w.r.t. $x^{\pi}_{p,r,t}$ *on* $[0, \alpha^{b3}_{p,r,t})$ *if*

$$\frac{\partial \varphi}{\partial x^{\pi}_{p,r,t}}(\boldsymbol{x}^{\pi}_{r,t}) = 0 \quad \textit{for } \{\boldsymbol{x}^{\pi}_{r,t} | x^{\pi}_{p,r,t} = \alpha^{b1}_{p,r,t}\} \quad (3.11)$$

$$\lim_{x^{\pi}_{p,r,t} \to \alpha^{b2}_{p,r,t}} \frac{\partial \varphi}{\partial x^{\pi}_{p,r,t}}(\boldsymbol{x}^{\pi}_{r,t}) = 0. \quad (3.12)$$

Note that, in addition, $\phi_{p,r,t}$ *w.r.t.* $x^{\pi}_{p,r,t}$ *is differentiable on* $[0, \infty)$ *if*

$$\alpha^{\text{min\_quant}}_{p,r,t} = 0. \quad (3.13)$$

If $\alpha^{\text{max\_price}}_{p,r,t} < \alpha^{b2}_{p,r,t}$*, the domain of the demand function (3.8) reduces w.r.t.* $x^{\pi}_{p,r,t}$ *to the interval* $[0, \alpha^{\text{max\_price}}_{p,r,t}]$*.*
All in all, the demand is constrained by the consumer's capacity limits and zero

$$0 \leq \phi_{p,r,t}(\boldsymbol{x}^{\pi}_{r,t}) \leq \alpha^{\text{max\_quant}}_{p,r,t}. \quad (3.14)$$

In the next step, we turn our attention to financial constraints. In household consumption theory, income plays a major role in determining the demand and limits the purchase possibilities (cf. equation (2.1) in section 2.1.1 and section 2.1.2 for corresponding models). Regarding firms or industry in general, the available budget $\alpha^{budget}_{r,t}$ gets important. Therefore, a further common constraint on the demand functions $\phi_{p,r,t},\ p \in P$, has to be included in the model

$$\sum_p x^{\pi}_{p,r,t} \cdot \phi_{p,r,t}(\boldsymbol{x}^{\pi}_{r,t}) \leq \alpha^{budget}_{r,t}. \quad (3.15)$$

Here, we assume that the budget is fixed and cannot change on behalf of the consumer in case of unexpected price developments.[11]

[11]Basically, the available budget $\alpha^{budget}_{r,t}$ can comprise credits or savings that will only be used in case

3.4.1 Influence of Price Expectation and Contracts

The focus of this section is to propose supplementary demand model components in order to incorporate the influence of the consumer's expectation on the price development as well as the impact of including contracts. Whereas the former aspect is, to our knowledge, quite a new approach in collecting demand dependencies, contracts are often part of contributions in management science (cf. [BF03, CL05]).
First, we assume that the consumer's expectation influences the demand at prices $x^{\pi}_{p,r,t} \in [\alpha^{b1}_{p,r,t}, \infty)$.[12] To be more precise,

Assumptions 3.7. *Expectation on Price Development*
The personal expectation on the price development of the consumer is assumed to be equal to the common expectation in the market. In general, this aspect can be incorporated through growth forecasts provided by economic organizations or forecasts of economic indices.

This leads to the following characteristics.

Characteristics of demand 3.4. *Influence of the consumer's expectation*
Let $\alpha^{E\pi}_{p,r,t}$ be the expectation on the price development at time t for time $t+z$, $z = 1, 2, \ldots$. We define

$$\alpha^{E\pi}_{p,r,t} := \begin{cases} -1 & \text{if the consumer expects a higher price in the future,} \\ 0 & \text{if the consumer has no influencing expectations on price development,} \\ 1 & \text{if the consumer expects a lower price in the future.} \end{cases}$$

Then, we rewrite the demand as

$$\phi^{E\pi}_{p,r,t}(\boldsymbol{x}^{\pi}_{r,t}) := \phi_{p,r,t}(\boldsymbol{x}^{\pi}_{r,t}) - \alpha^{E\pi}_{p,r,t} \cdot \phi^{q\_add}_{p,r,t}(\boldsymbol{x}^{\pi}_{r,t}) \tag{3.16}$$

where $\phi^{q\_add}_{p,r,t}(\boldsymbol{x}^{\pi}_{r,t})$ is the additional quantity he orders and the notation $\phi^{E\pi}_{p,r,t}$ indicates that the consumer's expectation on a price change influences the demand at time t. Note that the additional quantity depends on the price $x^{\pi}_{p,r,t}$ providing that $\phi^{E\pi}_{p,r,t}(\boldsymbol{x}^{\pi}_{r,t})$ satisfies the inequality (3.14).

While giving a description of consumer's influences on demand, it is indispensable to discuss the influence of contracts.[13] We show in the following that, in case of available

of very high prices, but are not planned to be spent for product p if $x^{\pi}_{p,r,t} \leq \alpha^{b2}_{p,r,t}$. Obviously, such an increase of capital influences the budget in the future, since, for example, the consumer will have further liabilities. However, analyzing these effects on budget and demand is beyond the scope of this thesis.

[12] For example, we suppose that if the customer expects prices to rise in the future, he is willing to purchase now a higher quantity and to store the surplus.

[13] Kannegiesser [Kan08] emphasized that the distinction between contract sales and spot sales plays an important role in the chemical industry. Therefore, he distinguished between consumption structured by contracts and consumption at the spot market described by linear demand functions, which automatically leads to different prices. In addition, he assumed that quantities can be sold at different prices in the spot market, too.

information about contracts, this can easily be embedded in our standard modeling approach. Therefore, we assume that the producer and the customer arrange that the consumer purchases a certain quantity $\alpha_{p,r,t}^{q\_con}$ at time t. In addition, this contract can include a price discount, but this is not mandatory.[14]

Characteristics of demand 3.5. *Including discount contracts we define the demand function as follows*

$$\phi_{p,r,t}^{\text{con}}(\boldsymbol{x}_{r,t}^{\pi}) := \phi_{p,r,t}(\boldsymbol{x}_{r,t}^{\pi}) - \alpha_{p,r,t}^{\text{con}} \cdot \alpha_{p,r,t}^{q\_\text{con}}, \tag{3.17}$$

where

$$\alpha_{p,r,t}^{\text{con}} := \begin{cases} 0 & \textit{if there is a bilateral contract,} \\ 1 & \textit{if there is no bilateral contract.} \end{cases}$$

The notation $\phi_{p,r,t}^{\text{con}}$ indicates that the possibility of contracts is included in the model.

Besides planning certainty, there can be more benefits for both customer and producer. If there is a price discount, the customer has to pay less, whereas the producer's advantage is reduction in storage costs and customer satisfaction, respectively customer loyalty.

3.5 Influences of Other Products' Prices on Demand: Price-based Substitutes

In addition to the influence of the own price of product p on its demand, prices of other products can also have an immense influence, e.g., if products are substitutes for each other. The issue of substitutes occurs in diverse contributions in neoclassical consumer theory (cf. section 2.1.2 and [DM80b, BS09]), but also assortment planning (cf. section 2.2 and [vRM99, NR03, HX08, KF07, Tra11]). Whereas, in the first field, the dependencies of the substitutes are expressed by the consumer's utility maximization, the publications in the second research area model substitution that is caused by the non-availability of products.

In this section, we develop a new approach to include the substitution aspect in our demand model, where substitution is controlled by price differences of substitutes. For that reason, we start with the formation of subsets consisting of all products that are substitutes to each other.

Suppose $\mathcal{P} = \{\mathcal{P}_1, ..., \mathcal{P}_m\}$ is a partition of the set P of all products such that

$$P = \mathcal{P}_1 \cup ... \cup \mathcal{P}_m,$$

where $\mathcal{P}_i \cap \mathcal{P}_j = \emptyset, i \neq j$, and so that if $p_{i_1} \in \mathcal{P}_i$ and $p_{i_2} \in \mathcal{P}_i$, p_{i_1} and p_{i_2} are substitutes. In the following, we consider a set $\mathcal{P}_i = \{p_{i_1}, \ldots, p_{i_n}\}$. To begin with, we write down our assumptions concerning the consumer's behavior in the case of substitution.

[14] For comparison, we refer to Cachon and Lariviere [CL05] for a presentation of different types of contracts in supply chain management (e.g., revenue-sharing contracts, buy-back contracts, price-discount contracts, or quantity discounts).

Assumptions 3.8. *Substitution*

- *The customer switches to the substitute if he can buy it at a lower price. Hence, in contrast to many other publications on substitution (see section 2.2 for examples), we consider substitution that is not due to the non-availability of products.*

- *If a product is substitutable, it is not necessarily substitutable for all applications, i.e., for each single application a (e.g., production process or end use). We split the total demand for p_{i_j} into a basis demand $\phi^b_{p_{i_j},r,t}$, which can only be satisfied by product p_{i_j}, and a substitutable demand $\phi^a_{\mathcal{P}_i,r,t}$. Whereas $\phi^b_{p_{i_j},r,t}$ only depends on the price of the product p_{i_j} under consideration, the substitutable demand is subject to both prices under consideration.*

- *The share of the substitutable demand assigned to the respective product depends on the corresponding price ratio.*

Note that from now on, our analysis is restricted to positive prices $x^{\pi}_{p_i,r,t} > 0,\ p_i \in \mathcal{P}_i$. In general, we distinguish between two types of substitution depending on the customer's situation: abrupt switching and gradual switching. Concerning gradual switching, we assume that some applications of the customer have a transition price range. This means, if prices of substitute products are in the same price range, a mixture of the products is required. In other words, switching does not happen completely and immediately if a certain price ratio barrier is crossed. We develop a modeling approach during the course of this section.

In case of complete switching, the full substitutable demand $\phi^a_{\mathcal{P}_i,r,t}$ needed for application a passes over to the cheaper product if the price ratio crosses the specified bound. In contrast to gradual switching, which solely depends on the prices, we assume that such an abrupt and complete change in demanding can also depend on time and costs of the switching process. This makes it more complex to develop a model, because, in theory, each application of the customer that provokes such a switch has different production factors.

In the following section, we briefly illustrate the emerging complexity of such a detailed modeling approach and discuss under which assumptions we can circumvent these difficulties by modeling the sum of all abrupt, complete switchings as a gradual switching process. In other words, we consider the aggregation of all applications leading to a complete change instead of each single switching process.

3.5.1 Abrupt Switching

In this section, we restrict our analysis to two substitute products, i.e., $\mathcal{P}_i = \{p_{i_1}, p_{i_2}\}$. In case of an abrupt and complete switching from one product to another, we can again distinguish between different application-specific cases. Thus, we consider the following situations.

1. Switching is costless and not time-consuming.

2. Switching is cost-intensive and not time-consuming.

3. Switching is cost-intensive and time-consuming.

Note that, in this section, we propose demand functions that include the effects of substitution caused by abrupt switching processes. These are, however, not differentiable with respect to prices.
Including the first case in our modeling approach is straightforward, since the customer simply switches to another production mode and uses the cheaper product. Consequently, we state the following characteristics.

Characteristics of demand 3.6. Model for abrupt switching 1
We assume that for application a switching from one product to its substitute product is costless and not time-consuming. If p_{i_j}, $j \in \{1,2\}$, was consumed at time $t-1$, i.e., $x^{\pi}_{p_{i_j},r,t-1} < x^{\pi}_{p_{i_{3-j}},r,t-1}$, the demand at time t is given by

$$\phi^{a,b}_{p_{i_j},r,t}(\boldsymbol{x}^{\pi}_{r,t}) = \begin{cases} \phi^{b}_{p_{i_j},r,t}(\boldsymbol{x}^{\pi}_{r,t}) & \text{if } x^{\pi}_{p_{i_{3-j}},r,t} < x^{\pi}_{p_{i_j},r,t}, \\ \phi^{a}_{\mathcal{P}_i,r,t}(\boldsymbol{x}^{\pi}_{r,t}) + \phi^{b}_{p_{i_j},r,t}(\boldsymbol{x}^{\pi}_{r,t}) & \text{if } x^{\pi}_{p_{i_{3-j}},r,t} \geq x^{\pi}_{p_{i_j},r,t}. \end{cases} \tag{3.18}$$

Remark 3.1. Given $\underline{x}^{\pi}_{p_i,r,t} := \min_{p_i \in \mathcal{P}_i}(x^{\pi}_{p_i,r,t})$ the substitutable demand is given by

$$\begin{aligned} \phi^{a}_{\mathcal{P}_i,r,t}(\boldsymbol{x}^{\pi}_{r,t}) = {} & \alpha^{\text{max\_quant}}_{\mathcal{P}_i,r,t} \mathbb{1}_{[0,\alpha^{b1}_{\mathcal{P}_i,r,t})}(\underline{x}^{\pi}_{p_i,r,t}) + \varphi_{p,r,t}(\boldsymbol{x}^{\pi}_{r,t}) \cdot \mathbb{1}_{[\alpha^{b1}_{\mathcal{P}_i,r,t},\alpha^{b2}_{\mathcal{P}_i,r,t})}(\underline{x}^{\pi}_{p_i,r,t}) \\ & + \alpha^{\text{min\_quant}}_{\mathcal{P}_i,r,t} \mathbb{1}_{[\alpha^{b2}_{\mathcal{P}_i,r,t},\alpha^{b3}_{\mathcal{P}_i,r,t})}(\underline{x}^{\pi}_{p_i,r,t}) + 0 \cdot \mathbb{1}_{[\alpha^{b3}_{\mathcal{P}_i,r,t},\infty)}(\underline{x}^{\pi}_{p_i,r,t}). \end{aligned} \tag{3.19}$$

So far, including a complete switching is simple. If we consider situations, in which such a product switching is cost-intensive, we have to take additional factors into account. Certainly, the most important influencing factors are additional switching costs $\alpha^{sc}_{p_{i_1},p_{i_2},t}$. Including these additional costs in the modeling leads to the following assumption.

Assumptions 3.9. *Switching is only profitable if at least one of the products' prices is element of the price range $[\alpha^{b1}_{\mathcal{P}_i,r,t}, \alpha^{b2}_{\mathcal{P}_i,r,t})$, i.e., $x^{\pi}_{p_{i_2},r,t} \in [\alpha^{b1}_{\mathcal{P}_i,r,t}, \alpha^{b2}_{\mathcal{P}_i,r,t}) \vee x^{\pi}_{p_{i_1},r,t} \in [\alpha^{b1}_{\mathcal{P}_i,r,t}, \alpha^{b2}_{\mathcal{P}_i,r,t})$.*

In all other cases, we assume that demand is price-insensitive, because other factors outweigh the prices (see section 3.4). Hence, switching mainly causes higher costs and procures no further benefit.

Characteristics of demand 3.7. Model for abrupt switching 2
If for application a switching from one product to its substitute product is cost-intensive but not time-consuming, we assume that the consumer does not switch immediately from the product in use to the possibly cheaper product, but switches if the corresponding price ratio $x^{\pi}_{p_{i_1},r,t}/x^{\pi}_{p_{i_2},r,t}$ crosses a specified barrier $\delta_{p_{i_1},p_{i_2},t} > 1$. Under the assumption that

product p_{i_1} was consumed at time $t-1$, i.e., $x^{\pi}_{p_{i_1},r,t-1} < \delta_{p_{i_1},p_{i_2},t-1} \cdot x^{\pi}_{p_{i_2},r,t-1}$ the demand for product p_{i_1} at time t is given by

$$\phi^{a,b}_{p_{i_1},r,t}(\boldsymbol{x}^{\pi}_{r,t}) = \begin{cases} \phi^{b}_{p_{i_1},r,t}(\boldsymbol{x}^{\pi}_{r,t}) & \text{if } \delta_{p_{i_1},p_{i_2},t} \cdot x^{\pi}_{p_{i_2},r,t} < x^{\pi}_{p_{i_1},r,t} \\ & \text{and } x^{\pi}_{p_{i_2},r,t} \in [\alpha^{b1}_{\mathcal{P}_i,r,t}, \alpha^{b2}_{\mathcal{P}_i,r,t}) \\ & \quad \vee x^{\pi}_{p_{i_1},r,t} \in [\alpha^{b1}_{\mathcal{P}_i,r,t}, \alpha^{b2}_{\mathcal{P}_i,r,t}) \\ \phi^{a}_{\mathcal{P}_i,r,t}(\boldsymbol{x}^{\pi}_{r,t}) + \phi^{b}_{p_{i_1},r,t}(\boldsymbol{x}^{\pi}_{r,t}) & \text{if } \delta_{p_{i_1},p_{i_2},t} \cdot x^{\pi}_{p_{i_2},r,t} \geq x^{\pi}_{p_{i_1},r,t}, \end{cases} \tag{3.20}$$

and for p_{i_2} by

$$\phi^{a,b}_{p_{i_2},r,t}(\boldsymbol{x}^{\pi}_{r,t}) = \begin{cases} \phi^{a}_{\mathcal{P}_i,r,t}(\boldsymbol{x}^{\pi}_{r,t}) + \phi^{b}_{p_{i_2},r,t}(\boldsymbol{x}^{\pi}_{r,t}) & \text{if } \delta_{p_{i_1},p_{i_2},t} \cdot x^{\pi}_{p_{i_2},r,t} < x^{\pi}_{p_{i_1},r,t} \\ & \text{and } x^{\pi}_{p_{i_2},r,t} \in [\alpha^{b1}_{\mathcal{P}_i,r,t}, \alpha^{b2}_{\mathcal{P}_i,r,t}) \\ & \quad \vee x^{\pi}_{p_{i_1},r,t} \in [\alpha^{b1}_{\mathcal{P}_i,r,t}, \alpha^{b2}_{\mathcal{P}_i,r,t}) \\ \phi^{b}_{p_{i_2},r,t}(\boldsymbol{x}^{\pi}_{r,t}) & \text{if } \delta_{p_{i_1},p_{i_2},t} \cdot x^{\pi}_{p_{i_2},r,t} \geq x^{\pi}_{p_{i_1},r,t}. \end{cases} \tag{3.21}$$

At this point, the question arises which factors have influence on $\delta_{p_{i_1},p_{i_2},t}$. To get a lower bound, we assume that the consumer switches from p_{i_1} to p_{i_2} at time t if

$$x^{\pi}_{p_{i_1},r,t} \cdot \phi^{a}_{\mathcal{P}_i,r,t}(\boldsymbol{x}^{\pi}_{r,t}) > x^{\pi}_{p_{i_2},r,t} \cdot \phi^{a}_{\mathcal{P}_i,r,t}(\boldsymbol{x}^{\pi}_{r,t}) + \alpha^{sc}_{p_{i_1},p_{i_2},t} \tag{3.22}$$

and if $x^{\pi}_{p_{i_2},r,t} \in [\alpha^{b1}_{\mathcal{P}_i,r,t}, \alpha^{b2}_{\mathcal{P}_i,r,t}) \vee x^{\pi}_{p_{i_1},r,t} \in [\alpha^{b1}_{\mathcal{P}_i,r,t}, \alpha^{b2}_{\mathcal{P}_i,r,t})$. Since $x^{\pi}_{p_{i_2},r,t} < x^{\pi}_{p_{i_1},r,t}$ we can set

$$\begin{aligned} \phi^{a}_{\mathcal{P}_i,r,t}(\boldsymbol{x}^{\pi}_{r,t}) &= \alpha^{\text{max\_quant}}_{\mathcal{P}_i,r,t} \cdot \mathbb{1}_{[0,\alpha^{b1}_{\mathcal{P}_i,r,t})}(x^{\pi}_{p2,r,t}) + \varphi^{a}_{\mathcal{P}_i,r,t}(\boldsymbol{x}^{\pi}_{r,t}) \cdot \mathbb{1}_{[\alpha^{b1}_{\mathcal{P}_i,r,t},\alpha^{b2}_{\mathcal{P}_i,r,t})}(x^{\pi}_{p2,r,t}) \\ &\leq \alpha^{\text{max\_quant}}_{\mathcal{P}_i,r,t}. \end{aligned}$$

This implies that switching from p_{i_1} to p_{i_2} is profitable if

$$\frac{x^{\pi}_{p_{i_1},r,t}}{x^{\pi}_{p_{i_2},r,t}} > 1 + \frac{\alpha^{sc}_{p_{i_1},p_{i_2},t}}{x^{\pi}_{p_{i_2},r,t} \cdot \phi^{a}_{\mathcal{P}_i,r,t}(\boldsymbol{x}^{\pi}_{r,t})} \geq 1 + \frac{\alpha^{sc}_{p_{i_1},p_{i_2},t}}{x^{\pi}_{p_{i_2},r,t} \cdot \alpha^{\text{max\_quant}}_{\mathcal{P}_i,r,t}}. \tag{3.23}$$

Hence, we obtain a lower bound for the price ratio indicating the change of consumption from p_{i_1} to its substitute p_{i_2} at time t

$$\delta^{\text{lower-bound}}_{p_{i_1},p_{i_2},t} = 1 + \frac{\alpha^{sc}_{p_{i_1},p_{i_2},t}}{x^{\pi}_{p_{i_2},r,t} \cdot \alpha^{\text{max\_quant}}_{\mathcal{P}_i,r,t}}. \tag{3.24}$$

Example 3.3. *Let $\mathcal{P}_i = \{p_{i_1}, p_{i_2}\}$. To illustrate a possible course of prices over multiple times we set for all $t = t_1, \ldots, t_9$ $\alpha^{sc}_{p_{i_1},p_{i_2},t} = \alpha^{sc}_{p_{i_2},p_{i_1},t} = 200$, $\alpha^{\text{max\_quant}}_{\mathcal{P},r,t} = 100$, $\alpha^{b1}_{\mathcal{P},r,t} = 7$ and $\alpha^{b2}_{\mathcal{P},r,t} = 25$. Furthermore, we set $\delta_{p_{i_1},p_{i_2},t} = \delta^{\text{lower-bound}}_{p_{i_1},p_{i_2},t}$. Figure 3.2 shows an exemplary course of the prices $x^{\pi}_{p_{i_1},r,t}$ and $x^{\pi}_{p_{i_2},r,t}$ at $t = t_1, \ldots, t_9$ for situation 1. The customer buys product p_{i_1} at t_1, t_5, t_6, t_7, t_8 and product p_{i_2} at t_2, t_3, t_4, t_9. The situation 2 is illustrated in figure 3.3. The consumer switches to the cheaper product if the lower bounds $\delta_{p_{i_1},p_{i_2},t}$ or $\delta_{p_{i_2},p_{i_1},t}$ are crossed. Consequently, he purchases product p_{i_1} at t_1, t_2, t_6, t_7, t_8 and product p_{i_2} at t_3, t_4, t_5, t_9.*

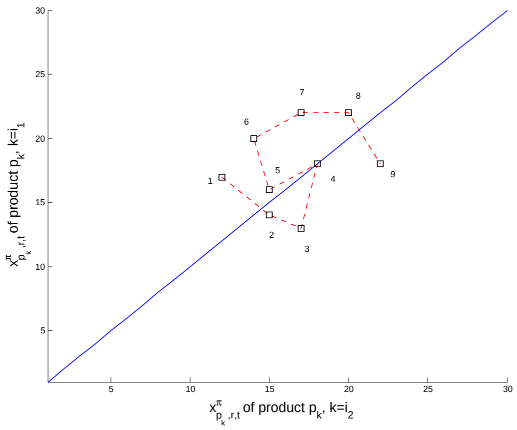

Figure 3.2: Illustration of a possible course of prices and the resulting purchase decision if switching from one product to another is costless and not time-consuming (situation 1)

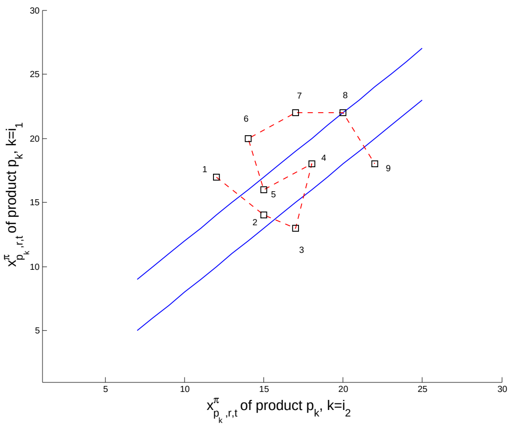

Figure 3.3: Illustration of a possible course of prices and the resulting purchase decision if switching from one product to another is cost-intensive and not time-consuming (situation 2)

Considering an application, in which switching from one product to another is both cost-intensive and time-consuming, requires still more information. We assume that the customer's decision depends, among others, on data of demand and prices before the possible switching as well as the expectation about the price development in the future. Moreover, technical details such as duration of the switching is crucial, since it takes some time until the switching process is terminated and production or final consumption proceeds. The need of all this additional data implies that explicitly modeling such a complex decision-making is quite difficult if not impossible unless stochastic components are included. Therefore, we restrict ourselves to describe an exemplary scheme of a cost-intensive and time-consuming switching (see example 3.4) before proceeding to aggregate single abrupt switches to a gradual switching.

Example 3.4. *Cost-intensive and time-consuming substitution*
In the following table, we draft a scenario in which the customer reprocessing p_{i_1} and p_{i_2} decides to switch his production mode from p_{i_1} to p_{i_2} at time t, which is both cost-intensive and time-consuming. z_1 denotes the time period for which the customer expects a positive price development. z_2 denotes the time needed to change the production process so that production with the substitute is possible. Moreover, let $\delta_{p_{i_1},p_{i_2},\tau} > 1 \ \forall \tau = t-1,\ldots,t+z_2+1$.

Time	*Market situation and Customer's decision*
$t-1$	*If* $x^{\pi}_{p_{i_1},r,t-1} < \delta_{p_{i_1},p_{i_2},t} \cdot x^{\pi}_{p_{i_2},r,t-1}$*, he purchases* p_{i_1} *at time* $t-1$.
t	*If assumption 3.9 holds,* $\delta_{p_{i_1},p_{i_2},t} \cdot x^{\pi}_{p_{i_2},r,t} < x^{\pi}_{p_{i_1},r,t}$*, and* $\alpha^{E\pi}_{p_{i_2},r,t+z} \geq \alpha^{E\pi}_{p_{i_1},r,t+z}$ $\forall z = 1,\dots,z_1$*, i.e., he expects that* $x^{\pi}_{p_{i_2},r,t+z} < x^{\pi}_{p_{i_1},r,t+z}$ $\forall z = 1,\dots,z_1$*, he switches and reduces his consumption, i.e.,* $\phi^{a,b}_{p_{i_1},r,t}(\boldsymbol{x}^{\pi}_{r,t}) = \phi^{b}_{p_{i_1},r,t}$ *and* $\phi^{a,b}_{p_{i_2},r,t}(\boldsymbol{x}^{\pi}_{r,t}) = \phi^{a,storage}_{\mathcal{P}_i,r,t}(\boldsymbol{x}^{\pi}_{r,t}) + \phi^{b}_{p_{i_2},r,t}$*, where* $\phi^{a,storage}_{\mathcal{P}_i,r,t(\boldsymbol{x}^{\pi}_{r,t})} < \phi^{a}_{\mathcal{P}_i,r,t}(\boldsymbol{x}^{\pi}_{r,t})$ *is the quantity he is able to store at time t until the production process is completed.*
$t{+}1$ *to* $t{+}z_2{-}1$	*Further reswitching is not profitable and causes loss. Hence, the consumer only purchases the basis demand* $\phi^{b}_{p_{i_1},r,\tau}$*,* $\tau = t{+}1,\dots,t{+}z_2{-}1$ *of* p_{i_1} *and* $\phi^{a,b}_{p_{i_2},r,t}(\boldsymbol{x}^{\pi}_{r,t}) = \phi^{a,storage}_{\mathcal{P}_i,r,\tau}(\boldsymbol{x}^{\pi}_{r,t}) + \phi^{b}_{p_{i_2},r,\tau}$*,* $\tau = t+1,\dots,t+z_2-1$.
$t+z_2$	*The switching is completed. The substitutable demand is completely satisfied by* p_{i_2}*, i.e.,* $\phi^{a,b}_{p_{i_2},r,t+1}(\boldsymbol{x}^{\pi}_{r,t+1}) = \phi^{a}_{\mathcal{P}_i,r,t+1}(\boldsymbol{x}^{\pi}_{r,t+1}) + \phi^{b}_{p_{i_2},r,t+1}$.
from $t+z_2+1$ *on*	*The customer is not willing to reswitch again, unless the market situation changes to a larger extent, i.e.,* $\tilde{\delta}_{p_{i_1},p_{i_2},t+z_2+n} \cdot x^{\pi}_{p_{i_2},r,t+z_2+n} > x^{\pi}_{p_{i_1},r,t+z_2+n}$ *where* $\tilde{\delta}_{p_{i_1},p_{i_2},t+z_2+n} < \delta_{p_{i_1},p_{i_2},t}$ *and* $n = 1,2,3,\dots$.

Note that we have no information about the storage opportunities, hence, it is possible that $\phi^{a,storage}_{\mathcal{P}_i,r,\tau}(\boldsymbol{x}^{\pi}_{r,t}) = 0,\ \tau = t,\dots,t+z_2-1$*. Summing up, the demand of products with applications for which substitution is cost-intensive and time-consuming, depends, among others, on the price ratio* $\delta_{p_{i_1},p_{i_2},t}$*, the switching costs, the expectation regarding the price development* $\alpha^{E\pi}_{p_{i_1},r,t+z}$ *and* $\alpha^{E\pi}_{p_{i_2},r,t+z}$ *for* $z = 1,\dots,z_1$*, and the duration of the switching process* z_2*.*

Remark 3.2. This example successfully shows the complexity of such switching processes, which are cost-intensive and time-consuming. Therefore, stochastic optimization models might be an appropriate tool in order to model the decision process of a customer because, obviously, he has to decide under uncertainty whether to switch the production process or not. In the following, we will explain how we circumvent this by aggregating the sum of all single abrupt substitutions.

As stated above, from now on, we do not consider each application explicitly, but aggregate all demand, which possibly arises from all applications of the customer.

Assumptions 3.10. Aggregation of substitutable demand
Under the assumption that there are a lot of applications differing in their production settings and switching features, the switching of the aggregated substitutable demand

$$\phi^{agg}_{\mathcal{P}_i,r,t}(\boldsymbol{x}^{\pi}_{r,t}) := \sum_{a} \phi^{a}_{\mathcal{P}_i,r,t}(\boldsymbol{x}^{\pi}_{r,t}) \tag{3.25}$$

can be approximately modeled by the gradual switching approach (described in the following section).

3.5.2 Gradual Switching

Again, we suppose we have two substitutes p_{i_1} and p_{i_2} with prices $x^{\pi}_{p_{i_1},r,t}$ and $x^{\pi}_{p_{i_2},r,t}$, respectively. If one of the products is clearly cheaper than the other product, the consumer's substitutable demand is absorbed by the cheaper one. If both prices are comparable, their common substitutable demand $\phi_{\mathcal{P}_i,r,t}$ is split. In the following, we aim to model this behavior by means of "splitting functions" $\rho_{p_{i_1}}$ and $\rho_{p_{i_2}}$ determining the share of the common demand for the products p_{i_1} and p_{i_2}.
Therefore, $\rho_{p_{i_1}}$ and $\rho_{p_{i_2}}$ have to satisfy certain properties, which we describe below.

Assumptions 3.11. *Necessary characteristics of $\rho_{p_{i_1}}$ and $\rho_{p_{i_2}}$*
For appropriate splitting functions $\rho_{p_{i_1}}: \mathbb{R}_0^+ \to [0,1]$ and $\rho_{p_{i_2}}: \mathbb{R}_0^+ \to [0,1]$, the following characteristics hold

- *$\rho_{p_{i_1}}$ and $\rho_{p_{i_2}}$ are functions of the ratio of the prices $x^{\pi}_{p_{i_1},r,t}$ and $x^{\pi}_{p_{i_2},r,t}$ and differentiable with respect to $x^{\pi}_{p_{i_1},r,t}$ and $x^{\pi}_{p_{i_2},r,t}$.*
- $\rho_{p_{i_1}}(1) = \rho_{p_{i_2}}(1) = \frac{1}{2}$.
- $\rho_{p_{i_1}}(y) + \rho_{p_{i_2}}(y) = 1$ *for* $y \in \mathbb{R}^+$.
- $\rho_{p_{i_1}}(y) = \rho_{p_{i_2}}\left(\frac{1}{y}\right)$ *for* $y \in \mathbb{R}^+$.

Having specified the required characteristics for $\rho_{p_{i_1}}(x^{\pi}_{p_{i_1},r,t}/x^{\pi}_{p_{i_2},r,t})$ and $\rho_{p_{i_2}}(x^{\pi}_{p_{i_1},r,t}/x^{\pi}_{p_{i_2},r,t})$ we can now build the demand model for gradual substitution.

Characteristics of demand 3.8. *Gradual substitution*
Let $\phi_{\mathcal{P}_i,r,t}: (\mathbb{R}_0^+)^{|P|} \times \mathbb{R} \times \mathbb{R}^I \times \mathbb{R}^I \times \mathbb{R}^C \to \mathbb{R}_0^+$, $\boldsymbol{x}^{\pi}_{r,t} \mapsto \phi_{\mathcal{P}_i,r,t}(\boldsymbol{x}^{\pi}_{r,t})$ be the demand function for the substitutable demand for all $p \in \mathcal{P}_i$, or the differentiable approximation of the substitutable demand function for $\phi^{agg}_{\mathcal{P}_i,r,t}(\boldsymbol{x}^{\pi}_{r,t})$, respectively.[15] *Assuming that the switching process is gradual, the demand for p_{i_1} is given by*

$$\phi^{\text{sub}}_{p_{i_1},r,t}(\boldsymbol{x}^{\pi}_{r,t}) = \rho_{p_{i_1}}\left(\frac{x^{\pi}_{p_{i_1},r,t}}{x^{\pi}_{p_{i_2},r,t}}\right) \cdot \phi_{\mathcal{P}_i,r,t}(\boldsymbol{x}^{\pi}_{r,t}) + \phi^{b}_{p_{i_1},r,t}(\boldsymbol{x}^{\pi}_{r,t}), \tag{3.26}$$

and for p_{i_2} by

$$\phi^{\text{sub}}_{p_{i_2},r,t}(\boldsymbol{x}^{\pi}_{r,t}) = \rho_{p_{i_2}}\left(\frac{x^{\pi}_{p_{i_2},r,t}}{x^{\pi}_{p_{i_1},r,t}}\right) \cdot \phi_{\mathcal{P}_i,r,t}(\boldsymbol{x}^{\pi}_{r,t}) + \phi^{b}_{p_{i_2},r,t}(\boldsymbol{x}^{\pi}_{r,t}), \tag{3.27}$$

where $\rho_{p_{i_1}}(x^{\pi}_{p_{i_1},r,t}/x^{\pi}_{p_{i_2},r,t})$ and $\rho_{p_{i_2}}(x^{\pi}_{p_{i_2},r,t}/x^{\pi}_{p_{i_1},r,t}) := 1 - \rho_{p_{i_1}}(x^{\pi}_{p_{i_1},r,t}/x^{\pi}_{p_{i_2},r,t})$ satisfy the assumptions 3.11.

Note that the superscript sub indicates that the effects of substitutes have been explicitly taken into account.

[15] Remember that we omit the parameters in the notation of the demand functions for a better comprehension.

Remark 3.3. Given $\mathcal{P}_i = \{p_{i_1}, p_{i_2}\}$. Provided that $\frac{\partial \phi_{\mathcal{P}_i,r,t}}{\partial x^{\pi}_{p_{i_1},r,t}} \left(\boldsymbol{x}^{\pi}_{r,t}\right) = \frac{\partial \phi_{\mathcal{P}_i,r,t}}{\partial x^{\pi}_{p_{i_2},r,t}} \left(\boldsymbol{x}^{\pi}_{r,t}\right)$,

$$\begin{aligned}\frac{\partial \phi^{\text{sub}}_{p_{i_2},r,t}}{\partial x^{\pi}_{p_{i_1},r,t}} \left(\boldsymbol{x}^{\pi}_{r,t}\right) &= \frac{\partial \rho_{p_{i_2}}}{\partial x^{\pi}_{p_{i_1},r,t}} \left(\frac{x^{\pi}_{p_{i_2},r,t}}{x^{\pi}_{p_{i_1},r,t}}\right) \cdot \phi_{\mathcal{P}_i,r,t}(\boldsymbol{x}^{\pi}_{r,t}) + \rho_{p_{i_2}} \left(\frac{x^{\pi}_{p_{i_2},r,t}}{x^{\pi}_{p_{i_1},r,t}}\right) \cdot \frac{\partial \phi_{\mathcal{P}_i,r,t}}{\partial x^{\pi}_{p_{i_1},r,t}} \left(\boldsymbol{x}^{\pi}_{r,t}\right) \\ &= \frac{\partial \rho_{p_{i_1}}}{\partial x^{\pi}_{p_{i_2},r,t}} \left(\frac{x^{\pi}_{p_{i_1},r,t}}{x^{\pi}_{p_{i_2},r,t}}\right) \cdot \phi_{\mathcal{P}_i,r,t}(\boldsymbol{x}^{\pi}_{r,t}) + \rho_{p_{i_1}} \left(\frac{x^{\pi}_{p_{i_1},r,t}}{x^{\pi}_{p_{i_2},r,t}}\right) \cdot \frac{\partial \phi_{\mathcal{P}_i,r,t}}{\partial x^{\pi}_{p_{i_2},r,t}} \left(\boldsymbol{x}^{\pi}_{r,t}\right) \\ &= \frac{\partial \phi^{\text{sub}}_{p_{i_1},r,t}}{\partial x^{\pi}_{p_{i_2},r,t}} \left(\boldsymbol{x}^{\pi}_{r,t}\right),\end{aligned}$$

since $\frac{\partial \phi^{b}_{p_{i_j},r,t}}{\partial x^{\pi}_{p_{i_k},r,t}}(\boldsymbol{x}^{\pi}_{r,t}) = 0$ (cf. assumptions 3.8). Consequently, in the case of substitutes, the cross-price derivatives are symmetric. This is automatically fulfilled for independent products p_k, p_l since $\frac{\partial \phi_{p_k,r,t}}{\partial x^{\pi}_{p_l,r,t}} = 0$ (cf. characteristics of demand 3.1).

Remark 3.4. In case more than two products are substitutes, the model (3.27) can be enhanced to n substitutes including n splitting functions instead of two. We obtain

$$\phi^{\text{sub}}_{p_{i_j},r,t}(\boldsymbol{x}^{\pi}_{r,t}) = \rho_{p_{i_j},\mathcal{P}_i}(x^{\pi}_{p_{i_1},r,t}, \ldots, x^{\pi}_{p_{i_n},r,t}) \cdot \phi_{\mathcal{P}_i,r,t}(\boldsymbol{x}^{\pi}_{r,t}) + \phi^{b}_{p_{i_j},r,t}(\boldsymbol{x}^{\pi}_{r,t}),\ j = 1, \ldots, n, \tag{3.28}$$

where $\mathcal{P}_i = \{p_{i_1}, \ldots, p_{i_n}\}$ and $\rho_{p_{i_j},\mathcal{P}_i}(x^{\pi}_{p_{i_1},r,t}, \ldots, x^{\pi}_{p_{i_n},r,t})$, $j = 1, \ldots, n$, satisfy, among others,

$$\rho_{p_{i_j},\mathcal{P}_i}(x^{\pi}_{p_{i_1},r,t}, \ldots, x^{\pi}_{p_{i_n},r,t}) = \frac{1}{n} \quad \text{if } x^{\pi}_{p_{i_1},r,t} = \ldots = x^{\pi}_{p_{i_n},r,t}$$

and

$$\sum_{j=1}^{n} \rho_{p_{i_j},\mathcal{P}_i}(x^{\pi}_{p_{i_1},r,t}, \ldots, x^{\pi}_{p_{i_n},r,t}) = 1.$$

To get a more detailed description further analysis is necessary. This, however, is beyond the scope of this thesis.

For the sake of completeness, we set up the following property concerning the dependency of the substitutes' prices.

Characteristics of demand 3.9. Influence of substitutes on demand
Let $\phi^{\text{sub}}_{p,r,t}$ be differentiable w.r.t. $x^{\pi}_{p,r,t}$, $p \in P$. Given the set of products P, if there are two products $\{p_s, p_l\} \in P$ with

$$\frac{\partial \phi^{\text{sub}}_{p_l,r,t}}{\partial x^{\pi}_{p_l,r,t}} \left(\boldsymbol{x}^{\pi}_{r,t}\right) \leq 0 \tag{3.29}$$

and

$$\frac{\partial \phi^{\text{sub}}_{p_l,r,t}}{\partial x^{\pi}_{p_s,r,t}} \left(\boldsymbol{x}^{\pi}_{r,t}\right) \geq 0, \tag{3.30}$$

and for all other products $p_m \in P \setminus \{p_l, p_s\}, m \neq l, s,$

$$\frac{\partial \phi^{\text{sub}}_{p_l,r,t}}{\partial x^{\pi}_{p_m,r,t}} \left(\boldsymbol{x}^{\pi}_{r,t}\right) = 0 \quad \text{for all } m = 1, \ldots, |P|, \quad m \neq l, s, \tag{3.31}$$

then p_s *is a substitute product for product* p_l *and the remaining products are independent, i.e., they are neither substitutes nor complements of these two products.*

For comparison, in economic studies, it is common to refer to goods as substitutes if the corresponding price elasticity (see definition 2.3) is positive. In contrast to derivatives, these measures capturing the demand responsiveness are unit-free. However, we restrict our analysis to the derivatives for the classification of the products assuming that prices are positive.
Note that our approach to including substitutes in the demand model implicates that this feature does not necessarily hold for all situations. In the case of aprubt cost-intensive switching, the substitution effect stated above gets lost in the presence of other effects such as high switching costs or a reverse expectation on the price development. This effect also occurs in the gradual modeling approach, because the effect of decreasing substitutable demand can superimpose the positive effect of the splitting function. We will elaborate this using the example of a specific demand function in the following chapter.

3.6 Influences of Other Products' Prices on Demand: Complements

In this section, we consider the case in which the consumer wants to purchase a set of products in a specified ratio, because he only needs or can reprocess a certain combination of these products. As with substitutes, such complements also arise in neoclassical consumer theory (cf. section 2.1.2 and [DM80b, BS09]).
Here, we present a new approach to include this dependence of multiple products in a phenomenological way. Again, we group the products under consideration. Let $\mathcal{C} = \{\mathcal{C}_1, \ldots, \mathcal{C}_m\}$ be a partition of the set P so that

$$P = \mathcal{C}_1 \cup \ldots \cup \mathcal{C}_m,$$

where $\mathcal{C}_i \cap \mathcal{C}_j = \emptyset$, $i \neq j$, and p_{i_1} and p_{i_2} are complementary products if $p_{i_1} \in \mathcal{C}_i$ and $p_{i_2} \in \mathcal{C}_i$. That means, the customer only demands them in a specified ratio $a^{\text{com}}_{p_{i_1},p_{i_2},t}$. Hence,

$$\phi^{\text{com}}_{p_{i_1},r,t}(\boldsymbol{x}^{\pi}_{r,t}) = a^{\text{com}}_{p_{i_1},p_{i_2},t} \cdot \phi^{\text{com}}_{p_{i_2},r,t}(\boldsymbol{x}^{\pi}_{r,t}), \tag{3.32}$$

where the superscript com implies that the demand function includes the effect of complementary products. Notably, so far, the additional basic demand for each product that can only be satisfied by each product separately has not been taken into account. We will return to this later on. In the following, we consider $\mathcal{C}_i = \{p_{i_1}, \ldots, p_{i_n}\}$.

Assumptions 3.12. *If the customer requires a product $p_{i_j} \in \mathcal{C}_i$, he simultaneously is in demand for a combination of all products of $\mathcal{C}_i$. Figuratively speaking, the customer demands a basket of products filled with the respective weight proportion $a^{\text{com}}_{p_{i_j},\mathcal{C}_i,t}$, $j = 1,\dots,n$, of the single products p_{i_j} he needs for further usage or processing.*
Consequently, the demand of this basket $\phi_{\mathcal{C}_i,r,t}$ and, hence, the demand for each single product p_{i_j} is influenced by the sum of all complementary products' prices $\Psi_{\mathcal{C}_i,r,t}(\boldsymbol{x}^\pi_{r,t}) = \sum_{k=1}^n a^{\text{com}}_{p_{i_k},\mathcal{C}_i,t} \cdot x^\pi_{p_{i_k},r,t}$, which is the cost function of the basket consisting of all products $p_{i_j} \in \mathcal{C}_i$.

Characteristics of demand 3.10. *Demand model for n complements*
Let $\phi_{\mathcal{C}_i,r,t}\colon (\mathbb{R}^+_0)^{|P|} \times \mathbb{R} \times \mathbb{R}^I \times \mathbb{R}^I \times \mathbb{R}^C \to \mathbb{R}^+_0, \boldsymbol{x}^\pi_{r,t} \mapsto \phi_{\mathcal{C}_i,r,t}(\boldsymbol{x}^\pi_{r,t})$ be the demand function for the mixture of products $p \in \mathcal{C}_i$ weighted by the respective factor $a^{\text{com}}_{p,\mathcal{C}_i,t}$ with respect to prices.[16] *Then, the demand for each single product $p_{i_j} \in \mathcal{C}_i$ can be expressed by*

$$a^{\text{com}}_{p_{i_j},\mathcal{C}_i,t} \cdot \phi_{\mathcal{C}_i,r,t}\left(\boldsymbol{x}^\pi_{r,t}\right), \tag{3.33}$$

where $a^{\text{com}}_{p_{i_j},\mathcal{C}_i,t}$ represents the respective proportion of p_{i_j} in the mixture required. All in all, the total demand for a product $p_{i_j} \in \mathcal{C}_i$ is given by

$$\phi^{\text{com}}_{p_{i_j},r,t}(\boldsymbol{x}^\pi_{r,t}) = a^{\text{com}}_{p_{i_j},\mathcal{C}_i,t} \cdot \phi_{\mathcal{C}_i,r,t}\left(\boldsymbol{x}^\pi_{r,t}\right) + \phi^b_{p_{i_j},r,t}(\boldsymbol{x}^\pi_{r,t}), \tag{3.34}$$

where $\phi^b_{p_{i_j},r,t}(\boldsymbol{x}^\pi_{r,t})$ is the basis demand that can only be satisfied by p_{i_j}.

Remark 3.5. We assume that $\phi_{\mathcal{C}_i,r,t}\left(\boldsymbol{x}^\pi_{r,t}\right) = \phi^{\text{bundle}}_{\mathcal{C}_i,r,t}\left(\Psi_{\mathcal{C}_i,r,t}(\boldsymbol{x}^\pi_{r,t})\right)$, where $\phi^{\text{bundle}}_{\mathcal{C}_i,r,t}\colon \mathbb{R}^+_0 \times \mathbb{R} \times \mathbb{R}^I \times \mathbb{R}^I \times \mathbb{R}^C \to \mathbb{R}^+_0$, $y \mapsto \phi_{\mathcal{C}_i,r,t}(y)$, and $\Psi_{\mathcal{C}_i,r,t}\colon (\mathbb{R}^+_0)^{|P|} \to \mathbb{R}^+_0$, $\boldsymbol{x}^\pi_{r,t} \mapsto \sum_{k=1}^n a^{\text{com}}_{p_{i_k},\mathcal{C}_i,t} \cdot x^\pi_{p_{i_k},r,t}$. Then, given $p_{i_j}, p_{i_k} \in \mathcal{C}_i$,

$$\begin{aligned}
\frac{\partial \phi^{\text{com}}_{p_{i_j},r,t}}{\partial x^\pi_{p_{i_k},r,t}}\left(\boldsymbol{x}^\pi_{r,t}\right) &= a^{\text{com}}_{p_{i_j},\mathcal{C}_i,t} \cdot \frac{\partial \phi_{\mathcal{C}_i,r,t}}{\partial x^\pi_{p_{i_k},r,t}}(\boldsymbol{x}^\pi_{r,t}) \\
&= a^{\text{com}}_{p_{i_j},\mathcal{C}_i,t} \cdot \frac{\partial \phi^{\text{bundle}}_{\mathcal{C}_i,r,t}}{\partial y}\left(\Psi_{\mathcal{C}_i,r,t}(\boldsymbol{x}^\pi_{r,t})\right) \cdot \frac{\partial \Psi_{\mathcal{C}_i,r,t}}{\partial x^\pi_{p_{i_k},r,t}}\left(\boldsymbol{x}^\pi_{r,t}\right) \\
&= a^{\text{com}}_{p_{i_j},\mathcal{C}_i,t} \cdot \frac{\partial \phi^{\text{bundle}}_{\mathcal{C}_i,r,t}}{\partial y}\left(\Psi_{\mathcal{C}_i,r,t}(\boldsymbol{x}^\pi_{r,t})\right) \cdot a^{\text{com}}_{p_{i_k},\mathcal{C}_i,t} \\
&= \frac{\partial \phi^{\text{com}}_{p_{i_k},r,t}}{\partial x^\pi_{p_{i_j},r,t}}\left(\boldsymbol{x}^\pi_{r,t}\right),
\end{aligned}$$

since $\frac{\partial \phi^b_{p_{i_j},r,t}}{\partial x^\pi_{p_{i_k},r,t}}(\boldsymbol{x}^\pi_{r,t}) = 0$ (cf. assumptions 3.8). Thus, in the case of complements, the cross-price derivatives are also symmetric.

The following characteristics concerning complementary products completes our analysis.

[16] Note that we omit the parameters in the notation of the demand functions for sake of simplicity.

Characteristics of demand 3.11. *Influence of complements on demand*
Let P be the set of products in the market under consideration. Product p_c is a complement of product p_l, while the remaining products of P are neither substitutes nor complements of p_l if

$$\frac{\partial \phi^{\text{com}}_{p_l,r,t}}{\partial x^{\pi}_{p_l,r,t}} \left(\boldsymbol{x}^{\pi}_{r,t}\right) \leq 0, \tag{3.35}$$

$$\frac{\partial \phi^{\text{com}}_{p_l,r,t}}{\partial x^{\pi}_{p_c,r,t}} \left(\boldsymbol{x}^{\pi}_{r,t}\right) \leq 0, \tag{3.36}$$

and

$$\frac{\partial \phi^{\text{com}}_{p_l,r,t}}{\partial x^{\pi}_{p_m,r,t}} \left(\boldsymbol{x}^{\pi}_{r,t}\right) = 0 \quad \textit{for all } m = 1, \ldots, |P|, \quad m \neq l, c. \tag{3.37}$$

Remark 3.6. Remarks 3.3 and 3.5 as well as the characteristics of demand 3.1, 3.9, and 3.11 ensure that all cross-price derivatives of the demand function $\phi_{p,r,t}\left(\boldsymbol{x}^{\pi}_{r,t}\right)$ are symmetric.

3.7 Conclusion

In this section, we provide the fundamental framework that permits to develop precise demand models for commodities. As stated above, we prefer a phenomenological approach rather than establishing the utility function, as pursued by many approaches to modeling demand (cf. section 2.1.2). However, some characteristics of the *Marshallian* and *Hicksian* demand function are transferred to the phenomenological demand function $\phi_{p,r,t}$ (e.g., symmetry of the cross-price derivatives, negativity of the derivative with respect to each price (cf. section 2.1.1)).
To sum up, we examine the impacts of all prices in the market ranging from the own price to the prices of substitutes and complements. Likewise, we analyze the influences of changes in the economic situation and influences on behalf of the consumer, who is only able to purchase according to his background (e.g., his budget and capacities). In doing so, our framework explicitly allows for the representation of a nonlinear demand function with respect to price for commodities. Regarding substitution, the approaches to model substitution in assortment planning are not applicable to commodities in general (cf. section 2.2). Here, the question is rather how the total quantity is allocated to multiple products because of price differences. Therefore, we propose a demand model that incorporates price-based substitution.
So far, our analyses are based on the assumption that the demand in a market can be described by the demand behavior of one single consumer by aggregating the demand of all consumers. At this early stage, such a simplified model is necessary because there is not enough information available to break down all the complex processes in the demand formation. Provided that more knowledge is accessible, the usage of multi-agent models seems appropriate to investigate the effects of multiple consumers in the market in a further step.

Another elaborate opportunity to extend the model are stochastic components. Throughout this section, our analysis reveals that including stochastic components might be useful. For instance, stochastic modeling of the development of the economic situation improves forecasts. In addition, by describing the consumer's characteristics, it might be convenient to model components such as the maximum capacity $\alpha_{p,r,t}^{\text{max\_quant}}$, the maximum price $\alpha_{p,r,t}^{\text{max\_price}}$, or the existence of contracts $\alpha_{p,r,t}^{\text{con}}$ as random variables. Moreover, stochastic optimization models serve as an appropriate tool to display the decision process of a consumer, especially in case of complex switching decisions that include time-consuming and cost-intensive components.

4 Modeling a Supply-Demand Trade Network for Commodities

This chapter contains an overview of existing publications regarding decision-making in supply chain management or chemical engineering, i.e., procurement, production, distribution, and sales. Moreover, we present a new market optimization model that includes supply-demand interaction to determine optimal price and production quantity strategies that maximize profit in a commodity market. Among others, this model is applicable to the petrochemical industry that is characterized by production processes, which produce and reprocess various chemical products.

Concerning models of commodity prices in general, there exist two different approaches: "stochastic reduced form" models and fundamental market models. The first approach mentioned adapts methods of pricing assets in finance and models price dynamics by means of stochastic processes that reflect the statistical properties of the prices (see [Gem05, EW03, Pil07]). Such models often serve as a basis for derivative pricing (cf. [Bod12] or [Ruj08]), portfolio optimization (cf. [Lud13]), and risk management.

In contrast, fundamental market models determine the price as the intersection of supply and demand (cf. [Kra09]). Evidently, such explicit modeling of these market components requires extensive knowledge of market mechanisms as well as of consumption properties on the demand side, and procurement, production settings, storage, and distribution on the supply side. This elaborate approach, however, provides a detailed presentation of the complexity of price development, and helps us to understand which components have a significant influence on price formation.

Modeling and optimizing production input-output flows are also an important part of supply chain management. The respective modeling approaches often show a network structure where vertices represent distinct facilities (e.g., different production locations, warehouses and markets) and edges represent the conjunctions between them. In addition to input-output flows of the different vertices and transportation along the edges, operation settings within the vertices are also controlled to optimize the supply chain. We refer to Stadtler [Sta08] and Fleischmann et al. [FMW08] for an introduction to organizational tasks and planning efforts within such a supply network as well as an overview of various partial aspects along a typical supply chain. An expedient and important feature in this framework is demand planning, because, among others, input quantities or specific settings of a production process may have to be determined prior to real demand becoming known.[1] Kilger and Wagner [KW08] gave an overview of the requirements and procedures of demand planning. Given a forecast of future demand,

[1] In this context, corresponding studies with a focus on sales and services are often summarized under the heading "demand chain planning".

the overall objective in supply chain management is to optimize production and trading strategies in the whole system. In addition, pricing decisions are often included in the optimization problem if the decision-maker has a market-dominating role.
In section 4.1, we review distinct methods of modeling and solving production optimization problems in the field of supply chain management or chemical engineering. In this context, many distinct research fields play a decisive role: modeling demand forecast, network design and network optimization, optimization theory, stochastic programming, etc.
In section 4.2, we present our approach to determine optimal pricing, production and transportation quantities by including the nonlinear demand-price relationship in the model. Thus, we explicitly combine optimal production and pricing decisions. To be more precise, we determine prices and production quantities for the whole product range in each region of the market as well as transportation quantities between regions in case of multiple time periods. In doing so, we present a version of the supply-demand trade network optimization model that is tailored to reflect the influence of the relationship between demand and price and also serves as a basis for the model reduction methods developed by Kramer [Kra13].[2] Finally, we outline essential differences in modeling demand compared to the cited publications and investigate which requirements a demand model has to fulfill so that a solution of our emerging optimization model exists.

4.1 Literature Review and Model Approaches

This section summarizes distinct modeling and planning concepts with regard to production optimization and supply chain management. Besides models tailored to the particularities of refineries or chemical engineering, this summary comprises more general modeling approaches. Depending on the design and objectives, these complex decision-making problems can be further classified regarding different aspects:
In the first place, according to the time horizon of the decision-making process the variables of the optimization models under consideration can be categorized in strategic, tactical, or operational decisions. In addition, as already mentioned above, the models can be classified into models without pricing decisions (i.e., prices are fixed and exogenously given from outside the network) and models including prices as variables to be optimized subject to given demand (forecast). In connection with that, broader diversity is caused by different modeling assumptions on demand. At first, the publications can be distinguished depending on whether they presume that demand is price-inelastic or not. Evidently, the latter gives rise to a demand model dependent on price. In addition, there are publications supposing that demand is deterministic, whereas a wide range of studies considers demand as a source of uncertainty and prefers a stochastic modeling, which, in turn, requires stochastic programming methods. This leads to the last item: the methods used to solve the decision-making problems include linear, nonlinear, mixed-integer, and

[2] Since this optimization problem was accomplished together with Kramer [Kra13], her PhD thesis "Modeling Price Formation in a Multi-Commodity Market - A Graph-Theoretical Decomposition Approach to Complexity Reduction" also discusses some modeling aspects.

stochastic programming.
In the following, we present a selection of publications structured according to their incorporation of demand. To begin with, we present contributions based on the assumption that demand is price-insensitive.
Bertsimas and Thiele [BT06] test a robust optimization approach to determine optimal order decisions in a plant network subject to uncertain demand. By restricting the aggregated scaled deviation of the demand variables from the respective mean, their proposed deterministic model results in a (mixed-integer) linear program with a modified demand sequence compared to the case in which demand is fixed to the mean value. Their approach does not require much information about the distribution of demand so that it is applicable to a broad range of demand distributions.
In comparison, Gupta and Maranas [GM03] investigate the effects of uncertain demand in the tactical and operational planning process of a supply chain in chemical engineering under the assumption that the quantity required is normally distributed with a known mean and standard deviation. Their network model encompasses multiple sites, multiple products, and multiple periods. To determine optimal production and logistic quantities they set up a two-stage stochastic program. In the first place, production costs and the expected value of logistic costs are minimized by determining optimal manufacturing decisions before real demand is known. In the second place, the logistic decisions are made given production quantities and real demand. In an extension of their work, the model also serves as a tool for risk management.
In contrast, Guillèn et al. [GMB$^+$05] consider the supply chain at the strategic level and chose a multi-objective approach, i.e., they aim to maximize the net present value of the supply chain, to maximize demand satisfaction, and to minimize financial risk. On the basis of demand scenarios associated with the respective probability of occurrence, they determine the number, location, and capacities of plants, as well as production rates and flow of material. To solve their stochastic mixed integer optimization problem they make use of the ϵ-constraint method. In this way, their approach results in a set of Pareto-optimal solutions reflecting the trade-off among the multiple objectives.
Another scenario-based demand modeling approach integrated into a multi-objective optimization approach is studied by Chen and Lee [CL04]. To solve the supply chain network given uncertain demand and prices they propose a two-phase fuzzy decision-making method.
Now, we will summarize publications that explicitly take the demand-price relation into account. Kannegiesser et al. [KGvB$^+$09] (see also [Kan08]) develop a mixed-integer linear optimization model for sales and supply planning of chemical commodities. Therefore, the objective is to optimize expected profit by making decisions about monthly sales quantities and prices over a period of multiple months. Regarding the supply side, the production is assigned to different production facilities at different locations, and the production processes are modeled with linear raw material recipe functions reflecting the quantitative relationship of required raw material input and produced output. A minimum quantity to be produced guarantees stability. So far, they neglect inventory, transportation, and exchange rates.
Concerning demand, they distinguish contract and spot demand at each location. Whereas

the contract sales quantities and prices are fixed, spot demand and spot prices are unsure. Under certain assumptions concerning the spot market situation, they model the relation of aggregated spot demand and average spot price as linear function given control parameters for minimum and maximum spot demand. To incorporate the uncertainty of the spot prices, they add additional price factors associated with their respective probability of occurrence. Within this scenario-based model approach, the demand functions differ in each scenario, whereas the price elasticities remain identical.[3] In the next step, they approximate the resulting quadratic turnover function with a piecewise linear function and maximize expected profit using two optimization strategies. First, they incorporate the weighted average of all scenario-based approximated sales turnovers in the objective function. Alternatively, they propose a two-phase optimization strategy that first computes the minimum profit of all scenarios which then serves as lower bound in the subsequent optimization problem. In doing so, the supply decisions does not vary for each scenario, only the prices differ. Finally, with this modeling approach they are able to analyze the influence of different price developments, different price elasticities, and different raw material prices on profit.
Chakravarty [Cha05] also presents a quantitative model for optimal production and pricing, but, in addition, he incorporates strategic decisions in his model. Thus, the decision variables of the resulting profit maximization of a monopolist includes production quantities and prices of a certain product in multiple countries as well as investment decisions in each of these countries. Concerning the demand-price relation, he uses the general model $\text{Demand} = a \cdot \text{Price}^n$ with $a > 0$ and $n < 0$ given, which is intensively studied in different fields of economics or marketing theory (cf. Lilien et al. [LKM92]).[4] To ensure reasonable sales quantities, an upper bound depending on each country's population limits total demand.
Taking advantage of the special structure of his constrained nonlinear convex optimization model, he develops an algorithm based on grid search to find a fast solution. In doing so, his approach allows to investigate the influence of several factors including overhead allocation, import tariffs, and demand but also the effects of local content rules, local taxes, long-term exchange rates, and market size in a single country.
For comparison, Lakkhanawat and Bagajewicz [LB08] combine microeconomic and mathematical methods to integrate the demand-price relation in their planning and scheduling model for refinery operations. To be more precise, they propose a demand function derived from a common utility function with constant elasticity of substitution.[5] The decision variables of their optimization model are crude oil input, processing, inventory, blending quantities over discretized time periods, and prices. Many model components such as the demand function are linearized to speed up computation. In addition to a deterministic version, they also investigate the influence of stochastic demand components

[3]Price elasticities are interpreted as the relative change of the spot price divided by the relative change of the spot sales quantity (see also section 2.1.1 for the definition).
[4]This demand model provides a constant price elasticity, in fact the price elasticity is equal to n (cf. section 2.1.1).
[5]We refer to section 2.1.1 for an introduction to neoclassical consumer theory (as part of microeconomic theory) as well as the description of the terminology.

using a two-stage stochastic optimization approach. At the end, they apply concepts of financial risk management to include distinct attitudes towards risk in the model.

4.2 Supply-Demand Trade Network Optimization Model

In this section, we present a general optimization model including supply-demand interactions to determine prices and production quantities of commodities. This model was developed in cooperation with Kramer [Kra13] with the intention to apply the resulting supply-demand trade network optimization model to the petrochemical industry.
To begin with, the goal was to build a model that determines the optimal pricing, production and transport strategies for multiple time periods as to maximize the profit in a market consisting of various operating possibilities related to different production sites. In other words, we consider an interorganizational and interregional supply network in which the single operators cooperate with each other to maximize joint profit. Thus, we assume that all single production sites and all decisions are under the control of one decision maker. Hence, the objective function of the optimization problem is the profit of a monopolist.
We consider a set of products $p \in P^M$ produced, required and sold in different regions $r \in R$ at time periods $t \in T$. Since these products differ in their demand characteristics as well as in their utilization in the supply chain, we classify them into subgroups. The set P_{ex} contains all products, of which the prices $a^{\pi}_{p,r,t}$ are fixed and given from markets distinct from the market under consideration. Intermediate products $p \in P_{mid}$ are simply produced and reprocessed in the regarded market, but are not required by other markets and, hence, are not sold. Lastly, $p \in P_{out}$ are products that are in demand by other markets (e.g., industrial sectors, households), i.e., their demand is driven by the corresponding prices and we include their demand-price relation by means of a nonlinear function in the market model.
This application serves as basis for the further research in this PhD thesis. Since the incorporation of price-dependent demand requires a more comprehensive study of nonlinear modeling approaches for demand, we will return to this topic later on discussing the conditions of a suitable demand model in the context of the proposed optimization model. Besides, the development of an appropriate demand model is described in full detail in sections 3 and 6. At this point, we confine ourselves to the description of characteristics that are important for setting up our market model. As a matter of fact, the demand of a product is split into demand by different sectors, represented by different customers. Consequently, assuming that $|P| = 1$, we obtain the aggregated demand function as the sum of the single demand functions with respect to the product's price $x^{\pi}_{p_{out},r,t}$

$$\phi_{p_{out},r,t}(x^{\pi}_{p_{out},r,t}) = \sum_{c} \phi_{c,p_{out},r,t}(x^{\pi}_{p_{out},r,t}), \tag{4.1}$$

where the sectors or customers act independently, but are assumed to have the same preferences.[6] If their single behavior can be expressed by a demand model with identical

[6]For an overview of the implications of aggregation in neoclassical consumer theory see section 2.1.2.1.

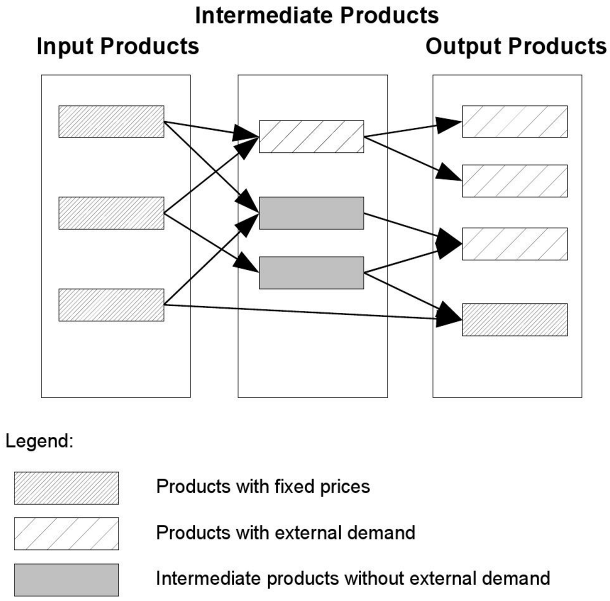

Figure 4.1: Illustration of a section of the product network

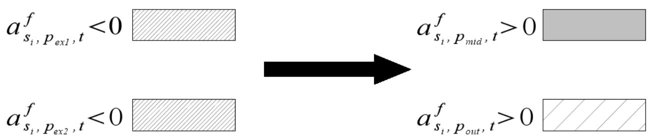

Figure 4.2: Illustration of a production process

consumer-related parameters $\lambda_i^{\phi_{c,p,r,t}}$, $i \in I$, their aggregated demand model equals to the demand of one single representative consumer given by

$$\phi_{p_{out},r,t}(x^{\pi}_{p_{out},r,t}) = |C| \cdot \phi_{c,p_{out},r,t}(x^{\pi}_{p_{out},r,t}), \tag{4.2}$$

where C is the set of consumers in the market. Regarding the supply side, the operations of production sites, i.e., the processing and production of the products, are given by corresponding processes $s \in S$. Figure 4.1 exemplarily illustrates the resulting connections for a selection of products. Here, if two products are linked by an arrow, the one on the left is a resource product and one on the right reflects an output product in a specific production process. In the model, corresponding operational process factors $a^f_{s,p,t}$ characterize each process s providing information about the relative quantities of inputs and outputs at time t. Consequently, input products of a process have negative factors and the factors for output products have positive a sign. An example is given in figure 4.2: two products with fixed prices are converted into an intermediate product and a product with external demand. The capacity of each production side is arbitrary

between zero and the maximum capacity. In other words, there is no minimum production quantity required to ensure the efficiency of the production sites and production is assigned to the cheapest operations. Moreover, we neglect fixed costs and consider production costs as variable costs. We approximate them by only considering the resource costs of a production process and neglect further costs (eg., removal costs, labor costs) or taxes. Furthermore, the model approach does not include integer decisions which indicate whether a production site is switched on or not. Likewise, we neglect the sequence of processes and aggregate the processes over the time period t (cf. [Kra13]).
Since fixed costs for a production site and transportation costs between plants of the same region are neglected, we assign their capacities directly to the respective processes and omit the specification of production sites in the optimization model. Likewise, the variable costs are directly related to the processes. In doing so, we transform the production network with plants as vertices to a product network with products as vertices linked by their respective production processes. Furthermore, we also include the possibility of trade between different regions. However, we neglect the possible occurrence of time lags in case the time period t exceeds the transit time from one region to each other. Transportation costs from one region to another are integrated being proportional to the transportation quantities and transport distance.
Summing up, our optimization problem is a profit maximization problem of a monopolist given aggregated demand functions with respect to the product's price for all products $p \in P_{out}$. The model combines tactical and operational decisions to determine optimal prices, production, and transport quantities, where the optimal production is constrained by the production capacities. Before formulating the supply-demand trade network optimization model, we conclude this introduction by characterizing the market under consideration.

Assumptions 4.1. *We consider a market that comprises producing and selling in multiple regions with the following characteristics*

1. *All consumers of a region r act independently and have the same demand behavior. Therefore, aggregation of their demand equals the demand of* ***one consumer*** *in each region.*
2. *The producers coordinate with each other and have a common objective, namely* ***overall profit maximization****.*
3. *There is interregional* ***trade****.*
4. *The products are connected by their* ***production processes*** *and possibly by their subsequent processing or by their end consumption.*
5. *The products are of standard quality and are in demand of* ***large quantities*** *with the price as main influencing factor for demand.*
6. *The market is* ***arbitrage-free****.*[7]

[7] A market is arbitrage free if there is no possibility to make risk-free profit because of price differences.

In the following, we present the nomenclature of our model.

Nomenclature of the Supply-Demand Trade Optimization Model

Sets:

P^M	products in the market ($P_{ex} \cup P_{mid} \cup P_{out}$)
P_{ex}	products with fixed prices, which are given from outside the network
P_{mid}	intermediate products without external demand
P_{out}	products with external demand
R	regions
S	processes
C	consumers
T	time periods
I	demand parameter indices

Parameters:

$a^{cap\_max}_{s,r,t}$	capacity of process s in region r at time t
$a^{\pi}_{p_{ex},r,t}$	price of product p_{ex} in region r at time t
$a^{f}_{s,p,t}$	input/output factor of product $p \in P_{ex} \cup P_{mid} \cup P_{out}$ in process s at time t
$a^{tr}_{r_1,r_2,t}$	transport costs to deliver one unit from region r_1 to region r_2 at time t
$a^{c\_stor}_{p,r,t}$	storage costs for a unit of product $p \in P_{mid} \cup P_{out}$ in region r at time t
$a^{cap\_stor}_{s,r,t}$	storage capacity for product $p \in P_{mid} \cup P_{out}$ in region r at time t

Variables:

$x^{\pi}_{p,r,t} \geq 0$	price of product $p \in P_{mid} \cup P_{out}$ in region r at time t
$x^{q}_{s,r,t} \geq 0$	production quantity of process s in region r at time t
$x^{tr}_{p,r_1,r_2,t} \geq 0$	transport quantity of product $p \in P_{mid} \cup P_{out}$ from r_1 to r_2 at time t
$x^{stor}_{p,r,t} \geq 0$	storage quantity of product $p \in P_{mid} \cup P_{out}$ in region r at time t

Functions:

$\phi_{c,p_{out},r,t}(\cdot)$	demand function of a single customer $c \in C$ w.r.t. $x^{\pi}_{p_{out},r,t}$, $\mathbb{R}^+_0 \to \mathbb{R}^+_0$, $x^{\pi}_{p_{out},r,t} \mapsto \phi_{c,p_{out},r,t}(x^{\pi}_{c,p_{out},r,t})$ for product p_{out} in region r at time t
$\phi_{p_{out},r,t}(\cdot)$	aggregated demand function w.r.t. $x^{\pi}_{p_{out},r,t}$, $\mathbb{R}^+_0 \to \mathbb{R}^+_0$, $x^{\pi}_{p_{out},r,t} \mapsto \phi_{p_{out},r,t}(x^{\pi}_{p_{out},r,t})$ for product p_{out} in region r at time t

Demand Parameters:

$\lambda_i^{\phi_{(c,)p,r,t}}$, $i \in I$	parameter of consumer c's demand function for product p_{out} in region r at time t

Regarding the optimization problem for one time period, we exclude the possibility of storage. In the following, we present the optimization model at time t comprising the profit function of the producer as the objective function and corresponding constraints that are explained in more detail below.

$$\max_{\substack{x^{\pi}_{p_{out},r,t},\ x^{q}_{s,r,t}\\ x^{tr}_{p_{out},r_1,r_2,t},\ x^{tr}_{p_{mid},r_1,r_2,t}}} \Bigg[\sum_{\substack{p_{out}\in P_{out}\\ r\in R}} x^{\pi}_{p_{out},r,t} \cdot \phi_{p_{out},r,t}(x^{\pi}_{p_{out},r,t}) + \sum_{\substack{p_{ex}\in P_{ex}\\ r\in R,\ s\in S}} x^{q}_{s,r,t} \cdot a^{f}_{s,p_{ex},t} \cdot a^{\pi}_{p_{ex},r,t} - \sum_{\substack{p\in P_{mid}\cup P_{out}\\ r_1\in R,\ r_2\in R}} x^{tr}_{p,r_1,r_2,t} \cdot a^{tr}_{r_1,r_2,t} \Bigg] \tag{4.3a}$$

subject to
$\forall s \in S,\ \forall r \in R$

$$x^{q}_{s,r,t} \leq a^{cap\_max}_{s,r,t}, \tag{4.3b}$$

$\forall p_{mid} \in P_{mid}, \forall r_1 \in R$

$$\sum_{r_2\in R} (x^{tr}_{p_{mid},r_1,r_2,t} - x^{tr}_{p_{mid},r_2,r_1,t}) \leq \sum_{s\in S} x^{q}_{s,r_1,t} \cdot a^{f}_{s,p_{mid},t}, \tag{4.3c}$$

$\forall p_{out} \in P_{out}, \forall r_1 \in R$

$$\phi_{p_{out},r_1,t}(x^{\pi}_{p_{out},r_1,t}) \leq \sum_{s\in S} x^{q}_{s,r_1,t} \cdot a^{f}_{s,p_{out},t} - \sum_{r_2\in R} (x^{tr}_{p_{out},r_1,r_2,t} - x^{tr}_{p_{out},r_2,r_1,t}), \tag{4.3d}$$

$\forall p \in P_{mid} \cup P_{out},\ \forall r_1 \neq r_2 \in R$

$$x^{\pi}_{p,r_1,t} \leq x^{\pi}_{p,r_2,t} + a^{tr}_{r_2,r_1,t}, \tag{4.3e}$$

and $\forall s \in S,\ \forall r \in R$

$$0 \leq x^{q}_{s,r,t} \cdot \Big(\sum_{p\in P_{mid}\cup P_{out}} a^{f}_{s,p,t} \cdot x^{\pi}_{p,r,t} + \sum_{p_{ex}\in P_{ex}} a^{f}_{s,p_{ex},t} \cdot a^{\pi}_{p_{ex},r,t} \Big). \tag{4.3f}$$

The profit as defined in the objective function (4.3a) is equal to the revenue of selling products with external demand and products with fixed prices minus the costs of producing these products minus the transport costs for quantities sold in regions other than the region of production. If there is p_{ex_i} with $a^{f}_{s,p_{ex_i},t} < 0$, the corresponding term of the second sum captures the input costs for p_{ex_i}. If, in contrast, $a^{f}_{s,p_{ex_j},t} > 0$, this term adds the revenue of selling product p_{ex_j} to the profit.
The restrictions from the production sites are included through the capacity constraint (4.3b). The production-transport constraint (4.3c) ensures that the net transport quantities of the intermediate products do not exceed the production quantities, whereas constraint (4.3d) guarantees that demand at the optimal price for each product in each region is met by production and transport. Concerning pricing, constraint (4.3e) ensures

that the difference in price in distinct regions is smaller than or equal to the respective transportation costs. Consequently, the market is arbitrage free. By means of constraint (4.3f) we include upper and lower bounds for the prices of intermediates in the model to guarantee that each production process is profitable. However, this model is not suited to uniquely determine the corresponding prices.

The modeling approach implicates that full demand is satisfied by the monopoly. Otherwise, if there is a difference in demand and sales quantity, the monopolist has the incentive to adjust his settings to optimize profit.[8]

In case contracts exist between the producer and some customers in the market under consideration, the corresponding quantity can be easily separated from the total quantity by establishing an extra term in the objective function and demand-related constraints. Provided that the demand function is differentiable with respect to the price, the proposed optimization problem can be solved by means of optimization methods based on derivatives such as SQP-methods or interior-point methods (see section 5.2 for description). For comparison, Kramer [Kra13] presented a more detailed formulation of the supply-demand trade network optimization model specifying each plant associated with corresponding production processes, capacity, and fixed costs for running a proceed at a plant. In this case, the optimization problem includes integer decisions which necessitates mixed-integer nonlinear optimization methods.

So far, optimization determines prices and production quantities for a fixed time period. Integrating the possibility of storage, the optimization model over a set of time periods $T = t_1, \dots, t_n$ is given by

$$\max_{\substack{x^{\pi}_{p_{out},r,t_i},\ x^{q}_{s,r,t_i}\\ x^{tr}_{p_{out},r_1,r_2,t_i},\ x^{tr}_{p_{mid},r_1,r_2,t_i}\\ x^{stor}_{p_{out},r,t_i},\ x^{stor}_{p_{mid},r,t_i},\ t_i\in T}} \Bigg[\sum_{t_i\in T} \Bigg(\sum_{\substack{p_{out}\in P_{out}\\ r\in R}} x^{\pi}_{p_{out},r,t_i} \cdot \phi_{p_{out},r,t_i}(x^{\pi}_{p_{out},r,t_i}) + \sum_{\substack{p_{ex}\in P_{ex}\\ r\in R,\ s\in S}} x^{q}_{s,r,t_i} \cdot a^{f}_{s,p_{ex},t_i} \cdot a^{\pi}_{p_{ex},r,t_i} - \sum_{\substack{p\in P_{mid}\cup P_{out}\\ r_1\in R,\ r_2\in R}} x^{tr}_{p,r_1,r_2,t_i} \cdot a^{tr}_{r_1,r_2,t_i} - \sum_{\substack{p\in P_{mid}\cup P_{out}\\ r\in R}} x^{stor}_{p,r,t_i} \cdot a^{c\_stor}_{p,r,t_i} \Bigg)\Bigg] \tag{4.4a}$$

subject to

$\forall s \in S,\ \forall r \in R, \forall t_i \in T$

$$x^{q}_{s,r,t_i} \leq a^{cap\_max}_{s,r,t_i}, \tag{4.4b}$$

$\forall p_{mid} \in P_{mid},\ \forall r_1 \in R,\ \forall t_i \in T$

$$\sum_{r_2\in R} (x^{tr}_{p_{mid},r_1,r_2,t_i} - x^{tr}_{p_{mid},r_2,r_1,t_i}) + x^{stor}_{p_{mid},r_1,t_i} - x^{stor}_{p_{mid},r_1,t_{i-1}} = \sum_{s\in S} x^{q}_{s,r_1,t_i} \cdot a^{f}_{s,p_{mid},t_i}, \tag{4.4c}$$

[8] This discrepancy is often denoted as lost demand (cf. Lakkhanawat [LB08]).

$\forall p_{out} \in P_{out},\ \forall r_1 \in R,\ \forall t_i \in T$

$$\phi_{p_{out},r_1,t_i}(x^{\pi}_{p_{out},r_1,t_i}) + \sum_{r_2 \in R}(x^{tr}_{p_{out},r_1,r_2,t_i} - x^{tr}_{p_{out},r_2,r_1,t_i}) + x^{stor}_{p_{out},r_1,t_i} - x^{stor}_{p_{out},r_1,t_{i-1}} = \sum_{s \in S} x^{q}_{s,r_1,t_i} \cdot a^{f}_{s,p_{out},t_i}, \quad (4.4d)$$

$\forall p \in P_{mid} \cup P_{out},\ \forall r_1 \neq r_2 \in R,\ \forall t_i \in T$

$$x^{\pi}_{p,r_1,t_i} \leq x^{\pi}_{p,r_2,t_i} + a^{tr}_{r_2,r_1,t_i}, \quad (4.4e)$$

$\forall s \in S,\ \forall r \in R,\ \forall t_i \in T$

$$0 \leq x^{q}_{s,r,t_i} \cdot (\sum_{p \in P_{mid} \cup P_{out}} a^{f}_{s,p,t_i} \cdot x^{\pi}_{p,r,t_i} + \sum_{p_{ex} \in P_{ex}} a^{f}_{s,p_{ex},t_i} \cdot a^{\pi}_{p_{ex},r,t_i}), \quad (4.4f)$$

and $\forall p_{out} \in P_{out},\ \forall r \in R,\ \forall t_i \in T$

$$x^{stor}_{p,r,t_i} \leq a^{cap\_stor}_{p,r,t_i}, \quad (4.4g)$$

where $x^{stor}_{p,r,t_0} = 0 \quad \forall p_{mid} \in P_{mid}, \forall r \in R$. The basic optimization model (4.3) changes as follows. In addition to the storage capacity constraints (4.4g) added, the constraints regarding the transportation-production(-sales) dependencies (4.3c) and (4.3d) change into constraints (4.4c) and (4.4d) to take the possibility of storage into account. Furthermore, the costs of storage are subtracted from the profit (cf. objective function (4.4a)). In the course of this thesis, we go back to the one-periodic model to analyze and test several modeling approaches for demand (cf. section 6.3). Therefore, it remains to specify the demand function to apply the optimization problem. In addition to the market-related characteristics, the structure of the proposed optimization model imposes some conditions to a useful demand model. These are discussed in the following section and compared to demand characteristics in the publications cited above.

4.3 Concluding Remarks - Distinctive Features of the Demand Function

To summarize, the modeling approaches of [KGvB+09, Cha05, LB08] most resemble the supply-demand optimization model proposed in the previous section. Since, among others, they explicitly include model components describing the demand-price relation, many assumptions and concepts agree with our optimization modeling approach. Regarding the work of Kannegiesser et al. [KGvB+09], they also group the consumers according to their regional or industry-specific sales locations. Likewise, their description of an intra-organizational production network with its frequently and continuously processed inputs is quite similar to our approach, but their value chain is not controlled by a monopolist. This feature is evident in the model of Chakravarty [Cha05] instead.

In the following, we limit ourselves to comparing and discussing the details of the approaches to modeling demand. As stated above, we explicity aim to incorporate the nonlinear aggregated demand-price relation in the optimization model, which necessitates nonlinear optimization methods. This concept also appears in the work of Chakravarty [Cha05] and Lakkhanawat [LB08]. Even, Kannegiesser et al. [KGvB+09] mention that demand could be nonlinearly modeled, and argue that a linear function is sufficient as a statistical fit.

In any case, it is necessary to take note of some requirements. First, the structure of the proposed optimization model necessitates the incorporation of saturation quantities in case of low prices as well as a maximum price for which the demand becomes zero. Otherwise, the optimization problem could get unbounded or may provide unreasonable solutions.[9] This can be realized by additional variable bounds preventing the respective quantities from becoming too extreme or by a demand model including the consumer's saturation quantity as well as the consumer's maximum price. In particular, the latter leads to a modeling approach that reflects demand behavior in every price range (see section 3.4). In contrast to our modeling approach, Chakravarty [Cha05] does not fix the production capacities but related it to investment quantities in each country. This, however, represents a lower bound for quantities and, thus, demand because he requires that the investment costs are covered by a selection of products produced in this country. To conclude, further advantageous characteristics of a demand function are differentiability and concavity. Kramer [Kra13] shows that if the demand function is concave, the optimization problem is convex and, therefore, a unique solution exists. In the remaining part, we will concentrate on differentiable functions so that optimization methods based on derivatives can be applied. Chapter 6 comprises a new explicit demand model for petrochemical products that is tailored to the proposed optimization model. Simulation results are presented in section 6.3.

[9] We suggest that selling an infinitesimal quantity at very high prices is unrealistic concerning the customer's and the supplier's preferences.

5 Constrained Optimization - Theory, Algorithms, and Application

The scope of this chapter is to explain the methodology that is applied to solve the diverse inequality constrained optimization problems arising in the course of this thesis. In addition to the network optimization problem (4.3) presented in section 4.2, these will also occur in terms of parameter identification problems in section 7.
In section 5.1, we summarize the optimality conditions for constrained optimization problems, before we pass on to methods that solve inequality constrained optimization programs in section 5.2. For more detailed information, we refer to numerous textbooks about optimization methods, e.g., [NW06, Fle01, GMW08, BGLS06].
In section 5.3, we discuss the features of the least-squares method that is most often applied to parameter estimation and data fitting problems. In this context, we present the Gauss-Newton algorithm used to solve nonlinear least-squares problems. Furthermore, we outline a generalization to solve constrained least-squares problems.
We refer to [Str11, NW06] for more information on the concept of least-squares, and to [Boc87, BKS07] for more details on the generalized Gauss-Newton algorithm for constrained least-squares problems.

5.1 Optimality Conditions for Constrained Optimization Problems

In general, most textbooks about optimization include sections on these optimality conditions, e.g., [NW06, Fle01, GMW08, BGLS06]. Principally, we sketch this section on [NW06], chapter 12. To begin with, the general optimization problem reads as

$$\min_{\boldsymbol{x}\in\mathbb{R}^n} f(\boldsymbol{x}) \tag{5.1a}$$

subject to

$$c_i(\boldsymbol{x}) = 0,\ i \in \mathcal{E} \quad c_i(\boldsymbol{x}) \geq 0,\ i \in \mathcal{I}, \tag{5.1b}$$

where $f, c_i \colon \mathbb{R}^n \to \mathbb{R}$ are smooth and $\mathcal{E}$ and $\mathcal{I}$ are finite sets of indices. In the following, the first-order derivative w.r.t. $\boldsymbol{x}$ is denoted by ∇ and the second-order derivative w.r.t. $\boldsymbol{x}$ by ∇^2. Obviously, $\Omega = \{\boldsymbol{x}|c_i(\boldsymbol{x}) = 0, i \in \mathcal{E}; c_i(\boldsymbol{x}) \geq 0,\ i \in \mathcal{I}\}$ is the set of all feasible points of problem (5.1). Additionally, the following definitions are used to characterize solutions of problem (5.1).

Definition 5.1. *Local Solution*
If $\boldsymbol{x}^* \in \{\boldsymbol{x}|c_i(\boldsymbol{x}) = 0, i \in \mathcal{E}; c_i(\boldsymbol{x}) \geq 0,\ i \in \mathcal{I}\}$ *and there is a neighborhood* $\mathcal{N}$ *of* $\boldsymbol{x}^*$*, where*

$f(\boldsymbol{x}) \geq f(\boldsymbol{x}^*)$ for $\boldsymbol{x} \in \mathcal{N} \cap \{\boldsymbol{x}|c_i(\boldsymbol{x}) = 0, i \in \mathcal{E}; c_i(\boldsymbol{x}) \geq 0,\ i \in \mathcal{I}\}$, then $\boldsymbol{x}^*$ is a local solution of problem (5.1).

Moreover, we consider the set of indices for which the constraints are equal to zero, i.e.,

Definition 5.2. *Active Set*
The active set $\mathcal{A}(\boldsymbol{x})$ at $\boldsymbol{x}$ is given by

$$\mathcal{A}(\boldsymbol{x}) = \mathcal{E} \cup \{i \in \mathcal{I}|c_i(\boldsymbol{x}) = 0\}. \tag{5.2}$$

For a local minimizer $\boldsymbol{x}^*$ of an unconstrained optimization, it is necessary that $\nabla f(\boldsymbol{x}^*) = 0$ and $\nabla^2 f(\boldsymbol{x}^*)$ is positive semidefinite. To build the optimality conditions for constrained optimization problems, the Langrangian function is central.

Definition 5.3. *Lagrangian Function*
The Lagrangian function of problem (5.1) is defined as

$$\mathcal{L}(\boldsymbol{x}, \boldsymbol{\lambda}) = f(\boldsymbol{x}) + \sum_{i \in \mathcal{E} \cup \mathcal{I}} \lambda_i c_i(\boldsymbol{x}), \tag{5.3}$$

where $\lambda_i \in \mathbb{R}$, $i \in \mathcal{E} \cup \mathcal{I}$ are the Lagrange multipliers of the respective constraints $c_i(\boldsymbol{x})$, $i \in \mathcal{E} \cup \mathcal{I}$.

Definition 5.4. *Set of Linearized Feasible Directions*

$$\mathcal{F}(\boldsymbol{x}) = \{d|d^T \nabla c_i(\boldsymbol{x}) = 0,\ \forall i \in \mathcal{E}, d^T \nabla c_i(\boldsymbol{x}) \geq 0,\ \forall i \in \mathcal{A}(\boldsymbol{x}^*) \cap \mathcal{I}\}$$

is the set of linearized feasible directions.

In general, the first-order necessary optimality conditions can be established provided that certain qualification conditions at $\boldsymbol{x}^*$ hold (cf. [NW06, GMW08, BGLS06]). In the following, we define the linear independence constraint qualification following again Nocedal [NW06] who establishes the optimality conditions in terms of the following qualification constraint.

Definition 5.5. *LICQ*
The linear independence constraint qualification (LICQ) holds if the set of active constraint gradients $\{\nabla c_i(\boldsymbol{x}),\ i \in \mathcal{A}(\boldsymbol{x})\}$ is linearly independent.

Consequently, we outline the first-order necessary conditions given the LICQ defined above.

Theorem 5.1. *First-Order Necessary Conditions*
Under the assumption that $\boldsymbol{x}^*$ is a local solution of problem (5.1), where f and c_i are smooth, and that the LICQ holds at $\boldsymbol{x}^*$, there exists a Lagrange multiplier vector $\boldsymbol{\lambda}^*$ with components λ_i^*, $i \in \mathcal{E} \cup \mathcal{I}$, so that the following conditions are fulfilled at $(\boldsymbol{x}^*, \boldsymbol{\lambda}^*)$

$$\nabla \mathcal{L}(\boldsymbol{x}^*, \boldsymbol{\lambda}^*) = 0, \tag{5.4a}$$
$$c_i(\boldsymbol{x}^*) = 0, \quad \forall i \in \mathcal{E}, \tag{5.4b}$$
$$c_i(\boldsymbol{x}^*) \geq 0, \quad \forall i \in \mathcal{I}, \tag{5.4c}$$
$$\lambda_i^* \geq 0, \quad \forall i \in \mathcal{I}, \tag{5.4d}$$
$$\lambda_i^* c_i(\boldsymbol{x}^*) = 0, \quad \forall i \in \mathcal{E} \cup \mathcal{I}. \tag{5.4e}$$

Proof: see [NW06] (page 323ff).

These conditions (5.4) are called the Karush-Kuhn-Tucker (KKT) conditions and the point $(\boldsymbol{x}^*, \boldsymbol{\lambda}^*)$, for which the KKT-conditions hold, is called a Karush-Kuhn-Tucker (KKT) point. More precisely, the conditions (5.4e) are called complementarity conditions. They ensure that at least one of λ_i^* and $c_i(\boldsymbol{x}^*)$ is equal to zero. As a consequence, strict complementarity is defined as follows.

Definition 5.6. *Strict Complementarity*
Suppose $\boldsymbol{x}^*$ locally solves problem (5.1) and $\boldsymbol{\lambda}^*$ satisfies the KKT conditions. The strict complementarity conditions holds if either λ_i^* or $c_i(\boldsymbol{x}^*) = 0$. That means, $\lambda_i^* > 0$ for all $i \in \mathcal{I} \cap \mathcal{A}(\boldsymbol{x}^*)$.

The next theorem provides the necessary second-order conditions using the Hessian of the Lagrangian function of problem (5.1).

Theorem 5.2. *Second-Order Necessary Conditions*
Under the assumption that $\boldsymbol{x}^*$ is a local solution of problem (5.1), that the LICQ conditions hold, and that $\boldsymbol{\lambda}^*$ is the Lagrange multiplier vector for which the Karush-Kuhn-Tucker conditions hold,

$$\boldsymbol{w}^T \nabla^2 \mathcal{L}(\boldsymbol{x}^*, \boldsymbol{\lambda}^*) \boldsymbol{w} \geq 0, \quad \forall \boldsymbol{w} \in C(\boldsymbol{x}^*, \boldsymbol{\lambda}^*), \tag{5.5}$$

where

$$C(\boldsymbol{x}^*, \boldsymbol{\lambda}^*) := \{\boldsymbol{w} \in \mathcal{F}(\boldsymbol{x}^*) | \nabla c_i(\boldsymbol{x}^*)^T \boldsymbol{w} = 0, \text{ all } i \in \mathcal{A}(\boldsymbol{x}^*) \cap \mathcal{I} \text{ with } \lambda_i^* > 0\}. \tag{5.6}$$

Proof: see [NW06] (page 332f).

In addition, sufficient conditions can also be shown in terms of the Hessian of the Langrangian.

Theorem 5.3. *Second-Order Sufficient Conditions*
Under the assumption that for $\boldsymbol{x}^* \in \Omega$, there is a Langrange multiplier vector $\boldsymbol{\lambda}^*$ so that the KKT conditions hold. If

$$\boldsymbol{w}^T \nabla^2 \mathcal{L}(\boldsymbol{x}^*, \boldsymbol{\lambda}^*) \boldsymbol{w} > 0, \quad \forall \boldsymbol{w} \in C(\boldsymbol{x}^*, \boldsymbol{\lambda}^*), \; \boldsymbol{w} \neq \boldsymbol{0}, \tag{5.7}$$

where

$$C(\boldsymbol{x}^*, \boldsymbol{\lambda}^*) := \{\boldsymbol{w} \in \mathcal{F}(\boldsymbol{x}^*) | \nabla c_i(\boldsymbol{x}^*)^T \boldsymbol{w} = 0, \; \forall i \in \mathcal{A}(\boldsymbol{x}^*) \cap \mathcal{I} \text{ with } \lambda_i^* > 0\}, \tag{5.8}$$

$\boldsymbol{x}^*$ is a strict local solution for problem (5.1).

Proof: see [NW06] (page 333f).

For further information, we refer to [NW06, GMW08, BGLS06]. Likewise, Boyd and Vanderberghe [BV04] discuss the KKT conditions for convex problems.

Remark 5.1. Note that problem (5.1) is convex if the objective function $f(\boldsymbol{x})$ is convex, the inequality constraint functions $-c_i(\boldsymbol{x}) \leq 0,\ i \in \mathcal{I}$ are convex, and the equality constraints functions $c_i(\boldsymbol{x}) \geq 0,\ i \in \mathcal{E}$ are affine. Thus, the feasible set of a convex optimization problem is convex. As a consequence, a local solution of a convex optimization problem is a global solution (see [BNO03]).

5.2 Methods to Solve Inequality Constrained Problems

In this section, we summarize common methods to solve inequality constrained problems. According to Nocedal [NW06], there are two powerful algorithms to solve large-scale nonlinear optimization problems: SQP (sequential quadratic programming) methods and interior-point methods. To begin with, we briefly outline the concept of the active set method for quadratic optimization problems, which are often part of the more general SQP methods.

5.2.1 Active Set Method for Quadratic Programming

Following [NW06], we restrict our presentation to convex quadratic problems of the form

$$\min_{\boldsymbol{x}} q(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^T\boldsymbol{G}\boldsymbol{x} + \boldsymbol{x}^T\boldsymbol{c} \tag{5.9a}$$

subject to

$$\boldsymbol{a}_i^T\boldsymbol{x} = b_i, \quad i \in \mathcal{E}, \tag{5.9b}$$

$$\boldsymbol{a}_i^T\boldsymbol{x} \geq b_i, \quad i \in \mathcal{I}, \tag{5.9c}$$

where $\boldsymbol{G}$ is a positive semidefinite $n \times n$ matrix; $\mathcal{E}$ and $\mathcal{I}$ are finite sets of indices; $\boldsymbol{c}$, $\boldsymbol{x}$, and $\boldsymbol{a}_i,\ i \in \mathcal{E} \cup \mathcal{I}$, are vectors in $\mathbb{R}^n$, and $b_i \in \mathbb{R},\ i \in \mathcal{E} \cup \mathcal{I}$.
Subsequently, we summarize the primal active-set method for quadratic programming. Evidently, a solution $\boldsymbol{x}^*$ of the quadratic optimization problem (5.9) satisfies the KKT conditions

$$\boldsymbol{G}\boldsymbol{x}^* + \boldsymbol{c} - \sum_{i \in \mathcal{A}(\boldsymbol{x}^*)} \lambda_i^* \boldsymbol{a}_i = 0, \tag{5.10a}$$

$$\boldsymbol{a}_i^T\boldsymbol{x}^* = b_i, \quad \forall i \in \mathcal{A}(x^*), \tag{5.10b}$$

$$\boldsymbol{a}_i^T\boldsymbol{x}^* \geq b_i, \quad \forall i \in \mathcal{I} \setminus \mathcal{A}(x^*), \tag{5.10c}$$

$$\lambda_i^* \geq 0, \quad \forall i \in \mathcal{I} \cap \mathcal{A}(x^*). \tag{5.10d}$$

Note that theorem (5.1) was formulated assuming that the LICQ is satisfied. As mentioned above, there are alternative constraint qualifications (see also [NW06], section 12). For instance, linearity of the constraints ensure that theorem (5.1) holds, which is satisfied by the quadratic problem (5.9) (see [NW06], section 16).
In general, a step k of the active set method consists in solving a quadratic equality constrained subproblem, where all equality constraints and some inequality constraints

are included as equalities. The corresponding indices are summarized in the working set $\mathcal{W}_k$. To be more precise, provided that the given iterate $\boldsymbol{x}_k$ does not minimize $q(\boldsymbol{x})$ subject to $\boldsymbol{a}_i^T\boldsymbol{x} = b_i,\ i \in \mathcal{W}_k$, the following equality constrained subproblem is solved to compute a step $\boldsymbol{\Delta x}_k$

$$\min_{\boldsymbol{\Delta x}_k} \left[\frac{1}{2}\boldsymbol{\Delta x}_k^T\boldsymbol{G}\boldsymbol{\Delta x}_k + \boldsymbol{g}_k^T\boldsymbol{\Delta x}_k\right] \tag{5.11a}$$

subject to

$$\boldsymbol{a}_i^T\boldsymbol{\Delta x}_k = 0, \quad i \in \mathcal{W}_k, \tag{5.11b}$$

where $\boldsymbol{g}_k = \boldsymbol{G}\boldsymbol{x}_k + \boldsymbol{c}$. We refer to [NW06] for methods for computing the solution $\boldsymbol{\Delta x}_k$ of problem (5.11). Therefore, the new iterate for problem (5.9) is given by

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \alpha_k\boldsymbol{\Delta x}_k, \tag{5.12}$$

where

$$\alpha_k = \min\left[1, \min_{i\notin\mathcal{W}_k, \boldsymbol{a}_i^T\boldsymbol{\Delta x}_k<0} \frac{b_i - \boldsymbol{a}_i^T\boldsymbol{x}_k}{\boldsymbol{a}_i^T\boldsymbol{\Delta x}_k}\right], \tag{5.13}$$

i.e., the step-length α_k is the largest value in $[0,1]$ so that all constraints of problem (5.9) are satisfied. The iteration stops if $\boldsymbol{\Delta x}_k = 0$. Then, a solution $\hat{\boldsymbol{x}}$ is found that minimizes the quadratic objective function given the current working set $\hat{\mathcal{W}}$. Consequently, we get from the optimality conditions of problem (5.11)

$$\sum_{i\in\hat{\mathcal{W}}} \boldsymbol{a}_i\hat{\lambda}_i = \boldsymbol{G}\hat{\boldsymbol{x}} + \boldsymbol{c} \tag{5.14}$$

for some Lagrange multipliers $\hat{\lambda}_i,\ i \in \hat{\mathcal{W}}$. If the multipliers $\lambda_i,\ i \notin \mathcal{I}\cap\hat{\mathcal{W}}$ are set equal to zero for the inequalities constraints that are not imposed to be equalities, $\hat{\boldsymbol{x}}$ and $\hat{\boldsymbol{\lambda}}$ satisfy equation (5.10a). Moreover, since the computation of the step length ensures that (5.10b) and (5.10c) hold, it remains to verify the fourth KKT condition so that $(\hat{\boldsymbol{x}}, \hat{\boldsymbol{\lambda}})$ is a KKT point for the original problem. Thus, $(\hat{\boldsymbol{x}}, \hat{\boldsymbol{\lambda}})$ is a KKT point if $\hat{\lambda}_i \geq 0,\ i \in \hat{\mathcal{W}}\cap\mathcal{I}$. In this case, since $\boldsymbol{G}$ is positive semidefinite, $\hat{\boldsymbol{x}}$ is a global solution of the quadratic problem (5.9) (see Nocedal [NW06], chapter 16).

If there is $\lambda_j < 0,\ j \in \hat{\mathcal{W}}\cap\mathcal{I}$, the index j is removed from the working set and the subproblem is solved without the corresponding imposed equality constraint. In doing so, the following theorem shows that the resulting step is feasible with respect to the removed constraint.

Theorem 5.4. *Given $\hat{\mathcal{W}}$, suppose that the solution $\hat{\boldsymbol{x}}$ satisfies equation (5.14) and $\boldsymbol{a}_i^T\hat{\boldsymbol{x}} = b_i$ for all $i \in \hat{\mathcal{W}}$. In addition, suppose that the constraint gradients $\boldsymbol{a}_i,\ i \in \hat{\mathcal{W}}$, are linearly independent, and there is $\hat{\lambda}_j < 0$ for $j \in \hat{\mathcal{W}}$. If $\boldsymbol{\Delta x}$ is the solution of*

$$\min_{\boldsymbol{\Delta x}} \left[\frac{1}{2}\boldsymbol{\Delta x}^T\boldsymbol{G}\boldsymbol{\Delta x} + \boldsymbol{g}_k^T\boldsymbol{\Delta x}\right] \tag{5.15a}$$

subject to

$$\boldsymbol{a}_i^T\boldsymbol{\Delta x} = 0, \quad i \in \mathcal{W}_k \setminus \{j\}, \tag{5.15b}$$

then $\boldsymbol{a}_j^T \boldsymbol{\Delta x} \geq 0$. *Moreover,* $\boldsymbol{\Delta x}$ *is a descent direction, i.e.,* $\boldsymbol{a}_j^T \boldsymbol{\Delta x} > 0$ *if the second order conditions of (5.15) are satisfied by* $\boldsymbol{\Delta x}$.

Proof: see [NW06]

To conclude, we sum up the algorithm assuming that the objective function of problem (5.9) is bounded in the feasible set.

Algorithm 1 Active-set Method

Input: $\boldsymbol{x_0}$, $\mathcal{W}_0$

$k \leftarrow 0$
while no solution found **do**
  Solve $\min_{\boldsymbol{\Delta x}} \left[\frac{1}{2}\boldsymbol{\Delta x}^T \boldsymbol{G} \boldsymbol{\Delta x} + \boldsymbol{g}_k^T \boldsymbol{\Delta x}\right]$ subject to $\boldsymbol{a}_i^T \boldsymbol{\Delta x} = 0,\ i \in \mathcal{W}_k$
  if $\boldsymbol{\Delta x} = 0$ **then**
    Compute $\hat{\lambda}_i$ so that $\sum_{i \in \hat{\mathcal{W}}} \boldsymbol{a}_i \hat{\lambda}_i = \boldsymbol{G}\hat{\boldsymbol{x}} + \boldsymbol{c}$, where $\hat{\mathcal{W}} = \mathcal{W}_k$
    if $\hat{\lambda}_i \geq 0$ for all $i \in \mathcal{W}_k \cap \mathcal{I}$ **then**
      Solution found $\boldsymbol{x}^* = \boldsymbol{x}_k$
    else
      $j \leftarrow \arg\ \min_{j \in \mathcal{W}_k \cap \mathcal{I}} \hat{\lambda}_i$
      $x_{k+1} \leftarrow x_k$; $\mathcal{W}_{k+1} \leftarrow \mathcal{W}_k \setminus \{j\}$
    end if
  else
    Compute α_k from $\alpha_k = \min\left[1, \min_{i \notin \mathcal{W}_k, \boldsymbol{a}_i^T \boldsymbol{\Delta x}_k < 0} \frac{b_i - \boldsymbol{a}_i^T \boldsymbol{x}_k}{\boldsymbol{a}_i^T \boldsymbol{\Delta x}_k}\right]$
    if $\alpha_k < 1$ **then**
      $\mathcal{W}_{k+1} \leftarrow \mathcal{W}_k \cup \{i^*\}$
      $k + 1 \leftarrow k$
    end if
  end if
end while

5.2.2 Sequential Quadratic Programming

The sequential quadratic programming (SQP) is an effective method for nonlinearly constrained problems. Here, each iteration consists in solving a quadratic subproblem to generate a step. That means, the SQP method solves problem (5.1) by solving iteratively

$$\min_{\boldsymbol{\Delta x}} \left[f(\boldsymbol{x}_k) + \nabla f(\boldsymbol{x}_k)^T \Delta \boldsymbol{x} + \frac{1}{2}\Delta \boldsymbol{x}^T \nabla^2 \mathcal{L}(\boldsymbol{x}_k) \Delta \boldsymbol{x}\right] \tag{5.16a}$$

subject to

$$\nabla c_i(\boldsymbol{x}_k)^T \Delta \boldsymbol{x} + c_i(\boldsymbol{x}_k) = 0, \quad i \in \mathcal{E}, \tag{5.16b}$$

$$\nabla c_i(\boldsymbol{x}_k)^T \Delta \boldsymbol{x} + c_i(\boldsymbol{x}_k) \geq 0, \quad i \in \mathcal{I}. \tag{5.16c}$$

These resulting subproblems are solved using, for example, the active set method as described in the section above, which can also include *line-search* or *trust-region globalization*. The basic SQP algorithm is shown below. Instead of explicitly computing the Hessian of the Lagrangian, SQP algorithms often use approximated versions $\boldsymbol{H}(\boldsymbol{x}_k) \approx \nabla^2\mathcal{L}(\boldsymbol{x}_k)$. We also refer to [NW06] for more details on these extensions and refinements, and proceed to the convergence of the SQP methods. Excluding the inequalities, solving problem (5.1) using the SQP algorithm with exact Hessian of the Lagrangian is equivalent to the application of Newton's method to the KKT conditions of (5.1). Therefore, the SQP method converges quadratically for equality constrained problems.

Algorithm 2 Local SQP Algorithm

Input: $\boldsymbol{x}_0$, $\boldsymbol{\lambda}_0$

```
1: k ← 0
2: while no convergence test is satisfied do
3:     Compute f(x_k), ∇f(x_k), ∇²L(x_k, x_k) and c_i(x_k), ∇c_i(x_k) ∀i ∈ E ∪ I
4:     Solve quadratic problem (5.16) to derive Δx_k and Lagrange multiplier l_k
5:     x_{k+1} ← x_k + Δx_k, λ_{k+1} ← l_k
6:     k ← k + 1
7: end while
```

5.2.3 Interior Point Methods

In this section, we sum up the principle of the interior point method, where the general optimization problem (5.1) is written in the form

$$\min_{\boldsymbol{x}\in\mathbb{R}^n} f(\boldsymbol{x}) \tag{5.17a}$$

$$\text{subject to} \quad \boldsymbol{c_E}(\boldsymbol{x}) = 0, \tag{5.17b}$$

$$\boldsymbol{c_I}(\boldsymbol{x}) - \boldsymbol{s} = 0, \tag{5.17c}$$

$$\boldsymbol{s} \geq 0. \tag{5.17d}$$

Precisely, the vector $\boldsymbol{c_I}(\boldsymbol{x})$ consists of the scalar functions $c_i(\boldsymbol{x})$, $i \in \mathcal{I}$ and $\boldsymbol{c_E}(\boldsymbol{x})$ is formed by its components $c_i(\boldsymbol{x})$, $i \in \mathcal{E}$. There are two possibilities to interpret the interior point methods. First, the KKT conditions with $\boldsymbol{y}$ and $\boldsymbol{z}$ as Lagrange multipliers are pertubed by a factor μ

$$\nabla f(\boldsymbol{x}) - \boldsymbol{J_E}^T(\boldsymbol{x})\boldsymbol{y} - \boldsymbol{J_I}^T(\boldsymbol{x})\boldsymbol{z} = 0, \tag{5.18a}$$

$$\boldsymbol{S}\boldsymbol{z} - \mu\boldsymbol{e} = 0, \tag{5.18b}$$

$$\boldsymbol{c_E}(\boldsymbol{x}) = 0, \tag{5.18c}$$

$$\boldsymbol{c_I}(\boldsymbol{x}) - \boldsymbol{s} = 0, \tag{5.18d}$$

(5.18e)

with $\mu = 0$,

$$\boldsymbol{s} \geq 0, \quad \boldsymbol{z} \geq 0, \tag{5.19}$$

where $\boldsymbol{S}$ is the diagonal matrix with entries $\boldsymbol{s}$ and $\boldsymbol{Z}$ is the diagonal matrix with entries $\boldsymbol{z}$. If $\mu = 0$, the inequalities necessitate that optimal active sets have to be determined. If $\mu > 0$, $\boldsymbol{s}$ and $\boldsymbol{z}$ are positive. The aim is to solve the pertubed KKT conditions (5.18) for $\mu_k \to 0$ ensuring that $\boldsymbol{s}, \boldsymbol{z} > 0$. Under the assumption that the LICQ, the complementarity condition, and the second-order sufficient conditions are satisfied for a solution $(\boldsymbol{x}^*, \boldsymbol{s}^*, \boldsymbol{y}^*, \boldsymbol{z}^*)$, there is a locally unique solution $(\boldsymbol{x}(\mu), \boldsymbol{s}(\mu), \boldsymbol{y}(\mu), \boldsymbol{z}(\mu))$ of the system (5.18) for all sufficiently small positive μ in the neighborhood. Furthermore, $(\boldsymbol{x}(\mu), \boldsymbol{s}(\mu), \boldsymbol{y}(\mu), \boldsymbol{z}(\mu))$ converges to $(\boldsymbol{x}^*, \boldsymbol{s}^*, \boldsymbol{y}^*, \boldsymbol{z}^*)$ for $\mu \to 0$.

In addition, the interior point method is regarded as barrier method. Here, the problem (5.17) is solved by considering a sequence of auxiliary problems

$$\min_{\boldsymbol{x},\boldsymbol{s}} f(\boldsymbol{x}) - \mu \sum_{i=1}^{m} \log(s_i) \tag{5.20a}$$

$$\text{subject to} \quad \boldsymbol{c_E}(\boldsymbol{x}) = 0, \tag{5.20b}$$

$$\boldsymbol{c_I}(\boldsymbol{x}) - \boldsymbol{s} = 0, \tag{5.20c}$$

where $\mu > 0$. The barrier term $-\mu \sum_{i=1}^{m} \log(s_i)$ effects that the components are not too close to zero. The corresponding KKT conditions are

$$\nabla f(\boldsymbol{x}) - \boldsymbol{J_E}^T(\boldsymbol{x})\boldsymbol{y} - \boldsymbol{J_I}^T(\boldsymbol{x})\boldsymbol{z} = 0, \tag{5.21a}$$

$$-\mu \boldsymbol{S}^{-1}\boldsymbol{e} + \boldsymbol{z} = 0, \tag{5.21b}$$

$$\boldsymbol{c_E}(\boldsymbol{x}) = 0, \tag{5.21c}$$

$$\boldsymbol{c_I}(\boldsymbol{x}) - \boldsymbol{s} = 0. \tag{5.21d}$$

Multiplying equation (5.21b) with $\boldsymbol{S}$ leads to the same KKT conditions as the first method proposed.

In the following, we outline the basic concept of interior point algorithms. Applying the Newton method to equations (5.18) in the variables $\boldsymbol{x}_k, \boldsymbol{s}_k, \boldsymbol{y}_k, \boldsymbol{z}_k$ generates step $\boldsymbol{p} = (\boldsymbol{p^x}_k, \boldsymbol{p^s}_k, \boldsymbol{p^y}_k, \boldsymbol{p^z}_k)$ through

$$\begin{bmatrix} \nabla^2 \mathcal{L} & 0 & -\boldsymbol{J_E}^T(\boldsymbol{x}) & -\boldsymbol{J_I}^T(\boldsymbol{x}) \\ 0 & \boldsymbol{Z} & 0 & \boldsymbol{S} \\ \boldsymbol{J_E}(\boldsymbol{x}) & 0 & 0 & 0 \\ \boldsymbol{J_I}(\boldsymbol{x}) & -\mathbb{1} & 0 & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{p^x} \\ \boldsymbol{p^s} \\ \boldsymbol{p^y} \\ \boldsymbol{p^z} \end{bmatrix} = - \begin{bmatrix} \nabla f(\boldsymbol{x}) - \boldsymbol{J_E}(\boldsymbol{x})^T \boldsymbol{y} - \boldsymbol{J_I}(\boldsymbol{x})^T \boldsymbol{z} \\ \boldsymbol{S}\boldsymbol{z} - \mu \boldsymbol{e} \\ \boldsymbol{c_E}(\boldsymbol{x}) \\ \boldsymbol{c_I}(\boldsymbol{x}) - \boldsymbol{s} \end{bmatrix}. \tag{5.22}$$

Then, the new iterate is given by

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \alpha_k^{s,max} \boldsymbol{p^x}_k, \quad \boldsymbol{s}_{k+1} = \boldsymbol{s}_k + \alpha_k^{s,max} \boldsymbol{p^s}_k, \tag{5.23a}$$

$$\boldsymbol{y}_{k+1} = \boldsymbol{y}_k + \alpha_k^{z,max} \boldsymbol{p^y}_k, \quad \boldsymbol{z}_{k+1} = \boldsymbol{z}_k + \alpha_k^{z,max} \boldsymbol{p^z}_k, \tag{5.23b}$$

where

$$\alpha_k^{s,max} = \max\{\alpha \in (0,1] : s_k + \alpha \boldsymbol{p^s}_k \geq (1-\tau)\boldsymbol{s}_k\}, \tag{5.24a}$$
$$\alpha_k^{z,max} = \max\{\alpha \in (0,1] : z_k + \alpha \boldsymbol{p^z}_k \geq (1-\tau)\boldsymbol{z}_k\}, \tag{5.24b}$$

with $\tau \in (0,1)$. These conditions ensure that the variables s and z do not converge too quickly to zero. Given the error function based on the KKT conditions (5.18)

$$E(\boldsymbol{x}_k, \boldsymbol{s}_k, \boldsymbol{y}_k, \boldsymbol{z}_{k+1}) = \max\{\|\nabla f(\boldsymbol{x}) - \boldsymbol{J_E}(\boldsymbol{x})^T\boldsymbol{y} - \boldsymbol{J_I}(\boldsymbol{x})^T\boldsymbol{z}\|, \|\boldsymbol{Sz} - \mu\boldsymbol{e}\|, \|\boldsymbol{c_E}(\boldsymbol{x})\|, \|\boldsymbol{c_I}(\boldsymbol{x}) - \boldsymbol{s}\|\} \tag{5.25}$$

as proposed by Nocedal [NW06], the basic algorithm can be summarized as follows.

Algorithm 3 Basic Interior Point Algorithm

Input: $\boldsymbol{x}_0$, $\boldsymbol{s}_0 > 0$, $\mu_0 > 0$, $\sigma, \tau \in (0,1)$

```
Compute y_0 and z_0 > 0
k ← 0
while no convergence test is satisfied do
    while until E(x_k, s_k, y_k, z_k; μ_k) ≤ μ_k do
        Solve equation (5.22) to obtain p = (p^x_k, p^s_k, p^y_k, p^z_k)
        Compute α_k^{s,max}, α_k^{z,max} using (5.24)
        Compute (x_{k+1}, s_{k+1}, y_{k+1}, z_{k+1}) using (5.23)
        μ_{k+1} ← μ_k and k ← k + 1
    end while
    Choose μ_k ∈ (0, σμ_k)
end while
```

Here, μ_k is kept fixed until a approximated solution of the KKT-conditions is found $E(\boldsymbol{x}_k, \boldsymbol{s}_k, \boldsymbol{y}_k, \boldsymbol{z}_k; \mu_k) \leq \mu_k$. Alternatively, μ_k can be updated in each iteration depending on the progress. In case of more difficult problems, this strategy is more robust and described in more detail in [NW06].

We also refer to Nocedal [NW06] for the description of interior point methods including line search and trust region strategies. Moreover, he showed that under certain conditions, the barrier parameter μ can be controlled so that the iterates converge superlinearly to the solution $(\boldsymbol{x}^*, \boldsymbol{s}^*, \boldsymbol{y}^*, \boldsymbol{z}^*)$.

All in all, interior point methods are suitable for large-scale problems. Wächter and Biegler [WB06] implemented a line search filter interior point in Ipopt (see also [Wä09]).

5.3 Least-Squares Problems

As mentioned above, the method of least-squares is the most common method to solve parameter estimation and fitting problems in physics, chemistry, finance, or economics. Therefore, these kind of problems play an important role in optimization theory.

In this section, we present the fundamental concept of this technique and outline corresponding algorithms. For more information, we refer to [Str11], who provides a comprehensive introduction, or to standard optimization literature (e.g., [BV04, NW06]). Supplementary details on the characteristics of the resulting parameter estimators can be found in literature about regression methods (e.g., [FBM04, Fox97, FKL09, Rya97]). Special focus of this section lies in the Gauss-Newton algorithm for nonlinear least-squares problems. In section 5.3.4, we outline a generalization for constrained nonlinear least-squares problems, which was developed by Bock [Boc83, Boc87, BKS07].[1]

5.3.1 Concept of Least-Squares Method

This section is mainly sketched on [NW06, Str11]. To begin with, we explain the idea of the least-squares method on the basis of the following setting. Given a model function $\phi(x_i, \boldsymbol{p})\colon \mathbb{R}^n \times \mathbb{R}^l \to \mathbb{R}$ that describes the relation between a set of observations $y_i,\ i = 1, \ldots, n$ and its corresponding input data $x_i,\ i = 1, \ldots, n$, we assume that

$$y_i = \phi(x_i, \boldsymbol{p}) + \epsilon_i, \tag{5.26}$$

where $\epsilon_i \sim \mathcal{N}(0, \sigma_i^2)$ represents the error related to each observation y_i. To get an estimation for the parameters $\boldsymbol{p} \in \mathbb{R}^l$, the least-squares-approach minimizes the sum of the squared residual errors that are optionally weighted by corresponding factors $w_i \neq 0$

$$\min_{\boldsymbol{p}} f(\boldsymbol{p}) = \frac{1}{2} \sum_{i=1}^{n} [w_i \cdot (y_i - \phi(x_i, \boldsymbol{p}))]^2. \tag{5.27}$$

In theory, the weighting factor w_i is equal to $\frac{1}{\sigma_i}$. However, in practice, the true distribution of the errors is usually unknown and, therefore, the variances have to be estimated in advance. Alternatives to get rough estimates of the weights w_i are provided by Strutz [Str11].[2]

From now on, we write $r_i(\boldsymbol{p}) = w_i \cdot (y_i - \phi(x_i, \boldsymbol{p}))$ and assume that $r_i,\ i = 1, \ldots, n$, is smooth. Then, the Jacobian Matrix of $\boldsymbol{r}(\boldsymbol{p}) = (r_1(\boldsymbol{p}), \ldots, r_n(\boldsymbol{p}))^T$ is given by

$$\boldsymbol{J}(\boldsymbol{p}) = \left[\frac{\partial r_i}{\partial p_j}\right]_{\substack{i=1,\ldots,n \\ j=1,\ldots,l}} = \begin{bmatrix} \nabla r_1(\boldsymbol{p})^T \\ \nabla r_2(\boldsymbol{p})^T \\ \vdots \\ \nabla r_n(\boldsymbol{p})^T \end{bmatrix}. \tag{5.28}$$

Moreover, we obtain

$$\nabla f(\boldsymbol{p}) = \sum_{i=1}^{n} r_i(\boldsymbol{p}) \nabla r_i(\boldsymbol{p}) = \boldsymbol{J}(\boldsymbol{p})^T \boldsymbol{r}(\boldsymbol{p}) \tag{5.29}$$

[1] This method will be applied in the subsequent chapter, in which we develop methods to identify parameters for the nonlinear demand model presented in section 6.2.

[2] If all observations are equally reliable, then $\sigma_i = \sigma = 1$. However, this is not recommendable if the available data comprises outliers, which probably occurs in most cases.

and

$$\nabla^2 f(\boldsymbol{p}) = \sum_{i=1}^{n} \nabla r_i(\boldsymbol{p}) \nabla r_i(\boldsymbol{p})^T + \sum_{i=1}^{n} r_i(\boldsymbol{p}) \nabla^2 r_i(\boldsymbol{p})$$
$$= \boldsymbol{J}(\boldsymbol{p})^T \boldsymbol{J}(\boldsymbol{p}) + \sum_{i=1}^{n} r_i(\boldsymbol{p}) \nabla^2 r_i(\boldsymbol{p}). \tag{5.30}$$

If $r_i,\ i = 1, \ldots, n$, is almost affine or, in general, rather small, the second term of (5.30) can be neglected. Many algorithms tailored to solve least-squares problems (5.27) take advantage of this feature. In general, these algorithms are modifications of *Newton* or *quasi-Newton* methods including the strategies for global convergence *line search* and *trust region.*[3]

5.3.2 Linear Least-Squares Problems

In the simplified case that the model equation $\phi(\cdot)$ is linear. i.e.,

$$f(\boldsymbol{p}) = \frac{1}{2} \|\boldsymbol{W}(\boldsymbol{J}\boldsymbol{p} - \boldsymbol{y})\|_2^2, \tag{5.31}$$

where

$$\boldsymbol{W} = \begin{pmatrix} w_1 & & \\ & \ddots & \\ & & w_n \end{pmatrix} \tag{5.32}$$

and $\nabla f(\boldsymbol{p}) = \boldsymbol{J}^T \boldsymbol{W}(\boldsymbol{J}\boldsymbol{p} - \boldsymbol{y})$. Here, the solution $\boldsymbol{p}^*$ satisfies the normal equations

$$\boldsymbol{J}^T \boldsymbol{W} \boldsymbol{J} \boldsymbol{p}^* = \boldsymbol{J}^T \boldsymbol{W} \boldsymbol{y}$$

of problem (5.31). Nocedal [NW06] presents three possible algorithms to compute $\boldsymbol{p}^*$ provided that $n \geq l$ and $\boldsymbol{J}$ has full rank. These techniques are based on Cholesky factorization, QR factorization, and singular value decomposition. In case of large problems, iterative techniques such as the conjugate gradient method might be more efficient. For the description and advantages of these possible methods we refer to Nocedal [NW06]. Before studying the algorithms for constrained least-squares problem, we shortly consider statistical aspects of the resulting estimator.

5.3.2.1 Statistical Analysis of Linear Least-Squares Problems

In this section, we shortly present some important statistical results of the solutions of linear least-squares problems (cf. [FBM04, Fox97, FKL09, Rya97]).

[3] We refer to [NW06, BGLS06, GMW08] for a detailed description of *Newton methods* and *globalization strategies*.

- A linear regression model relates a dependent variable y with a number of independent variables $x_1, \ldots, x_l$, and an error ϵ_i, i.e.,

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots + \beta_l x_l + \epsilon.$$

If $y_i,\ i = 1, \ldots, n$ are observations for y and $x_{i,1}, \ldots, x_{i,l}$ are observations for $x_i,\ i = 0, \ldots, n$, we obtain

$$y_i = \beta_0 + \beta_1 x_{1,i} + \ldots + \beta_l x_{l,i} + \epsilon_i,$$

where $\epsilon_1, \ldots, \epsilon_n$, are uncorrelated random variables with $\mathbb{E}(\epsilon_i) = 0$ and $\mathrm{Var}(\epsilon_i) = \sigma^2$ for all $i = 1, \ldots, n$, and $\mathrm{Cov}(\epsilon_i, \epsilon_j) = 0$ if $i \neq j$.
Then, the Gauss-Newton theorem shows that the least-squares estimator provides the best linear unbiased estimator for $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_l)^T$. That means, this estimator has lowest variance. For more information, we refer to Falk et al. [FBM04].

- Let $\epsilon_i = \mathcal{N}(0, \sigma_i),\ i = 1, \ldots, n$. If, in addition, the errors are independent from each other, the resulting maximum-likelihood estimator is equal to the result of the least-squares estimation (see [Str11, Fox97]).

- According to Fox [Fox97], if $(\boldsymbol{J}^T \boldsymbol{W} \boldsymbol{J})$ is invertible and $\epsilon_i = \mathcal{N}\left(0, \frac{\sigma_\epsilon^2}{w_i^2}\right)$, the resulting estimators in the linear case (5.31) are

$$\hat{\boldsymbol{p}} = (\boldsymbol{J}^T \boldsymbol{W} \boldsymbol{J})^{-1} \boldsymbol{J}^T \boldsymbol{W} \boldsymbol{y}$$

and

$$\hat{\sigma}_\epsilon^2 = \frac{\sum((\boldsymbol{y} - \boldsymbol{J}\hat{\boldsymbol{p}})/w_i)^2}{n}.$$

The estimated asymptotic covariance matrix of $\hat{\boldsymbol{p}}$ is equal to

$$\mathrm{Cov}(\hat{\boldsymbol{p}}) = \hat{\sigma}_\epsilon^2((\boldsymbol{J}^T \boldsymbol{W} \boldsymbol{J}))^{-1}.$$

- Notably, the least-squares method is a heavy tool for many kinds of fitting problems. However, if the errors are nonnormally distributed, the Least-Squares estimator is less efficient, because heavy-tailed distributions lead to outliers. We refer to [Str11, Fox97] for possibilities to detect outliers, nonconstant variance, or nonnormality.

5.3.3 Nonlinear Least-Squares Problems

In general, there are two algorithms to compute the solution of nonlinear least-squares problems: Gauss- Newton and Levenberg-Marquardt.
The idea of the Gauss-Newton method is to solve the nonlinear least-squares problem by iteratively solving linearizations in each loop. That means, a problem of the form $\min_{\boldsymbol{p}} \frac{1}{2}\|\boldsymbol{r}(\boldsymbol{p})\|_2^2$ can be solved by means of the following linearized problem

$$\min_{\boldsymbol{\Delta p}_k} \frac{1}{2}\|\boldsymbol{r}(\boldsymbol{p}_k) + \boldsymbol{J}(\boldsymbol{p}_k)\boldsymbol{\Delta p}_k\|_2^2. \tag{5.33}$$

Then, the iteration $\boldsymbol{p}_k$ is replaced by

$$\boldsymbol{p}_{k+1} = \boldsymbol{p}_k + \lambda_k \boldsymbol{\Delta p}_k \quad (0 \leq \lambda_{min} \leq \lambda_k \leq 1). \tag{5.34}$$

According to Nocedal [NW06], possibilities for step length conditions in line search are *Armijo* or *Wolfe conditions*. In case that the Jacobian $\boldsymbol{J}(\boldsymbol{p})$ is (almost) rank-deficient, the Gauss-Newton method does not necessarily converge, since the Gauss-Newton step $\boldsymbol{\Delta p}_k$ is not unique. Alternatively, the Levenberg-Marquardt method can be used (cf. [NW06, BGLS06]). Here, the linearized subproblem at each iteration is given by

$$\min_{\boldsymbol{\Delta p}_k} \frac{1}{2} \|\boldsymbol{r}(\boldsymbol{p}_k) + \boldsymbol{J}(\boldsymbol{p}_k)\boldsymbol{\Delta p}_k\|_2^2, \quad \text{subject to } \|\boldsymbol{\Delta p}_k\|_2 \leq \Delta_k. \tag{5.35}$$

If for the solution of the Gauss-Newton algorithm $\|\boldsymbol{\Delta p}_k^{GN}\|_2 \leq \Delta_k$, then $\boldsymbol{\Delta p}^{GN}$ is also a solution of problem (5.35). Otherwise, Nocedal [NW06] proves that, given $\lambda > 0$ the solution of (5.35) satisfies $\|\boldsymbol{\Delta p}_k^{GN}\|_2 = \Delta_k$ and

$$(\boldsymbol{J}^T \boldsymbol{J} + \lambda_{LM} \mathbb{1})\boldsymbol{p} = -\boldsymbol{J}^T \boldsymbol{r}. \tag{5.36}$$

For more details (e.g., implementation and convergence), we refer to [NW06]. In case of large residuals, both algorithms are not appropriate because the second-order part of $\nabla^2 f(\boldsymbol{p})$ is too significant to be neglected in the quadratic term. Hence, the asymptotic convergence is only linear. Nocedal [NW06] proposes to use Newton or Quasi-Newton methods or hybrid algorithms, which combine Gauss-Newton and (Quasi-)Newton methods.

5.3.4 Constrained Nonlinear Least-Squares Problems

Bock [Boc83, Boc87] (see also [BKS07]) presents a generalization to solve constrained nonlinear optimization problems of the form

$$\min_{\boldsymbol{p}} \frac{1}{2} \|\boldsymbol{r_1}(\boldsymbol{p})\|_2^2 \tag{5.37a}$$

subject to

$$\boldsymbol{r_2}(\boldsymbol{p}) = 0, \tag{5.37b}$$

$$\boldsymbol{r_3}(\boldsymbol{p}) \geq 0, \tag{5.37c}$$

where $\boldsymbol{r_1} \colon \mathbb{R}^p \to \mathbb{R}^{n_1}$, $\boldsymbol{r_2} \colon \mathbb{R}^p \to \mathbb{R}^{n_2}$,and $\boldsymbol{r_3} \colon \mathbb{R}^p \to \mathbb{R}^{n_3}$. Given an initial guess $\boldsymbol{p}_0$, $\boldsymbol{p}_k$ is iteratively improved by

$$\boldsymbol{p_{k+1}} = \boldsymbol{p}_k + \lambda_k \boldsymbol{\Delta p}_k \tag{5.38}$$

where $0 < \lambda_{min} \leq \lambda_k \leq 1$ and $\boldsymbol{\Delta p}_k$ is the solution of

$$\min_{\boldsymbol{\Delta p}_k} \frac{1}{2} \|\boldsymbol{r_1}(\boldsymbol{p}_k) + \boldsymbol{J_1}(\boldsymbol{p}_k)\boldsymbol{\Delta p}_k\|_2^2 \tag{5.39a}$$

subject to

$$\boldsymbol{r_2}(\boldsymbol{p}_k) + \boldsymbol{J_2}(\boldsymbol{p}_k)\boldsymbol{\Delta p}_k = 0 \tag{5.39b}$$

$$\boldsymbol{r_3}(\boldsymbol{p}_k) + \boldsymbol{J_3}(\boldsymbol{p}_k)\boldsymbol{\Delta p}_k \geq 0. \tag{5.39c}$$

Therefore, each iteration consists in solving a quadratic subproblem (e.g., with active set methods). The algorithm is described below.

Algorithm 4 Gauss Newton Algorithm

Input: $\boldsymbol{p}_0$, TOL, $\boldsymbol{r_1}(\boldsymbol{p})$, $\boldsymbol{J_1}(\boldsymbol{p})$, $\boldsymbol{r_2}(\boldsymbol{p})$, $\boldsymbol{J_2}(\boldsymbol{p})$, $\boldsymbol{r_3}(\boldsymbol{p})$, $\boldsymbol{J_3}(\boldsymbol{p})$

```
1: k ← 0
2: while ‖Δp_k‖_2 > TOL do
3:     Compute r_i(p_k) and J_i(p_k) for all i = 1, ··· , 3
4:     min_{Δp_k} 1/2 ‖r_1(p_k) + J_1(p_k)Δp_k‖_2^2
5:     s.t. r_2(p_k) + J_2(p_k)Δp_k = 0, r_3(p_k) + J_3(p_k)Δp_k ≥ 0
6:     p_{k+1} ← p_k + Δp_k
7:     k = k + 1
8: end while
```

Principally, this method is analyzed and developed in the context of parameter estimation problems for nonlinear ordinary differential equations (see [Boc83, Boc87, BKS07]) and, therefore, this algorithm is applied in many areas. For example, Bauer [Bau99] and Körkel [Kö02] apply this method to estimate parameters for models in chemistry and process engineering in the context of optimum experimental design. Jäger [Jä08] uses the Gauss-Newton method with trust region globalization to estimate parameters in the field of commodity pricing. Regarding the trust region globalization strategy, the linearized subproblem of a nonlinear equality constrained least-squares problem is given by

$$\min_{\boldsymbol{\Delta p}_k} \frac{1}{2}\|\boldsymbol{r_1}(\boldsymbol{p}_k) + \boldsymbol{J_1}(\boldsymbol{p}_k)(\boldsymbol{\Delta p}_k)\|_2^2 \tag{5.40a}$$

subject to

$$\boldsymbol{r_2}(\boldsymbol{p}_k) + \boldsymbol{J_2}(\boldsymbol{p}_k)\boldsymbol{\Delta p}_k = (1-\alpha)\boldsymbol{r_2}(\boldsymbol{p}),\ 0 < \alpha \leq 1, \tag{5.40b}$$

and

$$\|\boldsymbol{\Delta p}_k\|_2^2 \leq \Delta^2, \tag{5.40c}$$

where Δ is the trust region radius and α is the relaxation factor that ensures feasibility. The corresponding Karush-Kuhn-Tucker conditions are given by

$$\begin{aligned} (\boldsymbol{J_1}^T(\boldsymbol{p})\boldsymbol{J_1}(\boldsymbol{p}) + \lambda_{LM}\mathbb{1})\boldsymbol{\Delta p}_k + \boldsymbol{J_2}^T(\boldsymbol{p})\boldsymbol{\lambda} &= -\boldsymbol{J_1}^T(\boldsymbol{p})\boldsymbol{r_1}(\boldsymbol{p}) \\ \boldsymbol{J_2}(\boldsymbol{p})\boldsymbol{\Delta p}_k &= -\alpha\boldsymbol{r_2}(\boldsymbol{p}), \end{aligned}$$

with $\lambda_{LM} = 0$ if $\|\boldsymbol{\Delta p}_k\| \leq \Delta$.

5.3.4.1 Analysis of Solutions for Linearized Problems

In this section, we summarize the results of analyzing the solutions obtained by using the Gauss-Newton method presented above. This section will be mainly sketched on [Boc83, Boc87, BKS07, Bau99, Kö02]. From now on, we write

$$\boldsymbol{r_c}(\boldsymbol{p}) :=\begin{pmatrix}\boldsymbol{r_2}(\boldsymbol{p})\\ \tilde{\boldsymbol{r}}_{\boldsymbol{3}}(\boldsymbol{p})\end{pmatrix},\quad \boldsymbol{J_c}(\boldsymbol{p}) :=\begin{pmatrix}\boldsymbol{J_2}(\boldsymbol{p})\\ \tilde{\boldsymbol{J}}_{\boldsymbol{3}}(\boldsymbol{p})\end{pmatrix}, \tag{5.41}$$

where $\tilde{\boldsymbol{r}}_{\boldsymbol{3}}(\boldsymbol{p})$ comprises the active inequality constraints at $\boldsymbol{p}$, $\tilde{\boldsymbol{J}}_{\boldsymbol{3}}(\boldsymbol{p})$ is the corresponding Jacobian matrix and $n_c := n_2 + \tilde{n}_3$, where $\tilde{n}_3$ is the number of active inequality constraints.

Remark 5.2. $(\boldsymbol{p}^*, \boldsymbol{\lambda}^*)$ is a Karush-Kuhn-Tucker point of problem (5.37) if and only if $(\boldsymbol{0}, \boldsymbol{\lambda}^*)$ is a Karush-Kuhn-Tucker point of (5.39) with $\boldsymbol{p}_k = \boldsymbol{p}^*$.

Bock [Boc87] demonstrates that the local convergence behavior of inequality constraint problem is equal to the behavior of the equality constraint problem. Hence, only the latter needs to be considered from now on. The solution of problem (5.39) can be written by means of a generalized inverse $\boldsymbol{J}^+$.

Theorem 5.5. *Existence of generalized inverse*
Given the linearized problem (5.39),

$$\text{[CQ] Constraint Qualification:}\quad \operatorname{rank} \boldsymbol{J_c} = n_c \tag{5.42}$$

and

$$\text{[PD] Positive Definiteness:}\quad \operatorname{rank}\begin{pmatrix}\boldsymbol{J_1}\\ \boldsymbol{J_c}\end{pmatrix} = l \tag{5.43}$$

([PD] $\Leftrightarrow \boldsymbol{y}^T \boldsymbol{J_1}^T \boldsymbol{J_1} \boldsymbol{y} > 0$ for all $\boldsymbol{y} \in \operatorname{Kern}(\boldsymbol{J_c}(\boldsymbol{p}) \setminus \{0\})$) hold. Then,

- *there exists one Karush-Kuhn-Tucker point $(\boldsymbol{\Delta p}^*, \boldsymbol{\lambda}^*)$ of problem (5.39) and $\boldsymbol{\Delta p}^*$ is a strict minimum and*
- *there is a linear mapping $\boldsymbol{J}^+ : \mathbb{R}^l \to \mathbb{R}^{n_1+n_c}$, such that*

$$\boldsymbol{\Delta p}^* = -\boldsymbol{J}^+ \begin{pmatrix}\boldsymbol{r_1}\\ \boldsymbol{r_c}\end{pmatrix}$$

is a solution of (5.39).

$$\boldsymbol{J}^+ = \begin{pmatrix}\mathbb{1} & 0\end{pmatrix}\begin{pmatrix}\boldsymbol{J_1}^T\boldsymbol{J_1} & \boldsymbol{J_2}^T\\ \boldsymbol{J_2} & 0\end{pmatrix}^{-1}\begin{pmatrix}\boldsymbol{J_1}^T & 0\\ 0 & \mathbb{1}\end{pmatrix} \tag{5.44}$$

satisfies $\boldsymbol{J}^+\boldsymbol{J}\boldsymbol{J}^+ = \boldsymbol{J}^+$ and is called generalized inverse of $\boldsymbol{J}$.

Proof: See [Boc87].

Remark 5.3. In case of $\boldsymbol{r_2} = \boldsymbol{J_2} = \boldsymbol{0}$, we obtain

$$\boldsymbol{J}^{+} = (\boldsymbol{J_1}^T \boldsymbol{J_1})^{-1} \boldsymbol{J_1}^T. \tag{5.45}$$

Likewise, Bock [Boc87] proves the following contraction theorem, which characterizes the convergence behavior of the generalized Gauss-Newton method.

Theorem 5.6. Local Contraction Theorem
Let $\boldsymbol{J}^{+}(\boldsymbol{p})$ be the generalized inverse of the Jacobian $\boldsymbol{J}(\boldsymbol{p})$ of $\boldsymbol{r}(\boldsymbol{p}) \in C^1(D)$. Under the assumption that the Lipschitz conditions for $\boldsymbol{J}$ resp. $\boldsymbol{J}^{+}$ for all $t \in [0,1]$ and for all $\boldsymbol{p}, \boldsymbol{p'}, \boldsymbol{p''} \in D,\ \boldsymbol{p} - \boldsymbol{p'} = \boldsymbol{J}^{+}(\boldsymbol{p})\boldsymbol{F}(\boldsymbol{p})$,

$$\|\boldsymbol{J}^{+}(\boldsymbol{p'})(\boldsymbol{J}(\boldsymbol{p} + t(\boldsymbol{p'} - \boldsymbol{p})) - \boldsymbol{J}(\boldsymbol{p}))(\boldsymbol{p'} - \boldsymbol{p})\| \leq \omega t \|\boldsymbol{p'} - \boldsymbol{p}\|^2 \tag{5.46}$$

and

$$\|(\boldsymbol{J}^{+}(\boldsymbol{p''}) - \boldsymbol{J}^{+}(\boldsymbol{p}))\boldsymbol{R}(\boldsymbol{p})\| \leq \kappa \|\boldsymbol{p''} - \boldsymbol{p}\|, \tag{5.47}$$

where $\boldsymbol{R}(\boldsymbol{p})\colon = \boldsymbol{r}(\boldsymbol{p}) - \boldsymbol{J}(\boldsymbol{p})\boldsymbol{J}^{+}(\boldsymbol{p})\boldsymbol{r}(\boldsymbol{p})$ and $\kappa < 1$, are satisfied. Then, for all $\boldsymbol{p}_0 \in D$ with

$$\delta_0\colon = \kappa + \frac{\alpha_0 \omega}{2} < 1 \quad (\alpha_j := \|\boldsymbol{J}^{+}(\boldsymbol{p}_j)\boldsymbol{r}(\boldsymbol{p}_j)\|) \tag{5.48}$$

and

$$D_0 := \bar{K}\left(\boldsymbol{p}_0, \frac{\alpha_0}{1 - \delta_0}\right) \subset D, \tag{5.49}$$

1. *the iteration $\boldsymbol{p}_{j+1} = \boldsymbol{p}_j + \boldsymbol{\Delta p}_j$, $\boldsymbol{\Delta p}_j = -\boldsymbol{J}^{+}(\boldsymbol{p}_j)\boldsymbol{r}(\boldsymbol{p_j})$, is well-defined and stays in D_0,*

2. *there is a $\boldsymbol{p}^* \in D_0$ so that $\boldsymbol{p}_j \to \boldsymbol{p}^*$, i.e., $\boldsymbol{J}^{+}(\boldsymbol{p}^*)\boldsymbol{F}(\boldsymbol{p}^*) = 0$,*

3. *the a-priori-estimate $\|\boldsymbol{p}_j - \boldsymbol{p}^*\| \leq \delta_0^j \frac{\alpha_0}{1 - \delta_0}$, and*

4. *the convergence is linear: $\|\boldsymbol{\Delta p}_{j+1}\| \leq \delta_k \|\boldsymbol{\Delta p}_j\| = (\frac{\alpha_j \omega}{2} + \kappa)\|\boldsymbol{\Delta p}_j\|$.*

Proof: see [Boc87].

Remark 5.4. Nonlinearity is expressed through ω, and κ is the incompatibility constant (see [Boc87, Kö02]).

Remark 5.5. Formulated in a generalized version this theorem characterizes the local convergence of Newton-type methods in general.

5.3.4.2 Statistical Analysis of Solutions for Linearized Problems

In this section, the analysis is described for the case $\boldsymbol{r_3} = \mathbf{0}$, but can also be applied to the generalized case. Since the residuals of the initial problem are random variables, the solution of the Gauss-Newton method is also random. It follows that $\boldsymbol{\Delta p} = -\boldsymbol{J}^+ \begin{pmatrix} \boldsymbol{r_1} \\ \boldsymbol{r_2} \end{pmatrix}$ follows a normal distribution with $\mathbb{E}(\boldsymbol{\Delta p}) = \mathbf{0}$ and (approximate) covariance matrix

$$\boldsymbol{C} = \boldsymbol{J}^+ \begin{pmatrix} \mathbb{1} & 0 \\ 0 & 0 \end{pmatrix} (\boldsymbol{J}^+)^T \tag{5.50}$$

(cf. [Kö02] for the computation). According to Bock [Boc87], given a parameter estimation problem with l variables and n_2 equality constraints, the linearized confidence region $G_L(\alpha)$ for the optimal solution $\boldsymbol{p}^*$ with significance level α is given by

$$G_L(\alpha) = \left\{ \boldsymbol{p}^* + \boldsymbol{\Delta p} \in \mathbb{R}^l \;\middle|\; \|\boldsymbol{J_1}(\boldsymbol{p}^*)\boldsymbol{\Delta p}\|_2^2 \le \gamma(\alpha), \boldsymbol{J_2}(\boldsymbol{p}^*)\boldsymbol{\Delta p} = 0 \right\} \tag{5.51}$$

$$= \left\{ \boldsymbol{p}^* + \boldsymbol{J}^+(\boldsymbol{p}^*) \begin{pmatrix} -\boldsymbol{J_1}(\boldsymbol{p}^*)\boldsymbol{\Delta p} \\ 0 \end{pmatrix} \;\middle|\; \|-\boldsymbol{J_1}(\boldsymbol{p}^*)\boldsymbol{\Delta p}\|_2^2 \le \gamma(\alpha) \right\} \tag{5.52}$$

with $\gamma(\alpha) := (l - n_2)F_{(1-\alpha)}(l - n_2, n_1 - (l - n_2))$, where $F_{(1-\alpha)}$ is the $(1-\alpha)$-quantile of the F-distribution (see [Boc87] for the proof). The following theorem provides an approximation of the confidence region.

Theorem 5.7. *Let*

$$\theta_i := \sqrt{c_{ii}\gamma(\alpha)}, \quad i = 1, \dots, n, \tag{5.53}$$

where c_{ii} is the entry of the i-th principal diagonal of the covariance matrix C. Then, the linearized confidence region is enclosed

$$G_L(\alpha) \subseteq [p_1^* - \theta_1, p_1^* + \theta_1] \times \ldots \times [p_l^* - \theta_l, p_l^* + \theta_l]. \tag{5.54}$$

Proof: see [Boc87]

Remark 5.6. In case the variances σ_i^2, $i = 1, \dots, n$, are only known up to a factor β^2, the approximating intervals for the confidence region 5.54 are given by

$$\theta_i = b \cdot \sqrt{c_{ii}\gamma(\alpha)}, \quad i = 1, \dots, n, \tag{5.55}$$

where $b^2 := \frac{\|r_1(\boldsymbol{p}^*)\|_2^2}{n_1 - (l - n_2)}$ is an estimator for β^2 (cf. [Boc87, Bau99]).

6 A Heuristic Demand Model for Petrochemical Products

Having collected characteristics and dependencies described in our general framework in chapter 3, we are in a position to develop a quantitative demand model for the petrochemical market that is applicable to our supply-demand optimization problem proposed in chapter 4. In other words, our demand model is supposed to reflect the demand-price relation of petrochemical products in the framework established in the previous chapter and is simultaneously suitable for the optimization problem applied to the petrochemical market. So far, this problem is a quite unexplored field of research, since most of the literature provides approaches to modeling demand, which are not suitable. So far, most demand models are price-insensitive or employ the concept of utility function (cf. section 2). Therefore, we will start by analyzing very basic model functions with preference given to a phenomenological approach.
Another challenge of modeling demand for petrochemical products lies in the missing information in consumer behavior under certain conditions. For example, there is no data available about the hypothetical situation that prices are close to zero. Hence, our modeling relies on additional a-priori assumptions.
For this purpose, this chapter is structured as follows. To gain a better insight, we will summarize the difficulties and the problems we are faced with before discussing our heuristic approach to modeling demand. In section 6.2, we propose a basic demand model for product p_i in region r at time t with respect to price $x^{\pi}_{p_i,r,t}$, the *tanh-demand model*, as well as enhancements to include the influences of the change of the economic situation $\boldsymbol{\Delta a^{\zeta}}_{r,t,J}$ and prices of other products $x^{\pi}_{p_j,r,t},\ j \neq i$. We are able to prove that our model satisfies the general characteristics defined in chapter 3 to the greatest extent. In section 6.3, we integrate our demand model in the supply-demand trade network optimization problem and simulate reasonable prices and sales quantities for different scenarios.

6.1 Preliminaries

Above all, developing explicit model functions benefits from detailed data analysis. However, we rely on a heuristic approach, because the available data only provides incomplete information. Figure 6.1 reflect the structure of stereotypical yearly price and sales data and reveal very well the difficulties with which we are faced. These include:

1. Data exhibits years in which prices are close but sales quantities differ considerably.

2. There are consecutive years in which sales quantities and prices rise or fall.

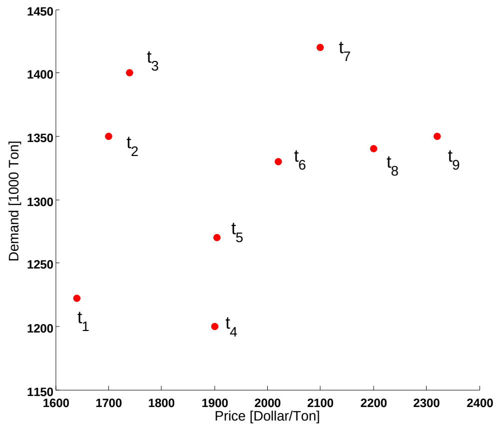

Figure 6.1: Exemplary price and consumption time series that display stereotypical features of yearly data

3. There is no information available about consumption in the whole price range.

Thus, we can draw the following conclusions, which makes straight modeling more complex.

1. There are definitely more factors which influence sales than solely price. In addition, these seem to partially overlap making it impossible to consider them separately.

2. The underlying nonlinear decreasing dependency of demand on price that we expect to exist is not evident. If the data exhibits a tendancy to express nonlinearity, it is not necessarily the hypothetical behavior of the consumer at a fixed time that we aim to model.

3. The historical data mainly provides information about the temporal process of demand data.

Reducing the study to the relationship between demand and price, there exist alternative models that do not imply that demand decreases if prices rise. For example, Huschto et al. [HFH$^+$11] develop a pricing model for conspicuous products, i.e., in which luxuries are purchases because of their reputation. Therefore, demand also increases if price increases. Such an assumption, however, is not adequate to describe the demand of commodities, which are of standard quality and purchased in large quantity for further processing or end consumption.
Hence, as Hildenbrand [Hil94] has already noted, we have to establish the demand function at a fixed time with the means of auxiliary a-priori assumptions.[1]

[1] In the framework of his studies on market demand, Hildenbrand also discusses the difficulties of modeling household demand given incomplete data. Since his empirical studies show the necessity of including demographic facts, but give no qualitative reference, his approach to modeling is also built on a-priori assumptions whenever necessary (see [Hil94], page 12ff).

On the basis of the assumptions made for our general approach to modeling in section 3, we set up a demand model that maps prices unambiguously to quantities required at these prices. In doing so, we keep in mind the incompleteness of information we have about the consumer and aim to avoid, as far as possible, parameters referring to influencing factors, which are not available.[2] This is also essential with regard to a robust parameter identification, which we discuss in section 7. To be more precise, we include the dependencies of prices and economic factors in the model.
Taking all aspects into account, we attribute the following characteristics to a quantitative demand function $\phi_{p,r,t}$ for product p in region r at time t in the petrochemical industry. In this section, we consider the demand functions for $|P| = 1$ und $|P| = 2$.

Assumptions 6.1. *Characteristics of the heuristic demand function*

1. *Demand and price are always non-negative.*
2. *The demand depends on prices and economic factors, which represent the economic situation.*
3. *The influence of price and economic factors may change in the course of time.*
4. *$\phi_{p,r,t}$ is nonlinear and continuous w.r.t. $x^{\pi}_{p,r,t}$.*
5. *We set $\alpha^{\text{min\_quant}}_{p,r,t} = 0$. More precisely, given $|P| = 1$, either there is a maximum price $\alpha^{\text{max\_price}}_{p,r,t}$ so that $\phi_{p,r,t}(\alpha^{\text{max\_price}}_{p,r,t}) = 0$ or, in case the model does not include the consumer's maximum price, $\phi_{p,r,t}(x^{\pi}_{p,r,t}) \to 0$ for $x^{\pi}_{p,r,t} \to \infty$.*
6. *In addition to the continuity of the demand function, $\phi_{p,r,t}$ is differentiable w.r.t. $x^{\pi}_{p,r,t}$.*
7. *$\phi_{p,r,t}$ satisfies the characteristics of demand 3.1 to 3.10 defined in section 3.*

As stated in section 3.1, petrochemical products are commodities and, hence, are offered, required, and purchased in large quantities of standard quality, thus we assume a continuous demand-price dependency. Moreover, we assume that the demand function satisfies the *law of demand*, i.e., it is decreasing. Its nonlinearity is due to the distinct consumer's behavior in the different price ranges.
As mentioned in section 4.3 the structure of the supply-demand trade network optimization model proposed in chapter 4.2 requires the inclusion of additional modeling aspects to prevent the problem from becoming unbounded. Therefore, we assume that $\phi_{p,r,t}$ converges to zero for high prices or that there is a maximum price that indicates the consumer's maximum willingness to pay. Otherwise, the optimum quantity can become infinitesimally small, sold at an infinitely high price. In addition, including a saturation quantity ensures that consumption is not infinite if prices are close to zero. In doing so, no additional constraints limiting the price are necessary in the optimization problem.
So far, the optimization model is deterministic in order to keep the complexity of the

[2]For instance, data about the budgets of firms which require petrochemical products is rarely available. Likewise, information concerning their subsequent production processes is not available.

optimization methods simple. Therefore, we do not include stochastic components as, for example, Domencich and McFadden [DM96] proposed in their explicit modeling for travel demand. Likewise, we require differentiability of the demand function. Consequently, we are able to solve the network optimization problem described in section 4.2 with optimization methods based on derivatives. Concerning the dynamic aspects, we include the specific time-dependent influence on demand in the parameter identification process (see chapter 7).
Note that some of these properties were already discussed or required in the characteristics of demand 3.1 to 3.10. However, we would like to put emphasis on properties as differentiability, nonlinearity, monotonicity, and dependency on time, because they are fundamental in our approach to modeling. In general, there are multiple options to determine a parametric demand model that satisfies the characteristics mentioned above:

- choose a suitable nonlinear function, or
- construct a suitable function by matching appropriate piecewise defined functions.

Since figure 3.1 in section 3.4 resembles to a class of functions consisting of different piecewise defined functions in each price region, the concept of piecewise defined models initially seems appropriate to explicitly model the demand-price relation. However, this approach to modeling is in general not appropriate due to several reasons outlined in the following. Above all, such approaches implicate a high number of parameters and are not necessarily differentiable.[3]
Alternatively, another option is to replace the linear terms in the second price range with a nonlinear function and to impose the condition of differentiability at the respective boundary points. However, the question arises why we do not take advantage out of a nonlinear function $\phi_{p,r,t}(x^{\pi}_{p,r,t})$ that displays the shape we have in mind for the demand, i.e., a function with two points of deflection and convergence if $x^{\pi}_{p,r,t} \to \infty$. For instance, the *hyperbolic tangent* function seems appropriate. In the following section, we show that it can be adapted to satisfy these properties as well as the assumptions 6.1. Moreover, such a modeling gets by with less parameters. For example, the saturation quantity in case of low prices is well reflected (see also section 6.2). This simplifies the parameter identification but also the interpretation of the parameters.[4]

6.2 The Tanh-Demand Model

This section contains the presentation of our approach to modeling demand that is applicable to the supply-demand trade network optimization model described in section 4.2. To begin with, we concentrate on the demand-price relation by separately considering

[3]This, in combination with the current data availability, complicates a parameter identification. However, by means of sufficient data, a piecewise linear function can provide an adequate approximation of real demand, which also can have kinks.

[4]Note that the hyperbolic function can also be expressed in terms of the exponential function, which provides a basis for many mathematical approaches to modeling. We prefer the hyperbolic tangent, because its parameters allow intuitive interpretation (see below).

a single petrochemical product and neglect the effects of prices of substitutes and complements as well as economic factors on demand in section 6.2.1. Accordingly, section 6.2.2 provides an extended model including economic factors. In addition, the inclusion of dependencies on substitutes and complements is examined in section 6.2.3.

6.2.1 Modeling Dependencies on the Product's Price

Since we assume that demand is nonlinear in prices the way described in section 3.4 (cf. figure 3.1), we select the negative hyperbolic tangent function as starting point for the demand model. Therefore, given $|P| = 1$, we set up the following basic model

$$\phi_{p,r,t}(x^{\pi}_{p,r,t}) = \max\left[\lambda_1^{\phi_{p,r,t}} \cdot \tanh\left(\frac{\lambda_2^{\phi_{p,r,t}} - x^{\pi}_{p,r,t}}{\lambda_3^{\phi_{p,r,t}}}\right) + \lambda_4^{\phi_{p,r,t}}, 0\right], \tag{6.1}$$

where $\phi_{p,r,t}(x^{\pi}_{p,r,t})\colon \mathbb{R}_0^+ \to \mathbb{R}_0^+$ and $\lambda_3^{\phi_{p,r,t}} > 0$. Furthermore, we assume that $\lambda_i^{\phi_{p,r,t}} \geq 0,\ i = 1, 2, 4$. This parameterization has some advantages regarding the interpretation of the values: to be more precise, we can relate the consumer's saturated demand quantity $\alpha^{\text{max\_quant}}_{p,r,t}$ and the consumer's maximum willingness to pay $\alpha^{\text{max\_price}}_{p,r,t}$, which we have both introduced in section 3.4, to the proposed parameters. First, since

$$\phi_{p,r,t}(0) = \lambda_1^{\phi_{p,r,t}} \cdot \tanh\left(\frac{\lambda_2^{\phi_{p,r,t}}}{\lambda_3^{\phi_{p,r,t}}}\right) + \lambda_4^{\phi_{p,r,t}},$$

we derive

$$\phi_{p,r,t}(0) = \alpha^{\text{max\_quant}}_{p,r,t} < \lambda_1^{\phi_{p,r,t}} + \lambda_4^{\phi_{p,r,t}} \quad \text{since } \tanh\left(\frac{\lambda_2^{\phi_{p,r,t}}}{\lambda_3^{\phi_{p,r,t}}}\right) < 1. \tag{6.2}$$

Thus, $\lambda_1^{\phi_{p,r,t}} + \lambda_4^{\phi_{p,r,t}}$ provides an upper bound for the consumer's saturated demand quantity. Likewise, given that $\lambda_4^{\phi_{p,r,t}} < \lambda_1^{\phi_{p,r,t}}$, we have $\phi_{p,r,t}(\alpha^{\text{max\_price}}_{p,r,t}) = 0$, where

$$\alpha^{\text{max\_price}}_{p,r,t} = \lambda_2^{\phi_{p,r,t}} - \lambda_3^{\phi_{p,r,t}} \cdot \text{artanh}\left(\frac{-\lambda_4^{\phi_{p,r,t}}}{\lambda_1^{\phi_{p,r,t}}}\right) = \lambda_2^{\phi_{p,r,t}} + \lambda_3^{\phi_{p,r,t}} \cdot \text{artanh}\left(\frac{\lambda_4^{\phi_{p,r,t}}}{\lambda_1^{\phi_{p,r,t}}}\right) < \infty. \tag{6.3}$$

In the following, we check if the proposed model (6.1) satisfies the basic price-related characteristics summarized in assumptions 6.1 and adapt the model to the requirements if necessary.[5] Since $\lambda_i^{\phi_{p,r,t}}$ depends on time t for each $i \in \{1, \cdots, 4\}$, we make sure that the demand function $\phi_{p,r,t}$ changes in the course of time. Obviously, the demand function $\phi_{p,r,t}$ is nonlinear and continuous w.r.t. $x^{\pi}_{p,r,t}$. Next, we examine the demand at high prices. If $\lambda_4^{\phi_{p,r,t}} > \lambda_1^{\phi_{p,r,t}}$,

$$\lim_{x^{\pi}_{p,r,t} \to \infty} \phi_{p,r,t}(x^{\pi}_{p,r,t}) = \lambda_4^{\phi_{p,r,t}} - \lambda_1^{\phi_{p,r,t}} > 0,$$

[5] Note that, so far, we concentrate on the demand's dependency on own prices and integrate economic factors as well as the effects of substitutes and complements afterwards.

which contradicts the assumption 6.1. Thus, we have to require $\lambda_4^{\phi_{p,r,t}} \leq \lambda_1^{\phi_{p,r,t}}$ in the modeling approach.
However, given $\lambda_4^{\phi_{p,r,t}} \leq \lambda_1^{\phi_{p,r,t}}$ our proposed model (6.1) is not differentiable at

$$x_{p,r,t}^{\pi} = \lambda_2^{\phi_{p,r,t}} + \lambda_3^{\phi_{p,r,t}} \cdot \operatorname{artanh}\left(\frac{\lambda_4^{\phi_{p,r,t}}}{\lambda_1^{\phi_{p,r,t}}}\right).$$

Consequently, to fulfill the assumption of demand's differentiability with respect to prices we have to restrict the domain of $\phi_{p,r,t}(x_{p,r,t}^{\pi})$. Given $\lambda_4^{\phi_{p,r,t}} \leq \lambda_1^{\phi_{p,r,t}}$, $\phi_{p,r,t}(x_{p,r,t}^{\pi}) \geq 0$ if

$$x_{p,r,t}^{\pi} \leq \lambda_2^{\phi_{p,r,t}} - \lambda_3^{\phi_{p,r,t}} \cdot \operatorname{artanh}\left(\frac{-\lambda_4^{\phi_{p,r,t}}}{\lambda_1^{\phi_{p,r,t}}}\right) = \lambda_2^{\phi_{p,r,t}} + \lambda_3^{\phi_{p,r,t}} \cdot \operatorname{artanh}\left(\frac{\lambda_4^{\phi_{p,r,t}}}{\lambda_1^{\phi_{p,r,t}}}\right).$$

Thus, $\phi_{p,r,t}(x_{p,r,t}^{\pi})$ is differentiable at the interval $(0, \lambda_2^{\phi_{p,r,t}} + \lambda_3^{\phi_{p,r,t}} \cdot \operatorname{artanh}(\lambda_4^{\phi_{p,r,t}}/\lambda_1^{\phi_{p,r,t}}))$. In addition, given $\lambda_4^{\phi_{p,r,t}} < \lambda_1^{\phi_{p,r,t}}$, the left-sided limit of the derivative exists for $x_{p,r,t}^{\pi} \nearrow \alpha_{p,r,t}^{\text{max\_price}}$ and is equal to $\frac{\partial \phi_{p,r,t}}{\partial x_{p,r,t}^{\pi}}(\alpha_{p,r,t}^{\text{max\_price}})$. Likewise, if $x_{p,r,t}^{\pi} \searrow 0$, the right-sided limit of the derivative exists and is equal to $\frac{\partial \phi_{p,r,t}}{\partial x_{p,r,t}^{\pi}}(0)$. Thus, we set

$$D_{1,p,r,t} := \begin{cases} \left[0, \lambda_2^{\phi_{p,r,t}} + \lambda_3^{\phi_{p,r,t}} \cdot \operatorname{artanh}\left(\frac{\lambda_4^{\phi_{p,r,t}}}{\lambda_1^{\phi_{p,r,t}}}\right)\right] & \text{if } \lambda_4^{\phi_{p,r,t}} < \lambda_1^{\phi_{p,r,t}} \\ \mathbb{R}_0^+ & \text{if } \lambda_4^{\phi_{p,r,t}} = \lambda_1^{\phi_{p,r,t}}. \end{cases} \tag{6.4}$$

Consequently,

$$\phi_{p,r,t}(x_{p,r,t}^{\pi}) \colon D_{1,p,r,t} \to D_{2,p,r,t},$$

where

$$D_{2,p,r,t} := \begin{cases} \left[0, \lambda_1^{\phi_{p,r,t}} \cdot \tanh\left(\frac{\lambda_2^{\phi_{p,r,t}}}{\lambda_3^{\phi_{p,r,t}}}\right) + \lambda_4^{\phi_{p,r,t}}\right] & \text{if } \lambda_4^{\phi_{p,r,t}} < \lambda_1^{\phi_{p,r,t}} \\ \left(0, \lambda_1^{\phi_{p,r,t}} \cdot \tanh\left(\frac{\lambda_2^{\phi_{p,r,t}}}{\lambda_3^{\phi_{p,r,t}}}\right) + \lambda_4^{\phi_{p,r,t}}\right] & \text{if } \lambda_4^{\phi_{p,r,t}} = \lambda_1^{\phi_{p,r,t}}, \end{cases} \tag{6.5}$$

is differentiable. It remains to examine the accordance with the characteristics of demand 3.1 and 3.3 defined in section 3. Since

$$\frac{\partial \phi_{p,r,t}}{\partial x_{p,r,t}^{\pi}}(x_{p,r,t}^{\pi}) = \left(\frac{-\lambda_1^{\phi_{p,r,t}}}{\lambda_3^{\phi_{p,r,t}}}\right) \cdot \operatorname{sech}^2\left(\frac{\lambda_2^{\phi_{p,r,t}} - x_{p,r,t}^{\pi}}{\lambda_3^{\phi_{p,r,t}}}\right) \leq 0$$

for $\lambda_1^{\phi_{p,r,t}}/\lambda_3^{\phi_{p,r,t}} \geq 0$, the model is decreasing in the price. Moreover,

$$0 \leq \phi_{p,r,t}(x_{p,r,t}^{\pi}) \leq \alpha_{p,r,t}^{\text{max\_quant}}$$

if $\alpha_{p,r,t}^{\text{max\_quant}} = \phi_{p,r,t}(0) = \lambda_1^{\phi_{p,r,t}} \cdot \tanh(\lambda_2^{\phi_{p,r,t}}/\lambda_3^{\phi_{p,r,t}}) + \lambda_4^{\phi_{p,r,t}}$. Thus, $\phi_{p,r,t}$ satisfies the characteristics of demand 3.3. Hence, we are able to establish the following theorem for the demand model.

Theorem 6.1. <u>*Demand model*</u>
Under the assumption that the influence of the economic situation is equal to zero and all products p are required independently from each other, the demand model given by $\phi_{p,r,t}(x^{\pi}_{p,r,t})\colon D_{1,p,r,t} \to D_{2,p,r,t}$,

$$\phi_{p,r,t}(x^{\pi}_{p,r,t}) = \lambda_1^{\phi_{p,r,t}} \cdot \tanh\left(\frac{\lambda_2^{\phi_{p,r,t}} - x^{\pi}_{p,r,t}}{\lambda_3^{\phi_{p,r,t}}}\right) + \lambda_4^{\phi_{p,r,t}} \tag{6.6}$$

and $\alpha^{\text{max\_quant}}_{p,r,t} = \lambda_1^{\phi_{p,r,t}} \cdot \tanh(\lambda_2^{\phi_{p,r,t}}/\lambda_3^{\phi_{p,r,t}}) + \lambda_4^{\phi_{p,r,t}}$ *satisfies the characteristics of a demand function stated in assumption 6.1 if*

$$0 \leq \lambda_2^{\phi_{p,r,t}},\ 0 < \lambda_3^{\phi_{p,r,t}},\ 0 \leq \lambda_4^{\phi_{p,r,t}} \leq \lambda_1^{\phi_{p,r,t}}.$$

In the following, we refer to equation (6.6) as *tanh-demand model.* An exemplary illustration of this model is shown in figure 6.2, together with the special case described in the following remark.

Remark 6.1. If, in some application of our optimization model, there is no need to model the demand close to zero consumption, a special case/simplification of the *tanh-demand model* can be used to reduce the number of parameters: Setting $\lambda_4^{\phi_{p,r,t}} = 0$, the demand function reduces to

$$\phi^{A}_{p,r,t}(x^{\pi}_{p,r,t}) = \lambda_1^{\phi_{p,r,t}} \cdot \tanh((\lambda_2^{\phi_{p,r,t}} - x^{\pi}_{p,r,t})/\lambda_3^{\phi_{p,r,t}}), \tag{6.7}$$

where $\phi_{p,r,t}(x^{\pi}_{p,r,t})\colon [0, \lambda_2^{\phi_{p,r,t}}] \to [0, \lambda_1^{\phi_{p,r,t}} \cdot \tanh(\lambda_2^{\phi_{p,r,t}}/\lambda_3^{\phi_{p,r,t}})]$. Likewise, $\alpha^{\text{max\_quant}}_{p,r,t} = \lambda_1^{\phi_{p,r,t}} \cdot \tanh(\lambda_2^{\phi_{p,r,t}}/\lambda_3^{\phi_{p,r,t}})$ and $\alpha^{\text{max\_price}}_{p,r,t} = \lambda_2^{\phi_{p,r,t}}$.
Thus, if the domain of the demand function is restricted in the optimization model, $\lambda_4^{\phi_{p,r,t}}$ can become redundant. This version is denoted by $\phi^{A}_{p,r,t}$ and is also illustrated in figure 6.2. In the following, we refer to equation (6.7) as *tanh-demand model A*.

Example 6.1. *To present an example of the tanh-demand model in figure 6.2 we set* $\lambda_1^{\phi_{p,r,t}} = 200$, $\lambda_2^{\phi_{p,r,t}} = 300$, $\lambda_3^{\phi_{p,r,t}} = 50$ *and* $\lambda_4^{\phi_{p,r,t}} = 190$. *Likewise, we select the following values* $\lambda_1^{\phi_{p,r,t}} = 390$, $\lambda_2^{\phi_{p,r,t}} = 300$ *and* $\lambda_3^{\phi_{p,r,t}} = 50$ *to illustrate tanh-demand model A.*

In the following, we integrate the change of the economic situation (section 6.2.2) and the effects of other products' prices (section 6.2.3.1) separately from each other in the basic demand model proposed in theorem 6.1.

6.2.2 Modeling Dependencies on Economic Factors

In the next step, we include the influence of the economic development on the demand. Therefore, we select two macroeconomic time series that represent well the economic

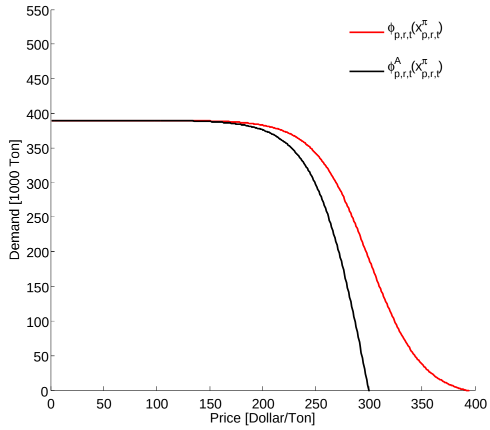

Figure 6.2: Illustration of *tanh-demand model* and *tanh-demand model A* that both reflect the nonlinear relationship between demand and price

development from our point of view: the gross domestic product (GDP) and an index representing the state of industrial production (IndPro).[6] That means, we set

$$\boldsymbol{\Delta a^{\zeta}}_{r,t,J} := (\Delta a^{\text{GDP}}_{r,t,J}, \Delta a^{\text{IndPro}}_{r,t,J}).$$

To include these economic factors in the model we make the following assumption.

Assumptions 6.2. *Inclusion of economic data in the demand function*
The change of GDP influences the willingness to pay and the change of an index for industrial production influences the quantities in demand.

Consequently, our model function (6.6) turns into

$$\phi^{\text{eco}}_{p,r,t}(x^{\pi}_{p,r,t}) =$$
$$(\lambda_1^{\phi_{p,r,t}} + \lambda_{\text{IndPro}}^{\phi_{p,r,t}} \cdot \Delta a^{\text{IndPro}}_{r,t,J}) \cdot \tanh\left(\frac{\lambda_2^{\phi_{p,r,t}} + \lambda_{\text{GDP}}^{\phi_{p,r,t}} \cdot \Delta a^{\text{GDP}}_{r,t,J} - x^{\pi}_{p,r,t}}{\lambda_3^{\phi_{p,r,t}}}\right) + \lambda_4^{\phi_{p,r,t}}, \quad (6.8)$$

where $\lambda_{\text{GDP}}^{\phi_{p,r,t}} \geq 0$ and $\lambda_{\text{IndPro}}^{\phi_{p,r,t}} \geq 0$. The superscript eco indicates that the economic factors are included in the explicit demand model. In doing so, the relation of parameters to consumer's saturated demand quantity $\alpha^{\text{max\_quant}}_{p,r,t}$ and the consumer's maximum willingness to pay $\alpha^{\text{max\_price}}_{p,r,t}$ changes into

$$\alpha^{\text{max\_quant}}_{p,r,t} < \lambda_1^{\phi_{p,r,t}} + \lambda_{\text{IndPro}}^{\phi_{p,r,t}} \cdot \Delta a^{\text{IndPro}}_{r,t,J} + \lambda_4^{\phi_{p,r,t}} \quad (6.9)$$

[6]To compare, we refer to Pindyck [Pin79] who investigated the structure of energy demand. He emphasized that the causal relationship between macroeconomic indices and energy demand is mutual, i.e., energy growth also influences the GDP growth.

since $\tanh((\lambda_2^{\phi_{p,r,t}} + \lambda_{\text{GDP}}^{\phi_{p,r,t}} \cdot \Delta a_{r,t,J}^{\text{GDP}})/\lambda_3^{\phi_{p,r,t}}) < 1$ and, provided that $\lambda_4^{\phi_{p,r,t}} < \lambda_1^{\phi_{p,r,t}}$,

$$\alpha_{p,r,t}^{\text{max\_price}} = \lambda_2^{\phi_{p,r,t}} + \lambda_{\text{GDP}}^{\phi_{p,r,t}} \cdot \Delta a_{r,t,J}^{\text{GDP}} + \lambda_3^{\phi_{p,r,t}} \cdot \text{artanh}\left(\frac{\lambda_4^{\phi_{p,r,t}}}{\lambda_1^{\phi_{p,r,t}} + \lambda_{\text{IndPro}}^{\phi_{p,r,t}} \cdot \Delta a_{r,t,J}^{\text{IndPro}}}\right). \tag{6.10}$$

In analogy with theorem 6.1, we define

$$D_{1,p,r,t}^{eco} := \begin{cases} \left[0, d_{1,p,r,t}^{eco}\right] & \text{if} \lambda_4^{\phi_{p,r,t}} < \lambda_1^{\phi_{p,r,t}}, \\ \mathbb{R}_0^+ & \text{if} \lambda_4^{\phi_{p,r,t}} = \lambda_1^{\phi_{p,r,t}}, \end{cases} \tag{6.11}$$

where

$$d_{1,p,r,t}^{eco} : = \lambda_2^{\phi_{p,r,t}} + \lambda_{\text{GDP}}^{\phi_{p,r,t}} \cdot \Delta a_{r,t,J}^{\text{GDP}} + \lambda_3^{\phi_{p,r,t}} \cdot \text{artanh}\left(\frac{\lambda_4^{\phi_{p,r,t}}}{\lambda_1^{\phi_{p,r,t}} + \lambda_{\text{IndPro}}^{\phi_{p,r,t}} \cdot \Delta a_{r,t,J}^{\text{IndPro}}}\right), \tag{6.12}$$

and

$$D_{2,p,r,t}^{eco} := \begin{cases} \left[0, d_{2,p,r,t}^{eco}\right] & \text{if} \lambda_4^{\phi_{p,r,t}} < \lambda_1^{\phi_{p,r,t}}, \\ \left(0, d_{2,p,r,t}^{eco}\right] & \text{if} \lambda_4^{\phi_{p,r,t}} = \lambda_1^{\phi_{p,r,t}}, \end{cases} \tag{6.13}$$

where

$$d_{2,p,r,t}^{eco} := (\lambda_1^{\phi_{p,r,t}} + \lambda_{\text{IndPro}}^{\phi_{p,r,t}} \cdot \Delta a_{r,t,J}^{\text{IndPro}}) \cdot \tanh\left(\frac{\lambda_2^{\phi_{p,r,t}} + \lambda_{\text{GDP}}^{\phi_{p,r,t}} \cdot \Delta a_{r,t,J}^{\text{GDP}}}{\lambda_3^{\phi_{p,r,t}}}\right) + \lambda_4^{\phi_{p,r,t}}, \tag{6.14}$$

to establish the following theorem.

Theorem 6.2. *Demand model including the influence of the economic situation*
The demand model comprising the influence of the economic situation given by $\phi_{p,r,t}^{\text{eco}} : D_{1,p,r,t}^{eco} \to D_{2,p,r,t}^{eco}$,

$$\phi_{p,r,t}^{\text{eco}}(x_{p,r,t}^{\pi}) = (\lambda_1^{\phi_{p,r,t}} + \lambda_{\text{IndPro}}^{\phi_{p,r,t}} \cdot \Delta a_{r,t,J}^{\text{IndPro}}) \cdot \tanh\left(\frac{\lambda_2^{\phi_{p,r,t}} + \lambda_{\text{GDP}}^{\phi_{p,r,t}} \cdot \Delta a_{r,t,J}^{\text{GDP}} - x_{p,r,t}^{\pi}}{\lambda_3^{\phi_{p,r,t}}}\right) + \lambda_4^{\phi_{p,r,t}} \tag{6.15}$$

with

$$\alpha_{p,r,t}^{\text{max\_quant}} = (\lambda_1^{\phi_{p,r,t}} + \lambda_{\text{IndPro}}^{\phi_{p,r}} \cdot \Delta a_{r,t,J}^{\text{IndPro}}) \cdot \tanh\left(\frac{\lambda_2^{\phi_{p,r,t}} + \lambda_{\text{GDP}}^{\phi_{p,r,t}} \cdot \Delta a_{r,t,J}^{\text{GDP}}}{\lambda_3^{\phi_{p,r,t}}}\right) + \lambda_4^{\phi_{p,r,t}}$$

satisfies the assumptions 6.1 if

$$\lambda_1^{\phi_{p,r,t}} + \lambda_{\text{IndPro}}^{\phi_{p,r,t}} \cdot \Delta a_{r,t,J}^{\text{IndPro}} \geq \lambda_4^{\phi_{p,r,t}} \geq 0,$$
$$\lambda_2^{\phi_{p,r,t}} + \lambda_{\text{GDP}}^{\phi_{p,r,t}} \cdot \Delta a_{r,t,J}^{\text{GDP}} \geq 0,$$
$$\lambda_3^{\phi_{p,r,t}} \geq 0,$$
$$\lambda_{\text{GDP}}^{\phi_{p,r,t}} \geq 0,$$
$$\lambda_{\text{IndPro}}^{\phi_{p,r,t}} \geq 0.$$

Proof: It remains to verify that our model approach satisfies the characteristics of demand 3.1 and 3.2. First, we have

$$\frac{\partial \phi^{\text{eco}}_{p,r,t}}{\partial x^{\pi}_{p,r,t}}(x^{\pi}_{p,r,t}) = \\ \frac{-(\lambda_1^{\phi_{p,r,t}} + \lambda_{\text{IndPro}}^{\phi_{p,r,t}} \cdot \Delta a^{\text{IndPro}}_{r,t,J})}{\lambda_3^{\phi_{p,r,t}}} \cdot \operatorname{sech}^2\left(\frac{\lambda_2^{\phi_{p,r,t}} + \lambda_{\text{GDP}}^{\phi_{p,r,t}} \cdot \Delta a^{\text{GDP}}_{r,t,J} - x^{\pi}_{p,r,t}}{\lambda_3^{\phi_{p,r,t}}}\right) \leq 0$$

since $\frac{\lambda_1^{\phi_{p,r,t}} + \lambda_{\text{IndPro}}^{\phi_{p,r,t}} \cdot \Delta a^{\text{IndPro}}_{r,t,J}}{\lambda_3^{\phi_{p,r,t}}} \geq 0$. Furthermore,

$$\frac{\partial \phi^{\text{eco}}_{p,r,t}}{\partial \Delta a^{\text{IndPro}}_{r,t,J}}(x^{\pi}_{p,r,t}) = \lambda_{\text{IndPro}}^{\phi_{p,r,t}} \cdot \tanh\left(\frac{\lambda_2^{\phi_{p,r,t}} + \lambda_{\text{GDP}}^{\phi_{p,r,t}} \cdot \Delta a^{\text{GDP}}_{r,t,J} - x^{\pi}_{p,r,t}}{\lambda_3^{\phi_{p,r,t}}}\right) \geq 0$$

since $\lambda_{\text{IndPro}}^{\phi_{p,r,t}} \geq 0$ and $\lambda_1^{\phi_{p,r,t}} + \lambda_{\text{IndPro}}^{\phi_{p,r,t}} \cdot \Delta a^{\text{IndPro}}_{r,t,J} \geq 0$. Likewise,

$$\frac{\partial \phi^{\text{eco}}_{p,r,t}}{\partial \Delta a^{\text{GDP}}_{r,t,J}}(x^{\pi}_{p,r,t}) = \\ \frac{\lambda_{\text{GDP}}^{\phi_{p,r,t}} \cdot (\lambda_1^{\phi_{p,r,t}} + \lambda_{\text{IndPro}}^{\phi_{p,r,t}} \cdot \Delta a^{\text{IndPro}}_{r,t,J})}{\lambda_3^{\phi_{p,r,t}}} \cdot \operatorname{sech}^2\left(\frac{\lambda_2^{\phi_{p,r,t}} + \lambda_{\text{GDP}}^{\phi_{p,r,t}} \cdot \Delta a^{\text{GDP}}_{r,t,J} - x^{\pi}_{p,r,t}}{\lambda_3^{\phi_{p,r,t}}}\right) \geq 0$$

since $\lambda_{\text{GDP}}^{\phi_{p,r,t}} \geq 0$.

In the following, we refer to model (6.15) as *tanh-demand model eco*.

Example 6.2. *Figure 6.3 illustrates tanh-demand model eco (6.15). In this example,* $\lambda_1^{\phi_{p,r,t}} = 200$, $\lambda_2^{\phi_{p,r,t}} = 300$, $\lambda_3^{\phi_{p,r,t}} = 50$, $\lambda_4^{\phi_{p,r,t}} = 190$, $\lambda_{\text{IndPro}}^{\phi_{p,r,t}} \cdot \Delta a^{\text{IndPro}}_{r,t,J} = 40$, *and* $\lambda_{\text{GDP}}^{\phi_{p,r,t}} \cdot \Delta a^{\text{GDP}}_{r,t,J} = 50$.

6.2.3 Modeling Dependencies on Prices of Other Products

The following section comprises the integration of the demand's dependency on substitutes (section 6.2.3.1) and complements (section 6.2.3.2). In doing so, we restrict our modeling approach to the case of two products, i.e., $|P| = 2$, and exclude the economic influence. Whereas the extension to the case of n products is straightforward for complements (cf. section 3.6), modeling demand in case of n substitutes requires further examination of the respective dependencies. However, this is beyond the scope of the thesis.

6.2.3.1 Substitutes

In this section, we transfer the general modeling approach for two substitutable products proposed in section 3.5 to the explicit *tanh-demand model*. Under the assumption

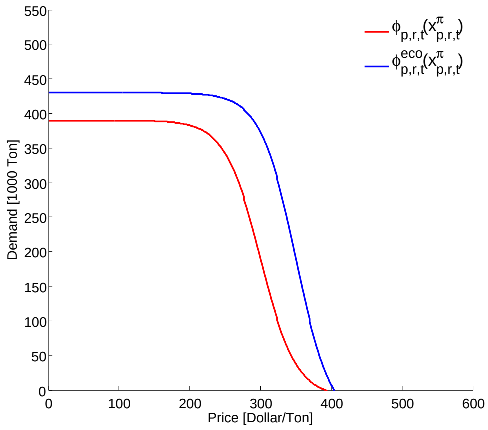

Figure 6.3: Illustration of *tanh-demand model eco* that reflects the nonlinear relationship between demand and price and, in contrast to *tanh-demand model*, includes influences of economic factors

that the sum of all abrupt changes can be covered by modeling gradual substitution, we integrate appropriate splitting functions such that the characteristics of demand 3.8 are satisfied. Note that from now on, we restrict our modeling to positive prices. The following proposition comprises appropriate splitting functions in the case of two substitutable products.

Proposition 6.1. *Let* $\mathcal{P} = \{p_i, p_{3-i}\}$ *be a set of substitutable products with prices* $x^{\pi}_{p_i,r,t} > 0,\ i = 1, 2$. *A rational function of the form*

$$\rho_{p_i}\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right) = \frac{1 + \sum\limits_{k=1}^{m} \binom{n}{k} \left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right)^k}{\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}} + 1\right)^n}, \tag{6.16}$$

where $i = 1, 2$, $n \in \mathbb{N}$, *and* $m = \lfloor 0.5 \cdot n \rfloor$, *satisfies the assumptions 3.11.*

Proof: Obviously, $0 \leq \rho_{p_i}\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right) \leq 1,\ i = 1, 2$. Likewise,

$$\rho_{p_{3-i}}\left(\left(\frac{x^{\pi}_{p_{3-i},r,t}}{x^{\pi}_{p_i,r,t}}\right)^{-1}\right) = \frac{1 + \sum\limits_{k=1}^{m} \binom{n}{k} \left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right)^k}{\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}} + 1\right)^n} = \rho_{p_i}\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right).$$

Moreover, given $m = \lfloor 0.5 \cdot n \rfloor$

$$\rho_{p_i}\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right) + \rho_{p_{3-i}}\left(\frac{x^{\pi}_{p_{3-i},r,t}}{x^{\pi}_{p_i,r,t}}\right)$$

$$=\frac{1+\sum_{k=1}^{m}\binom{n}{k}\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right)^k}{\left(\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right)+1\right)^n}+\frac{1+\sum_{k=1}^{m}\binom{n}{k}\left(\frac{x^{\pi}_{p_{3-i},r,t}}{x^{\pi}_{p_i,r,t}}\right)^k}{\left(\left(\frac{x^{\pi}_{p_{3-i},r,t}}{x^{\pi}_{p_i,r,t}}\right)+1\right)^n}$$

$$=\frac{1+\sum_{k=1}^{m}\binom{n}{k}\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right)^k+\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right)^n+\sum_{k=1}^{m}\binom{n}{k}\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right)^{n-k}}{\left(\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right)+1\right)^n}$$

$$=\frac{1+\sum_{k=1}^{m}\binom{n}{k}\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right)^k+\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right)^n+\sum_{k=m+1}^{n-1}\binom{n}{k}\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right)^{k}}{\left(\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right)+1\right)^n}$$

$$=\frac{\sum_{k=0}^{n}\binom{n}{k}\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right)^k}{\left(\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right)+1\right)^n}=1.$$

As a consequence, if $x^{\pi}_{p_i,r,t}=x^{\pi}_{p_{3-i},r,t}$,

$$\rho_{p_i}(1)=\rho_{p_{3-i}}(1)=1-\rho_{p_i}(1).$$

Thus, $\rho_{p_i}(1)=\rho_{p_{3-i}}(1)=\frac{1}{2}$.

Example 6.3. *Inserting $n=3$, equation (6.4) implies*

$$\rho_{p_i}\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right)=\frac{1+3\cdot\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right)}{\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}+1\right)^3},\quad i=1,2, \tag{6.17}$$

and given $n=5$, we obtain

$$\rho_{p_i}\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right)=\frac{1+5\cdot\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right)+10\cdot\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right)^2}{\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}+1\right)^5},\quad i=1,2. \tag{6.18}$$

We illustrate the shape of these splitting functions in figure 6.4 as well as the splitting functions for $n=15$ and $n=19$. Note that for small n the fraction that is associated with the more expensive product decreases slower than for large n.

Based on equation (3.26), which is established in the characteristics of demand 3.8, the substitutable demand $\phi^{\text{sub}}_{p_i,r,t}$, $i=1,2$, is composed of the demand that can be satisfied

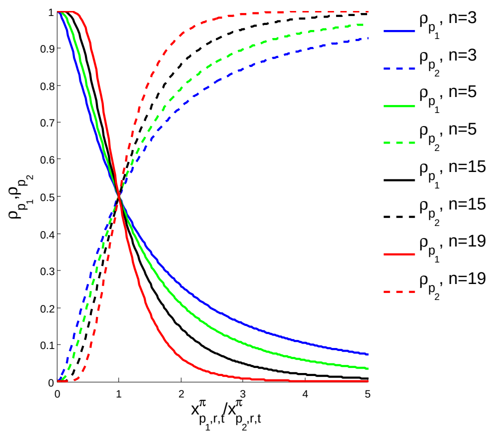

Figure 6.4: Illustration of the splitting functions (6.16) for $n = 3$, $n = 5$, $n = 15$, and $n = 19$ that indicate the allocation of the substitutable demand for two products p_1 and p_2 dependent on their prices.

by all substitutes and a basic demand only associated with p_i

$$\phi^{\text{sub}}_{p_i,r,t}(x^{\pi}_{p_i,r,t}, x^{\pi}_{p_{3-i},r,t}) = \rho_{p_i}\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right) \cdot \phi_{\mathcal{P},r,t}(x^{\pi}_{p_i,r,t}, x^{\pi}_{p_{3-i},r,t}) + \phi^{b}_{p_i,r,t}(x^{\pi}_{p_i,r,t}), \quad (6.19)$$

where $i = 1, 2$. Assuming that the substitutable demand is independent of all other products $p_j \neq p_i,\ i = 1, 2$, we can write the demand as function of $p_i,\ i = 1, 2$. Since the splitting function is not defined for $x^{\pi}_{p_i,r,t} = 0,\ i = 1, 2$, we restrict the domain of $\phi^{\text{sub}}_{p_i,r,t} \colon (x^{\pi}_{p_i,r,t}, x^{\pi}_{p_{3-i},r,t}) \mapsto \phi^{\text{sub}}_{p_i,r,t}(x^{\pi}_{p_i,r,t}, x^{\pi}_{p_{3-i},r,t}),\ i = 1, 2$, to $D^{\text{sub}}_{1,p_i,r,t}$, where

$$D^{\text{sub}}_{1,p_i,r,t} := \Big((D_{1,\mathcal{P},r,t} \setminus (0,0)) \cap \Big(D^{b}_{1,p_i,r,t} \times [0,\infty) \Big) \Big). \quad (6.20)$$

Note that $D^{b}_{1,p_i,r,t}$ is established according to equation (6.4). Correspondingly, given $\lambda_4^{\phi_{\mathcal{P},r,t}} = \lambda_1^{\phi_{\mathcal{P},r,t}}$ and $\lambda_4^{\phi^b_{p,r,t}} = \lambda_1^{\phi^b_{p,r,t}}$, we define

$$d^{sub}_{2,p_i,r,t} := \lambda_1^{\phi_{\mathcal{P},r,t}} \cdot \tanh\left(\frac{\lambda_2^{\phi_{\mathcal{P},r,t}}}{\lambda_3^{\phi_{\mathcal{P},r,t}}}\right) + \lambda_4^{\phi_{\mathcal{P},r,t}} + \lambda_1^{\phi^b_{p,r,t}} \cdot \tanh\left(\frac{\lambda_2^{\phi^b_{p,r,t}}}{\lambda_3^{\phi^b_{p,r,t}}}\right) + \lambda_4^{\phi^b_{p,r,t}},\ i = 1, 2, \quad (6.21)$$

and obtain

$$D^{\text{sub}}_{2,p_i,r,t} := \begin{cases} \big(0, d^{sub}_{2,p_i,r,t}\big) & \text{if } \lambda_4^{\phi_{\mathcal{P},r,t}} = \lambda_1^{\phi_{\mathcal{P},r,t}} \text{ and } \lambda_4^{\phi^b_{p,r,t}} = \lambda_1^{\phi^b_{p,r,t}} \\ \big[0, d^{sub}_{2,p_i,r,t}\big) & \text{otherwise.} \end{cases} \quad (6.22)$$

Concerning the modeling of $\phi_{\mathcal{P},r,t}(x^{\pi}_{p_i,r,t}, x^{\pi}_{p_{3-i},r,t})$, the following assumptions hold.

Assumptions 6.3. Modeling approach for the substitutable demand
So far, we have not specified the dependence of $\phi_{\mathcal{P},r,t}$ on the prices $x^{\pi}_{p_i,r,t}$ and $x^{\pi}_{p_{3-i},r,t}$. In general, we assume that demand is high if at least one of these prices is low and decreases if both prices increase. Therefore, we set

$$\phi_{\mathcal{P},r,t}(x^{\pi}_{p_i,r,t}, x^{\pi}_{p_{3-i},r,t}) = \lambda_1^{\phi_{\mathcal{P},r,t}} \cdot \tanh\left(\frac{\lambda_2^{\phi_{\mathcal{P},r,t}} - \min(x^{\pi}_{p_i,r,t}, x^{\pi}_{p_{3-i},r,t})}{\lambda_3^{\phi_{\mathcal{P},r,t}}}\right) + \lambda_4^{\phi_{\mathcal{P},r,t}}, \quad (6.23)$$

where

$$D_{1,\mathcal{P},r,t} :=$$
$$\left\{(x^{\pi}_{p_i,r,t}, x_{p_{3-i},r,t}) \in \mathbb{R}_0^+ \times \mathbb{R}_0^+ | \min(x^{\pi}_{p_i,r,t}, x^{\pi}_{p_{3-i},r,t}) \leq \lambda_2^{\phi_{\mathcal{P},r,t}} + \lambda_3^{\phi_{\mathcal{P},r,t}} \cdot \operatorname{artanh}\left(\frac{\lambda_4^{\phi_{\mathcal{P},r,t}}}{\lambda_1^{\phi_{\mathcal{P},r,t}}}\right)\right\}$$

Remark 6.2. This modeling approach for the substitutable demand (6.23) including the min-function does not satisfy the assumption that the demand function is differentiable. Therefore, to apply the demand function for substitutes in the optimization model in section 6.3, we will approximate the min-function by the differentiable function

$$f_{min}(x^{\pi}_{p_i,r,t}, x^{\pi}_{p_{3-i},r,t}) = \frac{1}{2}\left(x^{\pi}_{p_i,r,t} + x^{\pi}_{p_{3-i},r,t} - \sqrt{(x^{\pi}_{p_i,r,t} + x^{\pi}_{p_{3-i},r,t})^2}\right), \ i = 1, 2.$$

Example 6.4. *Let $\mathcal{P} = \{p_1, p_2\}$, $\lambda_1^{\phi_{\mathcal{P},r,t}} = 200$, $\lambda_2^{\phi_{\mathcal{P},r,t}} = 300$, $\lambda_3^{\phi_{\mathcal{P},r,t}} = 200$, $\lambda_4^{\phi_{\mathcal{P},r,t}} = 200$, and $\phi^b_{p_1,r,t} = \phi^b_{p_2,r,t} = 0$. Concerning the splitting function, we select $n = 5$, i.e., equation (6.18).*
Since we model the substitutable demand by means of the min-function (cf. figure 6.7), the following case differentiation is necessary.

$$\frac{\partial \phi_{\mathcal{P},r,t}}{\partial x^{\pi}_{p_{3-i},r,t}} = \begin{cases} 0 & \text{if } x^{\pi}_{p_i,r,t} < x^{\pi}_{p_{3-i},r,t} \\ -\frac{\lambda_1^{\phi_{\mathcal{P},r,t}}}{\lambda_3^{\phi_{\mathcal{P},r,t}}} \cdot \operatorname{sech}^2\left(\frac{\lambda_2^{\phi_{\mathcal{P},r,t}} - x^{\pi}_{p_{3-i},r,t}}{\lambda_3^{\phi_{\mathcal{P},r,t}}}\right) & \text{if } x^{\pi}_{p_i,r,t} > x^{\pi}_{p_{3-i},r,t} \end{cases} \quad (6.24)$$

Obviously, $\phi_{\mathcal{P},r,t}$ is not differentiable at $x^{\pi}_{p_i,r,t} = x^{\pi}_{p_{3-i},r,t}$. The resulting demand functions $\phi^{sub}_{p_1,r,t}$ and $\phi^{sub}_{p_2,r,t}$ are illustrated in figures 6.5 and 6.6. These illustrations reveal that in case $x^{\pi}_{p_i,r,t} > x^{\pi}_{p_{3-i},r,t}$ the demand decreases if the prices exceed a certain level. Figure 6.8 show the respective price combinations for which the derivative with respect to the substitute's price is negative. The red area represents the price combination for which the derivative is negative. Hence, for these prices, the demand decreases if the substitute's price rises.

This example reveals that, in general, our modeling approach does not provide

$$\frac{\partial \phi^{\text{sub}}_{p_i,r,t}}{\partial x^{\pi}_{p_{3-i},r,t}} = \frac{\partial \rho_{p_i}}{\partial x^{\pi}_{p_{3-i},r,t}} \cdot \phi_{\mathcal{P},r,t} + \rho_{p_i} \cdot \frac{\partial \phi_{\mathcal{P},r,t}}{\partial x^{\pi}_{p_{3-i},r,t}} \geq 0, \quad (6.25)$$

which is a characteristic that identifies substitutes (cf. the characteristics of demand 3.9). To conclude, we summarize the results of our investigation in the following theorem.

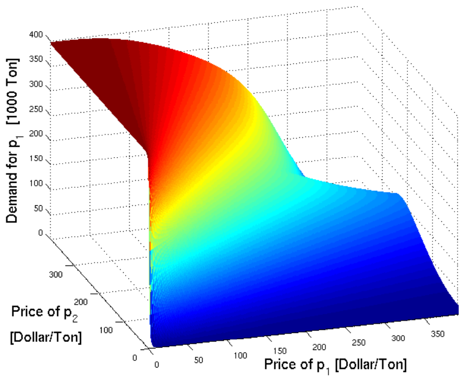

Figure 6.5: Illustration of the demand model $\phi^{sub}_{p_1,r,t}$ (6.19) with parameters given in example 6.4

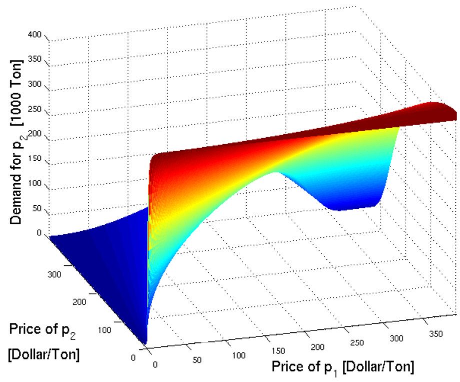

Figure 6.6: Illustration of the demand model $\phi^{sub}_{p_2,r,t}$ (6.19) with parameters given in example 6.4

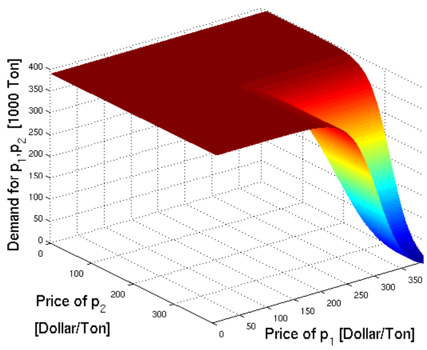

Figure 6.7: Illustration of the model for substitutable demand $\phi_{\mathcal{P},r,t}$ (6.23) with parameters given in example 6.4

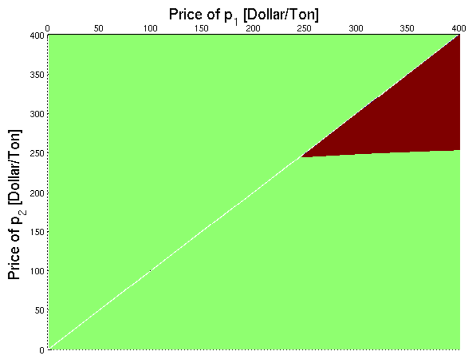

Figure 6.8: Illustration of the conversion of the derivative (6.24) with parameters given in example 6.4

Theorem 6.3. *Demand model for substitutable products*
Let $\mathcal{P} = \{p_i, p_{3-i}\}$ be a set of substitutes. Then, the demand function $\phi^{\text{sub}}_{p_i,r,t} \colon D^{\text{sub}}_{1,p_i,r,t} \to D^{\text{sub}}_{2,p_i,r,t}$,

$$\phi^{\text{sub}}_{p_i,r,t}(x^{\pi}_{p_i,r,t}, x^{\pi}_{p_{3-i},r,t}) = \rho_{p_i}\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right) \cdot \phi_{\mathcal{P},r,t}(x^{\pi}_{p_i,r,t}, x^{\pi}_{p_{3-i},r,t}) + \phi^{b}_{p_i,r,t}(x^{\pi}_{p_i,r,t}) \quad (6.26)$$

satisfies the assumptions 6.1 excluding differentiability at $x^{\pi}_{p_i,r,t} = x^{\pi}_{p_{3-i},r,t}$ if $\phi_{\mathcal{P},r,t}$ and $\phi^{b}_{p_i,r,t}$ fulfill the assumptions given by theorem 6.1 (excluding differentiability of $\phi_{\mathcal{P},r,t}$ at $x^{\pi}_{p_i,r,t} = x^{\pi}_{p_{3-i},r,t}$).

Proof: It remains to verify that $\frac{\partial \phi^{\text{sub}}_{p_i,r,t}}{\partial x^\pi_{p_i,r,t}}\left(x^\pi_{p_i,r,t}, x^\pi_{p_{3-i},r,t}\right) \leq 0$ if $x^\pi_{p_i,r,t} \neq x^\pi_{p_{3-i},r,t}$. We have

$$\frac{\partial \phi^{\text{sub}}_{p_i,r,t}}{\partial x^\pi_{p_i,r,t}} = \frac{\partial \rho_{p_i}}{\partial x^\pi_{p_i,r,t}} \cdot \phi_{\mathcal{P},r,t} + \rho_{p_i} \cdot \frac{\partial \phi_{\mathcal{P},r,t}}{\partial x^\pi_{p_i,r,t}} + \frac{\partial \phi^b_{p_i,r,t}}{\partial x^\pi_{p_i,r,t}},$$

given $x^\pi_{p_i,r,t} \neq x^\pi_{p_{3-i},r,t}$, where

$$\frac{\partial \phi_{\mathcal{P},r,t}}{\partial x^\pi_{p_i,r,t}}\left(x^\pi_{p_i,r,t}, x^\pi_{p_{3-i},r,t}\right) = \begin{cases} 0 & \text{if } x^\pi_{p_{3-i},r,t} < x^\pi_{p_i,r,t} \\ -\frac{\lambda_1^{\phi_{\mathcal{P},r,t}}}{\lambda_3^{\phi_{\mathcal{P},r,t}}} \cdot \operatorname{sech}^2\left(\frac{\lambda_2^{\phi_{\mathcal{P},r,t}} - x^\pi_{p_i,r,t}}{\lambda_3^{\phi_{\mathcal{P},r,t}}}\right) & \text{if } x^\pi_{p_{3-i},r,t} > x^\pi_{p_i,r,t}. \end{cases} \tag{6.27}$$

Thus, to prove that $\frac{\partial \phi^{\text{sub}}_{p_i,r,t}}{\partial x^\pi_{p_i,r,t}}\left(x^\pi_{p_i,r,t}, x^\pi_{p_{3-i},r,t}\right) < 0$ it remains to prove $\frac{\partial \rho_{p_i}}{\partial x^\pi_{p_i,r,t}}\left(\frac{x^\pi_{p_i,r,t}}{x^\pi_{p_{3-i},r,t}}\right) < 0$. We have

$$\begin{aligned}
&\frac{\partial \rho_{p_i}}{\partial x^\pi_{p_i,r,t}}\left(\frac{x^\pi_{p_i,r,t}}{x^\pi_{p_{3-i},r,t}}\right) \\
&= \frac{\left(\frac{x^\pi_{p_i,r,t}}{x^\pi_{p_{3-i},r,t}} + 1\right)^n \cdot \sum_{k=1}^{m} \binom{n}{k} k \frac{(x^\pi_{p_i,r,t})^{k-1}}{(x^\pi_{p_{3-i},r,t})^k}}{\left(\frac{x^\pi_{p_i,r,t}}{x^\pi_{p_{3-i},r,t}} + 1\right)^{2n}} \\
&\qquad - \frac{\left(\frac{x^\pi_{p_i,r,t}}{x^\pi_{p_{3-i},r,t}} + 1\right)^{n-1} \cdot \frac{n}{x^\pi_{p_{3-i},r,t}} \cdot \sum_{k=0}^{m} \binom{n}{k} \left(\frac{x^\pi_{p_i,r,t}}{x^\pi_{p_{3-i},r,t}}\right)^k}{\left(\frac{x^\pi_{p_i,r,t}}{x^\pi_{p_{3-i},r,t}} + 1\right)^{2n}} \\
&= \frac{\left(\frac{x^\pi_{p_i,r,t}}{x^\pi_{p_{3-i},r,t}} + 1\right) \cdot \sum_{k=1}^{m} \binom{n}{k} k \frac{(x^\pi_{p_i,r,t})^{k-1}}{(x^\pi_{p_{3-i},r,t})^k} - \frac{n}{x^\pi_{p_{3-i},r,t}} \cdot \sum_{k=0}^{m} \binom{n}{k} \left(\frac{x^\pi_{p_i,r,t}}{x^\pi_{p_{3-i},r,t}}\right)^k}{\left(\frac{x^\pi_{p_i,r,t}}{x^\pi_{p_{3-i},r,t}} + 1\right)^{n+1}} \\
&= \frac{\left(\frac{x^\pi_{p_i,r,t}}{x^\pi_{p_{3-i},r,t}} + 1\right) \cdot \sum_{k=1}^{m} \binom{n}{k-1} \left(\frac{x^\pi_{p_i,r,t}}{x^\pi_{p_{3-i},r,t}}\right)^{k-1} - n \cdot \sum_{k=0}^{m} \binom{n}{k} \left(\frac{x^\pi_{p_i,r,t}}{x^\pi_{p_{3-i},r,t}}\right)^k}{\left(x^\pi_{p_{3-i},r,t}\right) \cdot \left(\frac{x^\pi_{p_i,r,t}}{x^\pi_{p_{3-i},r,t}} + 1\right)^{n+1}} \\
&= \frac{\left(\frac{x^\pi_{p_i,r,t}}{x^\pi_{p_{3-i},r,t}} + 1\right) \cdot \sum_{k=0}^{m-1} \binom{n}{k} \left(\frac{x^\pi_{p_i,r,t}}{x^\pi_{p_{3-i},r,t}}\right)^k - n \cdot \sum_{k=0}^{m} \binom{n}{k} \left(\frac{x^\pi_{p_i,r,t}}{x^\pi_{p_{3-i},r,t}}\right)^k}{\left(x^\pi_{p_{3-i},r,t}\right) \cdot \left(\frac{x^\pi_{p_i,r,t}}{x^\pi_{p_{3-i},r,t}} + 1\right)^{n+1}}
\end{aligned}$$

$$= \frac{\sum_{k=0}^{m-1}\binom{n}{k}\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right)^{k+1} + \sum_{k=0}^{m-1}\binom{n}{k}\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right)^{k} - n\cdot\sum_{k=0}^{m}\binom{n}{k}\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right)^{k}}{\left(x^{\pi}_{p_{3-i},r,t}\right)\cdot\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}+1\right)^{n+1}}.$$

Since the prices are positive, only the numerator can be checked for negativity. We check this by equating coefficients of $\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right)^{\varepsilon}$, $\varepsilon = 0,\ldots,m$. We obtain

$$\begin{aligned}
\varepsilon = 0: \quad & 1-n<0\\
\varepsilon = 1,\ldots,m-1: \quad & \binom{n}{\varepsilon-1}+\binom{n}{\varepsilon}-n\cdot\binom{n}{\varepsilon}\\
&=\binom{n+1}{\varepsilon}-n\cdot\binom{n}{\varepsilon}\\
&=\frac{n!}{\varepsilon!(n-\varepsilon)!}\cdot\left(\frac{n+1}{n+1-\varepsilon}-n\right)\\
&=\frac{n!}{\varepsilon!(n-\varepsilon)!}\cdot\left(\frac{n+1-n^2-n+n\cdot\varepsilon}{n+1-\varepsilon}\right)\\
&<\frac{n!}{\varepsilon!(n-\varepsilon)!}\cdot\left(\frac{1-0.5\cdot n^2}{n+1-\varepsilon}\right)<0\\
\varepsilon = m: \quad & \binom{n}{m-1}-n\cdot\binom{n}{m}\\
&=\frac{n!}{(m-1)!(n-m)!}\cdot\left(\frac{1}{n-m+1}-\frac{n}{m}\right)\\
&=\frac{n!}{(m-1)!(n-m)!}\cdot\left(\frac{m-n^2+n\cdot m-n}{(n-m+1)\cdot m}\right)\\
&<\frac{n!}{(m-1)!(n-m)!}\cdot\left(\frac{0.5\cdot n-n+0.5\cdot n^2-n^2}{(n-m+1)\cdot m}\right)<0.
\end{aligned}$$

Thus,

$$\sum_{k=0}^{m-1}\binom{n}{k}\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right)^{k+1} + \sum_{k=0}^{m-1}\binom{n}{k}\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right)^{k} - n\cdot\sum_{k=0}^{m}\binom{n}{k}\left(\frac{x^{\pi}_{p_i,r,t}}{x^{\pi}_{p_{3-i},r,t}}\right)^{k} < 0.$$

From this it follows that $\frac{\partial\rho_{p_i}}{\partial x^{\pi}_{p_i,r,t}}\left(x^{\pi}_{p_i,r,t}/x^{\pi}_{p_{3-i},r,t}\right)<0$ and $\frac{\partial\phi_{\mathcal{P},r,t}}{\partial x^{\pi}_{p_i,r,t}}\left(x^{\pi}_{p_i,r,t},x^{\pi}_{p_{3-i},r,t}\right)<0$.

6.2.3.2 Complements

Finally, this section contains the enhancement of the model for products that are complementary to each other. On the basis of the modeling approach in section 3.6, we consider a set of two complements $\mathcal{C} = \{p_i, p_{3-i}\}$. Since the demand of these products is in a specified ratio representing the requirements for reprocessing, we consider the common demand of this mixture that is given by

$$\phi_{\mathcal{C},r,t}(x^{\pi}_{p_i,r,t}, x^{\pi}_{p_{3-i},r,t}) = \lambda_1^{\phi_{\mathcal{C},r,t}} \cdot \tanh\left(\frac{\lambda_2^{\phi_{\mathcal{C},r,t}} - \sum_{k=1}^{2} a^{\text{com}}_{p_k,\mathcal{C},t} \cdot x^{\pi}_{p_k,r,t}}{\lambda_3^{\phi_{\mathcal{C},r,t}}}\right) + \lambda_4^{\phi_{\mathcal{C},r,t}}. \tag{6.28}$$

The corresponding domain is given by

$$D_{1,\mathcal{C},r,t} := \begin{cases} \tilde{D}_{1,\mathcal{C},r,t} & \text{if } \lambda_4^{\phi_{\mathcal{C},r,t}} < \lambda_1^{\phi_{\mathcal{C},r,t}} \\ \mathbb{R}_0^+ \times \mathbb{R}_0^+ & \text{if } \lambda_4^{\phi_{\mathcal{C},r,t}} = \lambda_1^{\phi_{\mathcal{C},r,t}}, \end{cases} \tag{6.29}$$

where

$$\tilde{D}_{1,\mathcal{C},r,t} :=$$
$$\left\{(x^{\pi}_{p_i,r,t}, x^{\pi}_{p_{3-i},r,t}) \in \mathbb{R}_0^+ \times \mathbb{R}_0^+ | \sum_{k=1}^{2} a^{\text{com}}_{p_k,\mathcal{C},t} \cdot x^{\pi}_{p_k,r,t} \le \lambda_2^{\phi_{\mathcal{C},r,t}} + \lambda_3^{\phi_{\mathcal{C},r,t}} \cdot \operatorname{artanh}\left(\frac{\lambda_4^{\phi_{\mathcal{C},r,t}}}{\lambda_1^{\phi_{\mathcal{C},r,t}}}\right)\right\}.$$

Accordingly, the codomain is given by

$$D_{2,\mathcal{C},r,t} := \begin{cases} \left[0, \lambda_1^{\phi_{\mathcal{C},r,t}} \cdot \tanh\left(\frac{\lambda_2^{\phi_{\mathcal{C},r,t}}}{\lambda_3^{\phi_{\mathcal{C},r,t}}}\right) + \lambda_4^{\phi_{\mathcal{C},r,t}}\right] & \text{if } \lambda_4^{\phi_{\mathcal{C},r,t}} < \lambda_1^{\phi_{\mathcal{C},r,t}} \\ \left(0, \lambda_1^{\phi_{\mathcal{C},r,t}} \cdot \tanh\left(\frac{\lambda_2^{\phi_{\mathcal{C},r,t}}}{\lambda_3^{\phi_{\mathcal{C},r,t}}}\right) + \lambda_4^{\phi_{\mathcal{C},r,t}}\right] & \text{if } \lambda_4^{\phi_{\mathcal{C},r,t}} = \lambda_1^{\phi_{\mathcal{C},r,t}}. \end{cases} \tag{6.30}$$

Consequently, the demand for the single product $p_i,\ i = 1, 2$ can be expressed by

$$\phi^{\text{com}}_{p_i,r,t}(x^{\pi}_{p_i,r,t}, x^{\pi}_{p_{3-i},r,t}) = a^{\text{com}}_{p_i,\mathcal{C},t} \cdot \phi_{\mathcal{C},r,t}(a^{\text{com}}_{p_i,\mathcal{C},t} \cdot x^{\pi}_{p_i,r,t} + a^{\text{com}}_{p_{3-i},\mathcal{C},t} \cdot x^{\pi}_{p_{3-i},r,t}),\ i = 1, 2, \tag{6.31}$$

where $D^{\text{com}}_{1,p_i,r,t} := D_{1,\mathcal{C},r,t},\ i = 1, 2$, and

$$D^{\text{com}}_{2,p_i,r,t} := \begin{cases} \left[0, a^{\text{com}}_{p_i,\mathcal{C},t} \cdot \left(\lambda_1^{\phi_{\mathcal{C},r,t}} \cdot \tanh\left(\frac{\lambda_2^{\phi_{\mathcal{C},r,t}}}{\lambda_3^{\phi_{\mathcal{C},r,t}}}\right) + \lambda_4^{\phi_{\mathcal{C},r,t}}\right)\right] & \text{if } \lambda_4^{\phi_{\mathcal{C},r,t}} < \lambda_1^{\phi_{\mathcal{C},r,t}} \\ \left(0, a^{\text{com}}_{p_i,\mathcal{C},t} \cdot \left(\lambda_1^{\phi_{\mathcal{C},r,t}} \cdot \tanh\left(\frac{\lambda_2^{\phi_{\mathcal{C},r,t}}}{\lambda_3^{\phi_{\mathcal{C},r,t}}}\right) + \lambda_4^{\phi_{\mathcal{C},r,t}}\right)\right] & \text{if } \lambda_4^{\phi_{\mathcal{C},r,t}} = \lambda_1^{\phi_{\mathcal{C},r,t}},\ i = 1, 2. \end{cases} \tag{6.32}$$

Theorem 6.4. *Demand model for complementary products*
Let $\mathcal{C} = \{p_i, p_{3-i}\}$ be a set of complementary products. Then, the demand function $\phi^{\text{com}}_{p_i,r,t} \colon D^{\text{com}}_{1,p_i,r,t} \to D^{\text{com}}_{2,p_i,r,t}$,

$$\phi^{\text{com}}_{p_i,r,t}(x^{\pi}_{p_i,r,t}, x^{\pi}_{p_{3-i},r,t}) = a^{\text{com}}_{p_i,\mathcal{C},t} \cdot \phi_{\mathcal{C},r,t}(a^{\text{com}}_{p_i,\mathcal{C},t} \cdot x^{\pi}_{p_i,r,t} + a^{\text{com}}_{p_{3-i},\mathcal{C},t} \cdot x^{\pi}_{p_{3-i},r,t}),\ i = 1, 2, \tag{6.33}$$

with

$$\alpha^{\text{max\_quant}}_{p_i,r,t} = a^{\text{com}}_{p_i,\mathcal{C},t} \cdot (\lambda_1^{\phi_{\mathcal{C},r,t}} \cdot \tanh\left(\frac{\lambda_2^{\phi_{\mathcal{C},r,t}}}{\lambda_3^{\phi_{\mathcal{C},r,t}}}\right) + \lambda_4^{\phi_{\mathcal{C},r,t}}),\ i = 1, 2,$$

satisfies the assumptions 6.1 if $\phi_{\mathcal{C},r,t} \colon D_{1,\mathcal{C},r,t} \to D_{2,\mathcal{C},r,t}$ defined by model (6.28) and fulfills the assumptions required in theorem 6.1.

Proof: The accordance of equation (6.33) with the characteristics of demand 6.1 immediately results from its construction. Besides, the characteristics of demand 3.11 are satisfied because

$$\frac{\partial \phi^{\text{com}}_{p_i,r,t}}{\partial x^{\pi}_{p_{3-i},r,t}}(x^{\pi}_{p_i,r,t}, x^{\pi}_{p_{3-i},r,t}) =$$

$$\frac{-a^{\text{com}}_{p_{3-i},\mathcal{C},t} \cdot a^{\text{com}}_{p_i,\mathcal{C},t} \cdot \lambda_1^{\phi_{\mathcal{C},r,t}}}{\lambda_3^{\phi_{\mathcal{C},r,t}}} \cdot \operatorname{sech}^2\left(\frac{\lambda_2^{\phi_{\mathcal{C},r,t}} - a^{\text{com}}_{p_i,\mathcal{C},t} \cdot x^{\pi}_{p_i,r,t} - a^{\text{com}}_{p_{3-i},\mathcal{C},t} \cdot x^{\pi}_{p_{3-i},r,t}}{\lambda_3^{\phi_{\mathcal{C},r,t}}}\right) \leq 0$$

and in the same manner $\frac{\partial \phi^{\text{com}}_{p_{3-i},r,t}}{\partial x^{\pi}_{p_i,r,t}} \leq 0$.

Example 6.5. *Let* $\mathcal{C} = \{p_1, p_2\}$, $\lambda_1^{\phi_{\mathcal{C},r,t}} = 200$, $\lambda_2^{\phi_{\mathcal{C},r,t}} = 300$, $\lambda_3^{\phi_{\mathcal{C},r,t}} = 50$, $\lambda_4^{\phi_{\mathcal{C},r,t}} = 190$, *and* $\phi^b_{p_1,r,t} = \phi^b_{p_2,r,t} = 0$. *Then, given* $a^{\text{com}}_{p_1,\mathcal{C},t} = 1$ *and* $a^{\text{com}}_{p_2,\mathcal{C},t} = 2$ *the demand functions* $\phi^{\text{com}}_{p_1,r,t}$ *and* $\phi^{\text{com}}_{p_2,r,t}$ *are illustrated in figures 6.9 and 6.10.*

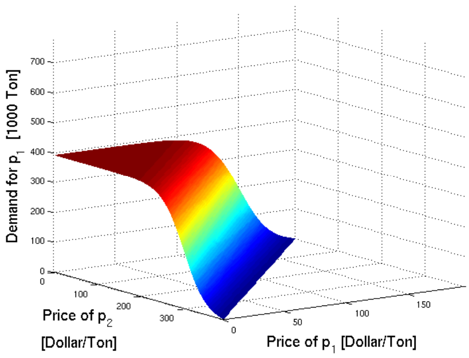

Figure 6.9: Illustration of $\phi^{\text{com}}_{p_1,r,t}$ (see model (6.33)) with parameters given in example 6.5

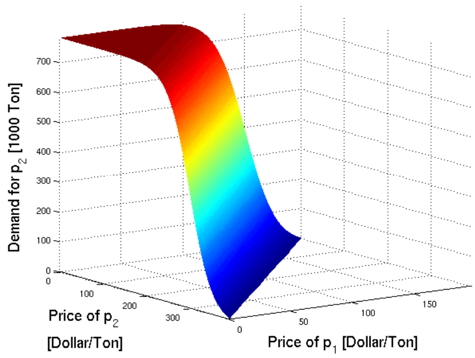

Figure 6.10: Illustration of $\phi^{\text{com}}_{p_2,r,t}$ (see model (6.33)) with parameters given in example 6.5

6.3 Including the Demand Models in the Supply-Demand Trade Network Optimization Problem

In this section, we apply the *tanh-demand model* (6.6), the *tanh-demand model eco* (6.15), the *tanh-demand model* for substitutes (6.26), and the *tanh-demand model* for complements (6.33) in the supply-demand trade network optimization model. Therefore, we first present the subsystem of the petrochemical network that we will use for the simulations of prices and sales quantities. For this network, we propose several demand scenarios for products with external demand and analyze the results of the respective profit maximization.

	Number
$\lvert P^M \rvert$	20
$\lvert P_{ext} \rvert$	15
$\lvert P_{mid} \rvert$	0
$\lvert P_{out} \rvert$	5
$\lvert R \rvert$	1
$\lvert S \rvert$	18
$\lvert C \rvert$	1
$\lvert T \rvert$	1

Table 6.1: Components of the petrochemical subnetwork under consideration

	Scale
$a_{s,r,t}^{cap\_max}$	$10^2 - 10^3$
$a_{p_{ex},r,t}^{\pi}$	$10^2 - 10^3$
$a_{s,p,t}^{f}$	10^0
$a_{p_{out},r,t}^{\pi}$	$10^2 - 10^3$
$a_{p_{out},r,t}^{q}$	$10^2 - 10^3$
$\Delta a_{r,t,1}^{\text{GDP}}$	10^2
$\Delta a_{r,t,1}^{\text{IndPro}}$	10^1

Table 6.2: Parameter scales of the petrochemical subnetwork under consideration

6.3.1 Description of the Subnetwork

We select a subnetwork of the petrochemical industry in cooperation with experts and add further estimates whenever historical data is not available. Applying the algorithm developed by Kramer [Kra13] to obtain a consistent network, the subnetwork includes the components summarized in table 6.1. For confidentiality reasons we do not provide the real notation and denote the respective components of the sets as follows: $T = \{t^{sim}\}$, $R = \{A\}$, and $P_{out} = \{1, 2, 3, 4, 5\}$. Likewise, we only give the scales of the data available for the network simulation.

The product network is shown in figure 6.11. Note that the reduction to one region causes some inconsistencies. In case the maximum capacity for producing a certain product is lower than historical sales quantities, we add an additional process with fixed costs and without inputs representing the purchase of the product from another region. To be more precise, the corresponding fixed costs are equal to a rough estimation of the production costs in another region plus the transportation costs to region A. Obviously, there is no further information about demand available. Therefore, we create some demand scenarios in the subsequent section.[7]

6.3.2 Simulation of Sales Quantities and Prices using Different Demand Scenarios

To integrate our demand model in the supply-demand trade network optimization problem, we propose different demand scenarios

- **Scenario basic**: all products $p \in P_{out}$ are required independently from each other, but have the same demand parameters $\lambda_1^{\phi_{p,r,t}} = 1000$, $\lambda_2^{\phi_{p,r,t}} = 3500$, $\lambda_3^{\phi_{p,r,t}} = 1500$, and $\lambda_4^{\phi_{p,r,t}} = 250$ for all $p \in P_{out}$.

[7] Motivated by the objective to investigate price formation of the past and forecast prices and sales quantities, we consider methods for identifying parameters of the demand function based on the data given in chapter 7.

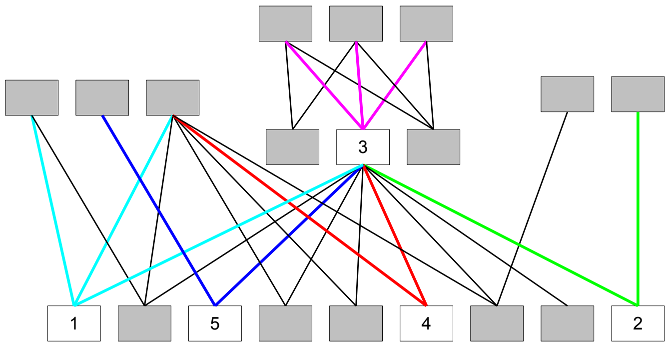

Figure 6.11: Illustration of the product network in the subsystem: the grey boxes depict product with fixed prices, the numbered boxes present products with external demand. The colored connections reflect their production processes, where inputs are above and outputs below.

- **Scenario eco**: all products $p \in P_{out}$ are required independently from each other, but have the same demand parameters $\lambda_1^{\phi_{p,r,t}} = 1000$, $\lambda_2^{\phi_{p,r,t}} = 3500$, $\lambda_3^{\phi_{p,r,t}} = 1500$, and $\lambda_4^{\phi_{p,r,t}} = 250$, $\lambda_{\text{GDP}}^{\phi_{p,r,t}} = 0.1$, and $\lambda_{\text{IndPro}}^{\phi_{p,r,t}} = 10$ for all $p \in P_{out}$. The change of the economic situation was calculated using $J = 1$: $\Delta a_{r,t,1}^{\zeta_i}$, $\zeta_i \in \{GDP, IndPr\}$.

- **Scenario sub 1**: let $\mathcal{P} = P_{sub} = \{p_1, p_2\}$, where $\lambda_1^{\phi_{\mathcal{P},r,t}} = 1000$, $\lambda_2^{\phi_{\mathcal{P},r,t}} = 3500$, $\lambda_3^{\phi_{\mathcal{P},r,t}} = 1500$, $\lambda_4^{\phi_{\mathcal{P},r,t}} = 250$. Additionally, $\lambda_1^{\phi^b_{p_{sub},r,t}} = 500$, $\lambda_2^{\phi^b_{p_{sub},r,t}} = 3500$, $\lambda_3^{\phi^b_{p_{sub},r,t}} = 1500$, and $\lambda_4^{\phi^b_{p_{sub},r,t}} = 250$ for all $p_{sub} \in P_{sub}$. That means, starting from **scenario basic**, half of the demand of products p_1 and p_2 is supposed to be substitutable. For the splitting function, we select $n = 19$. The remaining products $p_{out} \in P_{out} \setminus P_{sub}$ are required independently from each other. They have the same demand parameters $\lambda_1^{\phi_{p_{out},r,t}} = 1000$, $\lambda_2^{\phi_{p_{out},r,t}} = 3500$, $\lambda_3^{\phi_{p_{out},r,t}} = 1500$, and $\lambda_4^{\phi_{p_{out},r,t}} = 250$ for all $p_{out} \in P_{out} \setminus P_{sub}$.

- **Scenario sub 2**: let $\mathcal{P} = P_{sub} = \{p_1, p_2\}$, where $\lambda_1^{\phi_{\mathcal{P},r,t}} = 2000$, $\lambda_2^{\phi_{\mathcal{P},r,t}} = 3500$, $\lambda_3^{\phi_{\mathcal{P},r,t}} = 1500$, and $\lambda_4^{\phi_{\mathcal{P},r,t}} = 250$. As above, we select $n = 19$ for the splitting, but, this time, $\phi^b_{p_{sub},r,t}(x^{\pi}_{p,r,t}) = 0$ for all $p_{sub} \in P_{sub}$. Likewise, the remaining products $p_{out} \in P_{out} \setminus P_{sub}$ are required independently from each other, but have the same demand parameters $\lambda_1^{\phi_{p_{out},r,t}} = 1000$, $\lambda_2^{\phi_{p_{out},r,t}} = 3500$, $\lambda_3^{\phi_{p_{out},r,t}} = 1500$, and $\lambda_4^{\phi_{p_{out},r,t}} = 250$ for all $p_{out} \in P_{out} \setminus P_{sub}$.

- **Scenario com 1**: let $\mathcal{C} = P_{com} = \{p_1, p_2\}$ with $a^{\text{com}}_{p_i,P_{com},t} = 1$, $i = 1, 2$. Regarding the demand for these complements, we set $\lambda_1^{\phi_{P_{com},r,t}} = 1000$, $\lambda_2^{\phi_{P_{com},r,t}} =$

Scenario	Product 1	Product 2	Product 3	Product 4	Product 5	Total Profit
Basic	2648.10	2645.86	2635.87	2788.69	2633.37	$8.96 \cdot 10^6$
Eco	2700.56	2698.48	2688.49	2838.02	2686.16	$8.32 \cdot 10^6$
Sub 1	2524.70	2910.31	2639.25	2788.69	2633.37	$9.33 \cdot 10^6$
Sub 2	2633.97	3807.44	2639.25	2788.69	2633.37	$9.33 \cdot 10^6$
Com 1	2504.01	3046.44	2639.25	2788.69	2633.37	$9.95 \cdot 10^6$
Com 2	2844.59	2925.77	2641.14	2788.69	2645.68	$1.24 \cdot 10^7$

Table 6.3: Simulation results of prices and profit for each demand scenarios given the subnetwork described in section 6.3.1

$\sum_{p_i \in P_{com}} a^{\text{com}}_{p_i,P_{com},t} \cdot 3500 = 7000$, $\lambda_3^{\phi_{P_{com},r,t}} = 1500$, and $\lambda_4^{\phi_{P_{com},r,t}} = 250$.[8] The remaining products $p_{out} \in P_{out} \backslash P_{com}$ are required independently from each other, but have the same demand parameters $\lambda_1^{\phi_{p_{out},r,t}} = 1000$, $\lambda_2^{\phi_{p_{out},r,t}} = 3500$, $\lambda_3^{\phi_{p_{out},r,t}} = 1500$, and $\lambda_4^{\phi_{p_{out},r,t}} = 250$ for all $p_{out} \in P_{out} \setminus P_{com}$.

- **Scenario com 2**: let $\mathcal{C} = P_{com} = \{p_1, p_2\}$ with $a^{\text{com}}_{p_1,P_{com},t} = 1$ and $a^{\text{com}}_{p_2,P_{com},t} = 2$. Similarly to **scenario com 1** above, we select $\lambda_1^{\phi_{P_{com},r,t}} = 1000$, $\lambda_2^{\phi_{P_{com},r,t}} = \sum_{p_i \in P_{com}} a^{\text{com}}_{p_i,P_{com},t} \cdot 3500 = 10500$, $\lambda_3^{\phi_{P_{com},r,t}} = 1500$, and $\lambda_4^{\phi_{P_{com},r,t}} = 250$. The remaining products $p_{out} \in P_{out} \backslash P_{com}$ are required independently from each other, but have the same demand parameters $\lambda_1^{\phi_{p_{out},r,t}} = 1000$, $\lambda_2^{\phi_{p_{out},r,t}} = 3500$, $\lambda_3^{\phi_{p_{out},r,t}} = 1500$, and $\lambda_4^{\phi_{p_{out},r,t}} = 250$ for all $p_{out} \in P_{out} \setminus P_{com}$.

The optimization model was implemented in AMPL and solved using Ipopt-3.8.3 for each demand scenario. As initial values for the price variables, we select the prices from the previous year. Since the demand model for substitutes (6.26) is not differentiable at the whole domain $D^{\text{sub}}_{1,p_i,r,t}$, we approximate the min-function with

$$f_{min}(x^\pi_{p_i,r,t}, x^\pi_{p_{3-i},r,t}) = \frac{1}{2}\left(x^\pi_{p_i,r,t} + x^\pi_{p_{3-i},r,t} - \sqrt{(x^\pi_{p_i,r,t} + x^\pi_{p_{3-i},r,t})^2}\right),\ i = 1, 2.$$

Having established the scenarios we obtain the corresponding price and sales quantity simulations by solving the optimization problem (4.3) defined in section 4.2 for the subnetwork presented above. The results are shown in tables 6.3 and 6.4. Exemplarily, figures 6.12 to 6.19 illustrate the corresponding demand functions or the substitutable demand function, respectively, of products 1 and 2, together with the optimal solutions. All in all, the simulation results are satisfactory. In particular, we observe the following behavior.

- The demand functions in **scenario basic** and **scenario eco** are identical for all products $p \in P_{out}$. The differences of the optimal solutions are due to the produc-

[8] Basically, we assumed that almost all parameters are equal to **scenario basic** except $\lambda_2^{\phi_{P_{com},r,t}}$ as variable for the maximum price, which is set equal to $\sum_{p_i \in P_{com}} a^{\text{com}}_{p_i,P_{com},t} \cdot \lambda_2^{\phi_{p_i,r,t}}$.

Scenario	Product 1	Product 2	Product 3	Product 4	Product 5
Basic	763.839	764.936	769.814	691.593	771.030
Eco	795.946	796.972	801.89	724.701	803.034
Sub 1	923.008	621.729	768.168	691.593	771.030
Sub 2	1219.980	321.492	768.168	691.593	771.030
Com 1	997.104	997.104	768.168	691.593	771.030
Com 2	1084.440	2168.880	767.248	691.593	765.027

Table 6.4: Simulation results of sales quantities for each demand scenarios given the subnetwork described in section 6.3.1

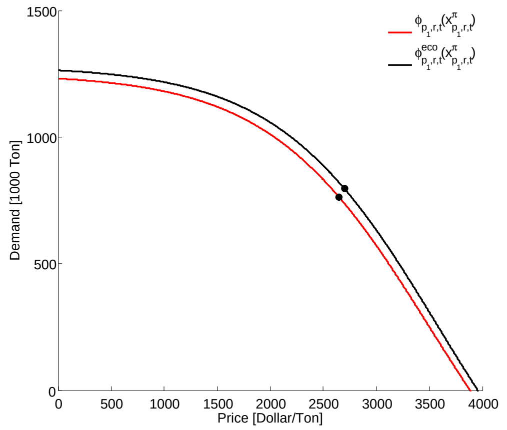

Figure 6.12: Demand $\phi_{p_1,r,t}$ for product 1 of **scenario basic** and **scenario eco**: change of optimal solution due to a change in the economic situation

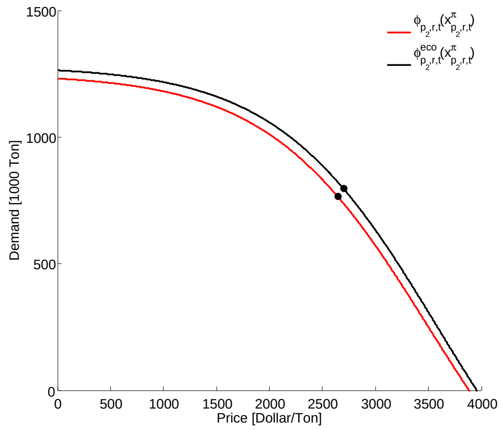

Figure 6.13: Demand $\phi_{p_2,r,t}$ for product 2 of **scenario basic** and **scenario eco**: change of optimal solution due to a change in the economic situation

tion processes. The results for products 1 and 2 are illustrated in the figures 6.12 and 6.13.

- Comparing the simulation results of **scenario basic** and **scenario eco**, the effects of a positive change in the economic situation is conspicuous. According to our model, the demand curve in **scenario eco** is shifted to the right compared to the respective demand function in **scenario basic**. This results in a higher price for slightly lower sales quantities.

- The model works well if the substitutable products are required independently from each other as proposed in **scenario sub 1**. Compared to the results of **scenario basic**, one of the substitutes becomes cheaper, whereas the other one becomes more expensive. This is plausible with regard to the substitutable demand that is driven and satisfied by the cheaper product. Consequently, the cheaper product

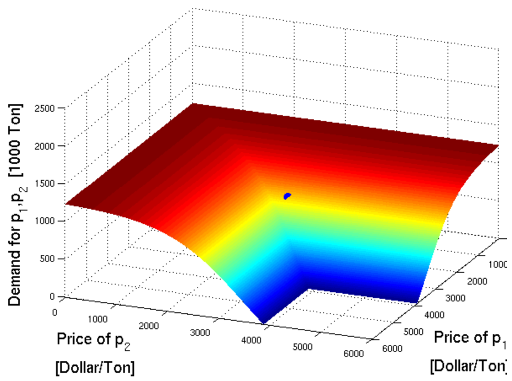

Figure 6.14: Substitutable demand $\phi_{\mathcal{P},r,t}$ for products 1 and 2 of **scenario sub 1**: optimal solution highlighted

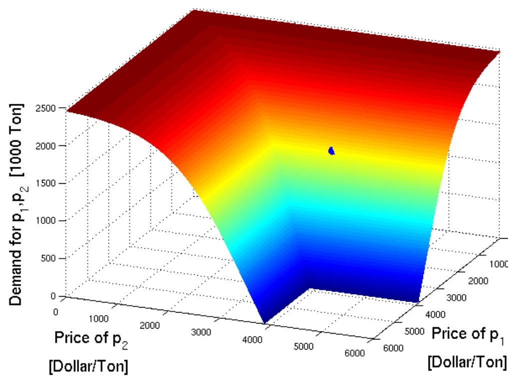

Figure 6.15: Substitutable demand $\phi_{\mathcal{P},r,t}$ for products 1 and 2 of **scenario sub 2**: optimal solution highlighted

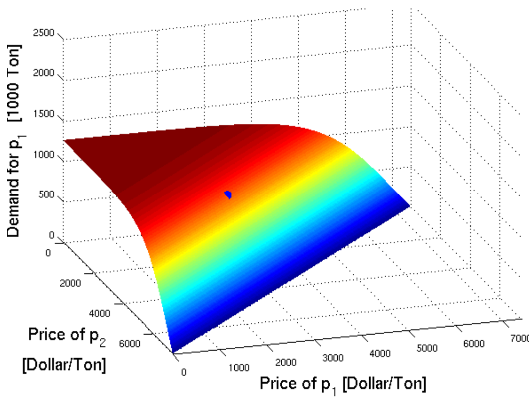

Figure 6.16: Demand $\phi^{\text{com}}_{p_1,r,t}$ for product 1 of **scenario com 1**: optimal solution highlighted

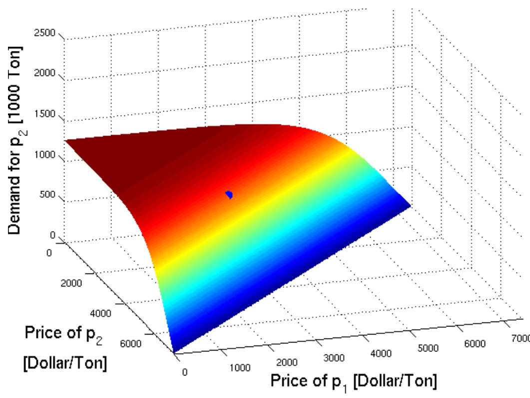

Figure 6.17: Demand $\phi^{\text{com}}_{p_2,r,t}$ for product 2 of **scenario com 1**: optimal solution highlighted

compensates the effect of increasing the price of the other product. As a result, the optimization results in higher profit compared to the profit of **scenario basic**.

- **Scenario sub 2** represents the case, in which the basis demand $\phi^b_{p_{sub},r,t}$ is zero for all $p_{sub} \in P_{sub}$. The demand model does not include a maximum price for the more expensive product, because the substitutable demand only limits the price of the cheaper product. Consequently, our optimization model indicates that the monopolist is tempted to drive up the price. The results reveal that this aspect has to be further analyzed in future research. Moreover, varying the initial values provokes a different local solution with a slightly lower or higher objective function

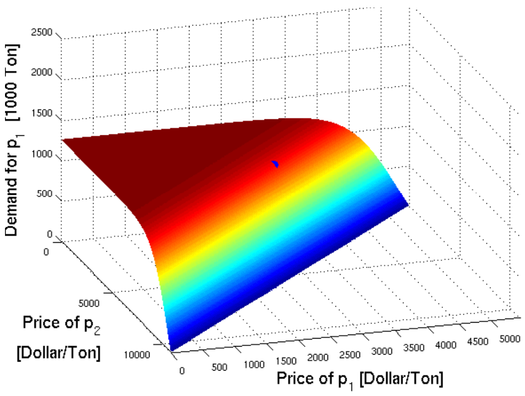

Figure 6.18: Demand $\phi^{\text{com}}_{p_1,r,t}$ for product 1 of **scenario com 2**: optimal solution highlighted

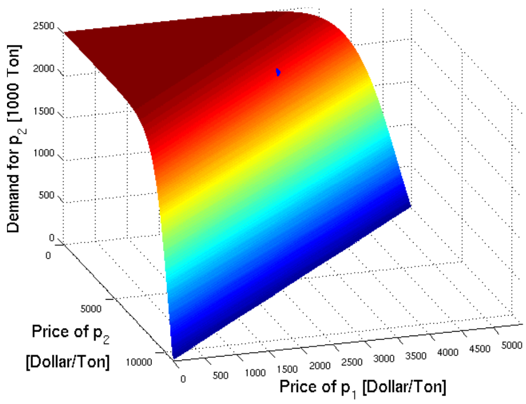

Figure 6.19: Demand $\phi^{\text{com}}_{p_2,r,t}$ for product 2 of **scenario com 2**: optimal solution highlighted

value. Clearly, the nonconvexity of the optimization problem comes from the fact the substitutable demand function is not concave (cf. figure 6.14 and 6.15).

- Likewise, the results of **scenario com 1** and **scenario com 2** are reasonable. However, the choice of the parameters induces that the demand is considerably high at high prices. This leads to higher sales quantities in the case of complements and also to a very high profit. Consequently, more data analysis is necessary to determine the demand parameters for complements. Especially, values for $\lambda_3^{\phi_{P_{com},r,t}}$ influence the shape of the demand function if $\lambda_1^{\phi_{P_{com},r,t}}$ and $\lambda_2^{\phi_{P_{com},r,t}}$ are fixed. It is, however, plausible that it is optimal for the producer to produce more of the products he sells in a "basket". For that reason, the prices of products 3 and 5 are increased so that higher quantities of complementary products 1 and 2 are produced and sold.

To conclude, our approach to modeling demand induces reasonable results. Thus, our demand model is applicable to the supply-demand trade network optimization model. Moreover, Kramer [Kra13] used the *tanh-demand model eco* in order to simulte prices and sales quantities in a three-region network over multiple time periods and obtained valuable results. However, it becomes obvious that more information about the products is necessary to create realistic scenarios for the multi-commodity demand models. Moreover, the identification of the model parameters is essential. Therefore, the subsequent chapter investigates methods for identifying the demand parameters of $\phi^{eco}_{p,r,t}(\boldsymbol{x}^{\pi}_{p,r,t})$.

6.4 Conclusion

In this section, we develop a quantitative demand model that is applicable in our optimization model and satisfies the characteristics summarized in the assumptions 6.1 to the greatest possible extent. To be more precise, we establish demand models including changes in the economic situation or considering the aspects of complementary products such that the model functions satisfy the demand characteristics summarized in assumptions 6.1. Including price-dependent substitutes is more complex than the other modeling approaches. Indeed, our approach to modeling demand of substitutes does not satisfy the requirement of being differentiable at the whole domain. Nevertheless, we are able to approximate the substitutable demand function by a differentiable function and insert this approximation in the network optimization model which leads to reasonable results in section 6.3.
Hence, our *tanh-demand model* offers a reasonable tool to simulate prices and sales quantities by providing the following advantages:

- The model function is bounded, nonlinear, continuous, and decreasing.
- The model function is differentiable with respect to the price almost everywhere. If this is not the case, an approximation for the demand function is offered to solve the optimization problem with algorithms based on derivatives.
- The model offers a saturation quantity.
- Including the demand model in the supply-demand trade network optimization model results in reasonable price and sales quantities simulations.
- The model function includes few parameters.

Nevertheless, to make statements about real price formation and provide price forecasts, it is necessary to estimate the parameters of the demand model. A prerequisite is, however, that sufficient information to estimate parameters is available. The subsequent chapter proposes two methods to identify the parameters that are tailored to the available data.

7 Methods to Identify the Demand Parameters of Petrochemical Products

Having established explicit demand models in chapter 6, our next step comprises the development of methods for identifying parameters. The objective of this identification process is not only to estimate the historical demand function given historical data, but also to provide a forecast of the future demand that is applicable in our supply-demand trade network optimization model presented in section 4.2 to simulate price and sales quantity forecasts in the petrochemical industry. In this chapter, our studies focus on identifying the parameters of the *tanh-demand model eco*

$$\phi^{eco}_{p,r,t}(x^{\pi}_{p,r,t}) = (\lambda_1^{\phi_{p,r,t}} + \lambda_{\text{IndPro}}^{\phi_{p,r,t}} \cdot \Delta a_{r,t,J}^{\text{IndPro}}) \cdot \tanh\left(\frac{\lambda_2^{\phi_{p,r,t}} + \lambda_{\text{GDP}}^{\phi_{p,r,t}} \cdot \Delta a_{r,t,J}^{\text{GDP}} - x^{\pi}_{p,r,t}}{\lambda_3^{\phi_{p,r,t}}}\right) + \lambda_4^{\phi_{p,r,t}}, \quad (7.1)$$

where $|P| = 1$. In section 7.1, to begin with, we discuss the emerging difficulties of identifying the parameters

$$\lambda_1^{\phi_{p,r,t_0}}, \lambda_2^{\phi_{p,r,t_0}}, \lambda_3^{\phi_{p,r,t_0}}, \lambda_4^{\phi_{p,r,t_0}}, \lambda_{\text{GDP}}^{\phi_{p,r,t_0}}, \text{ and } \lambda_{\text{IndPro}}^{\phi_{p,r,t_0}}$$

for a fixed time t_0 by means of data consisting of yearly prices, yearly sales quantities, and yearly economic indices. Obviously, the fact that the assumed nonlinear structure is not evident from available data poses a big challenge. Therefore, we propose two methods for parameter identification that we tailor to the available data set.

In section 7.2, we approximate the demand function by determining a range of possible parameter values on the basis of several data statistics (i.e., we make several a-priori assumptions) and recalculate the optimal price formation of preceding years for these parameter values by use of the supply-demand trade network optimization model (4.3) presented in section 4.2. Then, we calculate the average deviation of the resulting price and sales quantity simulations from the historical data for each parameter fit. Finally, we accept those parameter values that minimize the differences of the simulations to the historical values as the most appropriate parameters for time t_0.

Alternatively, in section 7.3, we propose an optimization problem with constraints that reflect assumptions on the shape of the demand function. Applying the generalized Gauss-Newton method for constrained weighted least-squares problems, we estimate the demand parameters for each product separately.

To conclude, in section 7.4, we integrate the respective demand functions obtained by both approaches for each product in the supply-demand trade network optimization problem (4.3) and compare the resulting price and sales quantity simulations with each other.

7.1 Difficulties of Realizing a Parameter Identification

We have already discussed the shortcomings of yearly data with regard to establishing explicit demand models in section 6.1. Likewise, identifying parameters of the demand model (7.1) gets also complicated by means of the available historical data as the following parameter identification-related issues reveal (using again the example of data shown in the figure 6.1).

1. The effect of prices on demand does not clearly arise from the given data. In other words, the demand-price relation is not distinguishable from other influencing factors.

2. There is no information available about consumption in high and low price ranges.

As a result, we draw the following conclusions for the identification process.

1. Two, possibly consecutive, price and sales quantity tuples at two different times result from different states of the economic and consumer-related influencing factors.

2. To estimate the parameters for a given fixed time we cannot rely on a high number of years in which the market situation is similar. Hence, we reduce the estimation input to price-sales combinations of years in which the market situation is comparable and additionally weight the data with a time-dependent factor if necessary.

3. Further information is essential for a reasonable approximation of the consumer's behavior in the unobserved price ranges.

Subsequently, we show how to tackle the problem in two different ways. Therefore, our research is restricted to the *tanh-demand model eco*, because

1. the available database does not provide information that indicates which products in the petrochemical network are substitutes or complements,[1] and,

2. as stated above, influences of prices and other influencing factors are not easily distinguishable. In other words, there is no consumption data available that is adjusted to changes in the economic situation,

Both of the following techniques require additional assumptions to provide an efficient parameter identification. Concering the data needed, the first technique is rather circumstantial and elaborate, because it includes numerous simulations of the whole market, whereas the second approach is more general and is only based on price and consumption data of the regarded petrochemical product as well as on economic factors.

[1] Kök and Fisher [KF07] also note that information about substitution of products, i.e., how much is required because of the substitution effect, usually is not available.

7.2 Simulation-based Approach to Approximate the Demand Parameters

This section comprises our concept to approximate the basic parameters $\lambda_1^{\phi_{p,r,t_0}}, \ldots, \lambda_4^{\phi_{p,r,t_0}}$ and subsequently $\lambda_{\text{GDP}}^{\phi_{p,r,t_0}}$ and $\lambda_{\text{IndPro}}^{\phi_{p,r,t_0}}$ based on historical market information. As stated in section 6.2, we assume that $\lambda_i^{\phi_{p,r,t}} \geq 0,\ i = 1, 2, 4,\ \lambda_3^{\phi_{p,r,t}} > 0$ and $\lambda_k^{\phi_{p,r,t_0}} \geq 0,\ k \in \{GDP, IndPro\}$. Under the assumption that the upper bound of consumer's maximum quantity, $\alpha_{p,r,t_0}^{\text{UB\_max\_quant}}$, and the consumer's maximum price, $\alpha_{p,r,t_0}^{\text{max\_price}}$, can be modeled as a function of past consumption, $a_{p,r,\tau}^q,\ \tau \in T_{t_0}$, and price data, $a_{p,r,\tau}^\pi,\ \tau \in T_{t_0}$, respectively, we have

$$\alpha_{p,r,t_0}^{\text{UB\_max\_quant}} = \alpha_{p,r,t_0}^{mq} \cdot f((a_{p,r,\tau}^q)_{\tau \in T_{t_0}}), \tag{7.2}$$

$$\alpha_{p,r,t_0}^{\text{max\_price}} = \alpha_{p,r,t_0}^{mp} \cdot f((a_{p,r,\tau}^\pi)_{\tau \in T_{t_0}}), \tag{7.3}$$

where T_{t_0} includes all years whose data is assumed to influence the consumer's characteristics at t_0. In doing so, we restrict our approximation to the case $\lambda_4^{\phi_{p,r,t_0}} < \lambda_1^{\phi_{p,r,t_0}}$. Basically, we propose formulas for the upper bound of the maximum consumption and the maximum price using historical data without taking into account the influences of economic factors so far. Having determined the basic demand parameters, we estimate the shift caused by changes in the economic situation using the method of least squares. In short, our way of proceeding is as follows. For different factors α_{p,r,t_0}^{mq} and α_{p,r,t_0}^{mp},

1. we propose modeling approaches for the upper bound of $\alpha_{p,r,t_0}^{\text{max\_quant}}$ as well as $\alpha_{p,r,t_0}^{\text{max\_price}}$

$$\alpha_{p,r,t_0}^{\text{UB\_max\_quant}} = \alpha_{p,r,t_0}^{mq} \cdot f((a_{p,r,\tau}^q)_{\tau \in T_{t_0}}) = \lambda_1^{\phi_{p,r,t_0}} + \lambda_4^{\phi_{p,r,t_0}} \tag{7.4}$$

$$\alpha_{p,r,t_0}^{\text{max\_price}} = \alpha_{p,r,t_0}^{mp} \cdot f((a_{p,r,\tau}^\pi)_{\tau \in T_{t_0}}) = \lambda_2^{\phi_{p,r,t_0}} + \lambda_3^{\phi_{p,r,t_0}} \cdot \operatorname{artanh}\left(\frac{\lambda_4^{\phi_{p,r,t_0}}}{\lambda_1^{\phi_{p,r,t_0}}}\right) \tag{7.5}$$

   and relate them with the basic demand parameters still excluding the influence of economic factors,

2. we determine $\lambda_1^{\phi_{p,r,t_0}}, \ldots, \lambda_4^{\phi_{p,r,t_0}}$ by assuming that the data of the previous year $t_0 - 1$ satisfies the demand function and the relations above,

3. we integrate economic factors and estimate $\lambda_{\text{GDP}}^{\phi_{p,r,t_0}}$ and $\lambda_{\text{IndPro}}^{\phi_{p,r,t_0}}$ using the method of least-squares described in section 5.3,

4. we simulate historical prices and sales quantities using the supply-demand trade network optimization model proposed in section 4.2 including the demand function, and

5. we compute the error, i.e., the deviation of the simulations from the historical data.

By computing error statistics, we determine the best parameter fit to be equal to those values that minimize the average deviation of simulations from the historical values. In the following, we explain our assumptions concerning the parameter identification and explicate our approach to determine the most appropriate parameter fit. Afterwards, we test this method using an exemplary subsystem of the petrochemical network.

7.2.1 Heuristic Principle to Approximate Parameters

We start with determining the parameters $\lambda_1^{\phi_{p,r,t_0}}, \dots, \lambda_4^{\phi_{p,r,t_0}}$ by expressing the upper bound of consumer's maximum quantity and the consumer's maximum price by a function of past consumption and price data, respectively. In doing so, we propose the following principle:

Assumptions 7.1. *Principle to determine parameters of the tanh-demand model A*
In section 6.2, we have established for the tanh-demand model A that

$$\lambda_1^{\phi_{p,r,t_0}} = \alpha_{p,r,t_0}^{\text{UB\_max\_quant}}, \quad \lambda_2^{\phi_{p,r,t_0}} = \alpha_{p,r,t_0}^{\text{max\_price}}. \tag{7.6}$$

That means, $\lambda_2^{\phi_{p,r,t_0}}$ displays the maximum price that the consumer is willing to pay at time t_0 and $\lambda_1^{\phi_{p,r,t_0}}$ displays the upper bound of the maximum capacity of the consumer at time t_0. On the basis of these definitions, we compute $\lambda_3^{\phi_{p,r,t_0}}$ in the following way: as long as no adaption to the economic changes has occurred yet we assume that the tuple of the previous year $(a^{\pi}_{p,r,t_0-1}, a^{q}_{p,r,t_0-1})$ satisfies the demand function for the current time t_0, i.e.,

$$a^{q}_{p,r,t_0-1} = \lambda_1^{\phi_{p,r,t_0}} \cdot \tanh\left(\frac{\lambda_2^{\phi_{p,r,t_0}} - a^{\pi}_{p,r,t_0-1}}{\lambda_3^{\phi_{p,r,t_0}}}\right). \tag{7.7}$$

Thus, $\lambda_3^{\phi_{p,r,t_0}}$ can be written in terms of the parameters $\lambda_1^{\phi_{p,r,t_0}}$, $\lambda_2^{\phi_{p,r,t_0}}$, and data given from the previous year:

$$\lambda_3^{\phi_{p,r,t_0}} = \frac{\lambda_2^{\phi_{p,r,t_0}} - a^{\pi}_{p,r,t_0-1}}{\operatorname{artanh}\left(\frac{a^{q}_{p,r,t_0-1}}{\lambda_1^{\phi_{p,r,t_0}}}\right)}. \tag{7.8}$$

Note that $\lambda_3^{\phi_{p,r,t_0}}$ exists and is positive if $\lambda_2^{\phi_{p,r,t_0}} = \alpha_{p,r,t_0}^{\text{max\_price}} > a^{\pi}_{p,r,t_0-1}$ and $\lambda_1^{\phi_{p,r,t_0}} > \alpha_{p,r,t_0}^{\text{UB\_max\_quant}} > a^{q}_{p,r,t_0-1}$ which holds for $a^{\pi}_{p,r,t_0-1} \in D_{1,p,r,t}$ and $a^{q}_{p,r,t_0-1} \in D_{2,p,r,t}$.

Concerning the general model (6.6), the following assumption holds.

Assumptions 7.2. *Principle to determine parameters of the tanh-demand model*
On the basis of the relations established in section 6.2 and assumptions 7.1, we set

$$\lambda_1^{\phi_{p,r,t_0}} = \alpha^{\text{shift}} \cdot \alpha_{p,r,t_0}^{\text{UB\_max\_quant}}, \quad \lambda_4^{\phi_{p,r,t_0}} = (1 - \alpha^{\text{shift}}) \cdot \alpha_{p,r,t_0}^{\text{UB\_max\_quant}} \tag{7.9}$$

where $0.5 < \alpha^{\text{shift}} < 1$. *By doing this, the upper bound for the maximum consumption is identical in both models and we make sure that* $\phi_{p,r,t_0}(\alpha^{\text{max\_price}}_{p,r,t_0}) = 0$. *Moreover,*

$$\lambda_2^{\phi_{p,r,t_0}} + \lambda_3^{\phi_{p,r,t_0}} \cdot \operatorname{artanh}\left(\frac{\lambda_4^{\phi_{p,r,t_0}}}{\lambda_1^{\phi_{p,r,t_0}}}\right) = \alpha^{\text{max\_price}}_{p,r,t_0}. \tag{7.10}$$

Assuming that the tuple of the previous year $(a^{\pi}_{p,r,t_0-1}, a^{q}_{p,r,t_0-1})$ *satisfies the demand function, we obtain*

$$a^{q}_{p,r,t_0-1} = \lambda_1^{\phi_{p,r,t_0}} \cdot \tanh\left(\frac{\lambda_2^{\phi_{p,r,t_0}} - a^{\pi}_{p,r,t_0-1}}{\lambda_3^{\phi_{p,r,t_0}}}\right) + \lambda_4^{\phi_{p,r,t_0}}. \tag{7.11}$$

By analogy with equation (7.8), substituting equation (7.10) into (7.11), $\lambda_3^{\phi_{p,r,t_0}}$ *is given by*

$$\lambda_3^{\phi_{p,r,t_0}} = \frac{\alpha^{\text{max\_price}}_{p,r,t_0} - a^{\pi}_{p,r,t_0-1}}{\operatorname{artanh}\left(\frac{\lambda_4^{\phi_{p,r,t_0}}}{\lambda_1^{\phi_{p,r,t_0}}}\right) + \operatorname{artanh}\left(\frac{a^{q}_{p,r,t_0-1} - \lambda_4^{\phi_{p,r,t_0}}}{\lambda_1^{\phi_{p,r,t_0}}}\right)}. \tag{7.12}$$

Note that $\lambda_3^{\phi_{p,r,t_0}}$ *exists and is positive if* $\alpha^{\text{max\_price}}_{p,r,t_0} > a^{\pi}_{p,r,t_0-1}$ *and* $\lambda_1^{\phi_{p,r,t_0}} > a^{q}_{p,r,t_0-1} - \lambda_4^{\phi_{p,r,t_0}} > 0$.

So far, in case there is no information about the consumer's characteristics available, we model $\alpha^{\text{UB\_max\_quant}}_{p,r,t_0}$ and $\alpha^{\text{max\_price}}_{p,r,t_0}$ on the basis of historical data.

Assumptions 7.3. *General modeling of consumer's characteristics*
We consider $\alpha^{\text{UB\_max\_quant}}_{p,r,t_0}$ *and* $\alpha^{\text{max\_price}}_{p,r,t_0}$ *and assume that these consumer's characteristics are proportional to specific statistics of the historical data (e.g., weighted mean or maximum). Furthermore, let* T_{t_0} *be a set of previous times whose data is supposed to influence the situation at present time* t_0, *let* $\alpha^{mq}_{p,r,t_0} > 1$ *be the maximum quantity factor, and let* $\alpha^{mp}_{p,r,t_0} > 1$ *be the maximum price factor. Consequently,*

$$\alpha^{\text{UB\_max\_quant}}_{p,r,t_0} = \alpha^{mq}_{p,r,t_0} \cdot \sum_{\tau \in T_{t_0}} w_\tau \cdot a^{q}_{p,r,\tau}, \tag{7.13}$$

$$\text{or} \quad \alpha^{\text{UB\_max\_quant}}_{p,r,t_0} = \alpha^{mq}_{p,r,t_0} \cdot \max(a^{q}_{p,r,\tau})_{\tau \in T_{t_0}} \tag{7.14}$$

are possible formulas, where examples for the weighting function w_τ *are given in example 3.2. Similarly,*

$$\alpha^{\text{max\_price}}_{p,r,t_0} = \alpha^{mp}_{p,r,t_0} \cdot \sum_{\tau \in T_{t_0}} w_\tau \cdot a^{\pi}_{p,r,\tau}, \tag{7.15}$$

$$\text{or} \quad \alpha^{\text{max\_price}}_{p,r,t_0} = \alpha^{mp}_{p,r,t_0} \cdot \max(a^{\pi}_{p,r,\tau})_{\tau \in T_{t_0}}. \tag{7.16}$$

In the following, we refer to equations (7.13) and (7.15) as modeling *mult_y* (multiple years). Using equation (7.14) and (7.16) is denoted by *max_y* (maximum year).

Example 7.1. *Given $T_{t_0} = \{t_0 - 1\}$ we obtain $\lambda_1^{\phi_{p,r,t_0}} = a_{p,r,t_0}^{mq} \cdot a_{p,r,t_0-1}^{q}$ and $\lambda_2^{\phi_{p,r,t_0}} = a_{p,r,t_0}^{mp} \cdot a_{p,r,t_0-1}^{\pi}$ using mult_ y. For tanh-demand model A, equation (7.8) simplifies to*

$$\lambda_3^{\phi_{p,r,t_0}} = \frac{(\alpha_{p,r,t_0}^{mp} - 1) \cdot a_{p,r,t_0-1}^{\pi}}{\operatorname{artanh}\left(\frac{1}{\alpha_{p,r,t_0}^{mq}}\right)}.$$

So far, using historical data, we obtain an approximation of the demand function, which rather corresponds to the demand-price relation of the previous year. The next step comprises the estimation of $\lambda_{\text{GDP}}^{\phi_{p,r,t_0}}$ and $\lambda_{\text{IndPro}}^{\phi_{p,r,t_0}}$ using the least squares approach to adjust the demand function to the economic situation at t_0.
In comparison to T_{t_0}, which includes all years that are assumed to influence the consumer's characteristics at t_0, let T_0 be the set of preceding years to be included in the parameter identification process for time t_0. To get a reasonable estimation, T_0 contains all years in which the market situation is comparable to that of t_0. Hence, the following simplification gets useful.

Assumptions 7.4. *Change in the economic situation for T_0*
$\lambda_{\text{GDP}}^{\phi_{p,r,t}}$ and $\lambda_{\text{IndPro}}^{\phi_{p,r,t}}$ are constant for all $t \in T_0 \cup t_0$.

Under this assumption we can omit the time index for these two parameters in the remaining section. As stated above, we determine the parameters $\lambda_1^{\phi_{p,r,t}}, \lambda_2^{\phi_{p,r,t}}, \lambda_3^{\phi_{p,r,t}}$, and $\lambda_4^{\phi_{p,r,t}}$ for all $t \in T_0$ under the assumption that they are not influenced by the change in the economic situation, i.e., using the principles explained in assumptions 7.1 and 7.2. Then, to add the change in the economic situation we estimate $\lambda_{\text{GDP}}^{\phi_{p,r}}$ and $\lambda_{\text{IndPro}}^{\phi_{p,r}}$ using the method of least squares (described in section 5.3).
Consequently, given $\lambda_1^{\phi_{p,r,t}}, \lambda_2^{\phi_{p,r,t}}, \lambda_3^{\phi_{p,r,t}}, \lambda_4^{\phi_{p,r,t}} \forall t \in T_0$, our parameter identification problem is

$$\min_{\lambda_{\text{GDP}}^{\phi_{p,r}}, \lambda_{\text{IndPro}}^{\phi_{p,r}}} \sum_{r \in R} \sum_{p \in P} \sum_{t \in T_0} (a_{p,r,t}^{q} - \phi_{p,r,t}^{eco}(a_{p,r,t}^{\pi}))^2 \tag{7.17a}$$

subject to

$$0 \le \lambda_{\text{GDP}}^{\phi_{p,r}}, \tag{7.17b}$$

$$0 \le \lambda_{\text{IndPro}}^{\phi_{p,r}}. \tag{7.17c}$$

This is a constrained least-squares problem that can be solved using the generalized Gauss-Newton method. We illustrate the formation of the basic demand function as well as the shifted demand function that reflects the influence of the economic factors in figure 7.1. Basically, the resulting upper bound for maximum consumption is equal to $\alpha_{p,r,t_0}^{\text{UB\_max\_quant}} + \lambda_{\text{IndPro}}^{\phi_{p,r}} \cdot a_{r,t,J}^{\text{IndPro}}$ and the maximum price at t_0 is equal to $\alpha_{p,r,t_0}^{\text{max\_price}} + \lambda_{\text{GDP}}^{\phi_{p,r}} \cdot a_{r,t,J}^{\text{GDP}}$. Note that all parameters $\lambda_1^{\phi_{p,r,t_0}}, \lambda_2^{\phi_{p,r,t_0}}, \lambda_3^{\phi_{p,r,t_0}}, \lambda_4^{\phi_{p,r,t_0}}, \lambda_{\text{GDP}}^{\phi_{p,r}}$, and $\lambda_{\text{IndPro}}^{\phi_{p,r}}$ are determined subject to a specific α_{p,r,t_0}^{mq} and α_{p,r,t_0}^{mp}.
To identify the most suitable factors for the current market situation, we propose several

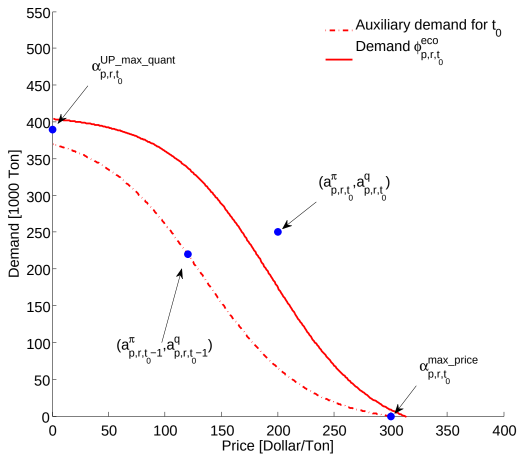

Figure 7.1: Illustration of the heuristic approach: approximation of the basic demand parameters and shift due to economic factors

factors for α^{mq}_{p,r,t_0} and α^{mp}_{p,r,t_0} and solve the supply-demand trade network optimization model developed in section 4.2 to simulate corresponding prices and sales quantities for each combination of α^{mq}_{p,r,t_0} and α^{mp}_{p,r,t_0}. In the following, these tuples are denoted by

$$(x^{\pi}_{p,r,t_0}(\alpha^{mq}_{p,r,t_0}, \alpha^{mp}_{p,r,t_0}), x^{q}_{p,r,t_0}(\alpha^{mq}_{p,r,t_0}, \alpha^{mp}_{p,r,t_0})).$$

To compare the results and detect the most reliable simulation, we further compute the deviations of the simulations from real data and construct quantitative indices that indicate the fit with the minimum deviation on average. Therefore, we compare the fits by means of three indices: the mean squared error[2] of prices $\text{MSE}_{\text{Price}}$ and sales quantities $\text{MSE}_{\text{Quantity}}$

$$\text{MSE}_{\text{Price}}(\alpha^{mq}_{p,r,t_0}, \alpha^{mp}_{p,r,t_0}) = \frac{1}{|R|}\sum_{r\in R}\left(\frac{1}{|P_{out}|}\sum_{p\in P_{out}}\left(\frac{1}{|T|}\sum_{t_0\in T}\left(1-\frac{x^{\pi}_{p,r,t_0}(\alpha^{mq}_{p,r,t_0}, \alpha^{mp}_{p,r,t_0})}{a^{\pi}_{p,r,t_0}}\right)^2\right)\right), \tag{7.18}$$

$$\text{MSE}_{\text{Quantity}}(\alpha^{mq}_{p,r,t_0}, \alpha^{mp}_{p,r,t_0}) = \frac{1}{|R|}\sum_{r\in R}\left(\frac{1}{|P_{out}|}\sum_{p\in P_{out}}\left(\frac{1}{|T|}\sum_{t_0\in T}\left(1-\frac{x^{q}_{p,r,t_0}(\alpha^{mq}_{p,r,t_0}, \alpha^{mp}_{p,r,t_0})}{a^{q}_{p,r,t_0}}\right)^2\right)\right), \tag{7.19}$$

as well as the average distance of the tuples $(x^{\pi}_{p,r,t}(\alpha^{mq}_{p,r,t_0}, \alpha^{mp}_{p,r,t_0}), x^{q}_{p,r,t}(\alpha^{mq}_{p,r,t_0}, \alpha^{mp}_{p,r,t_0}))$

[2] Note that, in some textbooks, the mean squared error is defined as the standard deviation of the model residuals (cf. Pilipovic [Pil07]).

and $(a^{\pi}_{p,r,t}, a^{q}_{p,r,t})$ in $D^{eco}_{1,p,r,t} \times D^{eco}_{2,p,r,t}$

$$\text{A\_Dis}(\alpha^{mq}_{p,r,t_0}, \alpha^{mp}_{p,r,t_0}) = \frac{1}{|R|} \sum_{r \in R} \left(\frac{1}{|P_{out}|} \sum_{p \in P_{out}} \left(\frac{1}{|T|} \sum_{t_0 \in T} \text{dist}(\alpha^{mq}_{p,r,t_0}, \alpha^{mp}_{p,r,t_0}) \right) \right), \quad (7.20)$$

where

$$\text{dist}(\alpha^{mq}_{p,r,t_0}, \alpha^{mp}_{p,r,t_0}) = \sqrt{\left(x^{q}_{p,r,t_0}(\alpha^{mq}_{p,r,t_0}, \alpha^{mp}_{p,r,t_0}) - a^{q}_{p,r,t_0}\right)^2 + \left(x^{\pi}_{p,r,t_0}(\alpha^{mq}_{p,r,t_0}, \alpha^{mp}_{p,r,t_0}) - a^{\pi}_{p,r,t_0}\right)^2}. \quad (7.21)$$

In contrast, this error measure includes both simulation results simultaneously and enables a straightforward comparison of the simulations.[3] Note that, in case we aim to determine the structure of historical demand real data of t_0 is available. To forecast the demand at time t_0 it is only possible to compare simulation of the previous times $t \in T_0$ with real data.
In the following section, we test this approach using the subsystem of the petrochemical industry already presented in section 6.3.1.

7.2.2 Application to the Petrochemical Market

We apply the approach proposed above to the subsystem presented in section 6.3.1. Thus, the optimization model simulating the price formation of this subsystem comprises the demand function of five different products $p \in P_{out} = \{1, 2, 3, 4, 5\}$ and all products are produced and sold in one region so that there is no trade included. As above, since the network under consideration has not sufficient capacity for all product, we add an additional process with fixed costs if necessary.
To solve the resulting supply-demand trade network optimization problem (cf. section 4.2), we make use of the interior point solver Ipopt-3.8.3 (see [WB06, Wä09]) through AMPL (see [FGK02]). In all examples, we assume $(\alpha^{mq}_{p,r,t_0}, \alpha^{mp}_{p,r,t_0})$ to be identical for all $p \in P_{out}$ and determine the demand parameters modeling the upper bound for the maximum quantity and the maximum price by means of max_y and the values

$$(\alpha^{mq}, \alpha^{mp}) \in \{1.3, 1.5, 1.7, 1.9\} \times \{1.2, 1.4, 1.6, 1.8\},$$

where we omit the indices for simplicity in the remaining section. Establishing the demand parameters for each combination (7.2.2), we obtain sixteen different demand models so that there are sixteen scenarios for the price formation in the petrochemical network. To distinguish, table 7.1 comprises the corresponding notation referring to each scenario according to the combination that determines the demand function. Furthermore, it remains to determine the default parameter settings for

[3] Using the distance of simulation and data tuple as error index is more suitable than comparing the profit resulting from the simulations to the historical profit. In this way, we prefer the simulations whose price and sales are both close to the original data. Analyzing, the profit is not appropriate, because, for example, a high price and a small amount can also achieve profit close to the historical one, although each single result is rather unrealistic.

	1.3	1.5	1.7	1.9
1.2	1.3_1.2	1.5_1.2	1.7_1.2	1.9_1.2
1.4	1.3_1.4	1.5_1.4	1.7_1.4	1.9_1.4
1.6	1.3_1.6	1.5_1.6	1.7_1.6	1.9_1.6
1.8	1.3_1.8	1.5_1.8	1.7_1.8	1.9_1.8

Table 7.1: Notation of the scenarios with reference to the composition used to determine the demand parameters

$$\alpha^{\text{shift}},\ T_0,\ (T_t)_{t\in T_0},\ \text{and } T.$$

to simulate prices and sales quantities of $p \in P_{out}$ for each of the sixteen scenarios by solving the supply-demand trade network optimization model. To compare the simulation results, we calculate the error statistics (7.18), (7.19), and (7.20) to which we refer as multi-product error statistics in the following. In addition, we also calculate the average distance A_Dis (error (7.20)) for each product separately by setting $P = \{p\},\ \forall p \in P_{out}$ in the formula. For this reason, the respective scenario that minimizes the average distance of the simulations to the historical values can be determined for each single product. Accordingly, we call these indices single-product error statistics. To better detect the results of each error statistic, we mark the minimum values in the respective tables with green color. Subsequently, we discuss two different applications. In section 7.2.2.1, we aim to approximate the demand function at time t^{sim} based on all information available at time t^{sim}. In section 7.2.2.2, our objective is to forecast the demand at time t^{sim} based on information up to time $t^{\text{sim}} - 1$. Obviously, the different approaches differ in T: whereas prices and sales at t^{sim} are known in the first approximation, we have to determine the optimal factors by comparing the simulations for preceding times $t \in T_0$ for which we assume that the change in the economic situation is constant in the second approach.

7.2.2.1 Approximation of Historical Demand

To summarize, we have $P_{out} = \{1, 2, 3, 4, 5\}$, $R = \{A\}$, $T_0 = \{t^{\text{sim}} - 7, \ldots, t^{\text{sim}} - 1\}$, and $T_t = \{t-4, \ldots, t-1\}$ for all $t \in T_0 \cup T$, where $T = \{t^{\text{sim}}\}$. Concerning the change in the economic situation, we set $J = 1$ (cf. section 3.3). Moreover, we assume that $\alpha^{\text{shift}} = 1$. The resulting values of the multi-product error statistics defined above are outlined in table 7.2. In general, these errors reveal that the price formation gets better results if the assumed maximum price is rather small. More precisely, for each value of α^{mq} fixed, the $\text{MSE}_{\text{Price}},\ P_{out}$ rises if α^{mp} rises. All in all, the $\text{MSE}_{\text{Price}},\ P_{out}$ achieves its minimum at combination 1.9_1.2, whereas $\text{MSE}_{\text{Quantity}},\ P_{out}$ is minimal for combination 1.3_1.6. Since these results differ, it is preferable to consider the error statistic A_Dis, P_{out} that combines both variables to get a unique decision guidance. Here, the best fit is achieved for combination 1.9_1.6. For this combination, table 7.3 provides the corresponding demand parameters. Regarding the demand parameters for the economic influence, we also present the standard deviation (STD_i) as well as values $\theta_i,\ i = \{GDP, IndPro\}$ so

Scenario	$\text{MSE}_{\text{Price}}$ P_{out}	$\text{MSE}_{\text{Quantity}}$ P_{out}	A_Dis P_{out}
1.3_1.2	0.052	0.119	534.49
1.3_1.4	0.088	0.089	485.75
1.3_1.6	0.150	0.031	496.13
1.3_1.8	0.237	0.047	672.52
1.5_1.2	0.046	0.136	559.29
1.5_1.4	0.076	0.102	486.34
1.5_1.6	0.132	0.035	467.76
1.5_1.8	0.213	0.050	638.00
1.7_1.2	0.042	0.150	577.25
1.7_1.4	0.069	0.111	490.75
1.7_1.6	0.122	0.037	451.23
1.7_1.8	0.199	0.051	618.09
1.9_1.2	0.039	0.162	589.61
1.9_1.4	0.064	0.119	496.51
1.9_1.6	0.115	0.038	440.49
1.9_1.8	0.191	0.052	605.18

Table 7.2: Multi-product error statistics A_Dis of the prices and sales quantities simulations given $\alpha^{\text{shift}} = 1$

that for the linearized confidence region $G_L(0.05)$ (cf. section 5.3.4.2 and [Boc87, Bau99, Kö02])

$$G_L(0.05) \subseteq [\lambda_{\text{GDP}}^{\phi_{p,r,t^{\text{sim}}}} - \theta_{\text{GDP}}, \lambda_{\text{GDP}}^{\phi_{p,r,t^{\text{sim}}}} + \theta_{\text{GDP}}] \times [\lambda_{\text{IndPro}}^{\phi_{p,r,t^{\text{sim}}}} - \theta_{IndPRo}, \lambda_{\text{IndPro}}^{\phi_{p,r,t^{\text{sim}}}} + \theta_{\text{IndPro}}]. \quad (7.22)$$

However, the overall result is not necessarily the best for each single product. Table 7.4 summarizes the error statistics A_Dis, $P = \{p\}$ for each single product $p \in P_{out}$ provided that the demand function for all products are determined with the same combination.[4] In this regard, solely A_Dis, $P = \{2\}$ is minimal for combination 1.9_1.6, whereas the resulting demand functions for the other products are quite different. The corresponding demand parameters together with the respective notation for the scenario combination are outlined in table 7.5. In comparison with the parameters minimizing the multi-product average distance, only the result for product 5 totally differs.
In general, we might expect that errors are smaller if the demand function for each single

[4]Since the input quantities for the market under consideration are constrained, the optimal prices and sales quantities can influence each other in case the input quantities are exhausted. Therefore, considering the price formation for each product separately does not necessarily provide an absolute decision guide.

p	$\lambda_1^{\phi_{p,r,t^{\text{sim}}}}$	$\lambda_2^{\phi_{p,r,t^{\text{sim}}}}$	$\lambda_3^{\phi_{p,r,t^{\text{sim}}}}$	$\lambda_4^{\phi_{p,r,t^{\text{sim}}}}$	$\lambda_{\text{GDP}}^{\phi_{p,r,t^{\text{sim}}}}$	$\lambda_{\text{IndPro}}^{\phi_{p,r,t^{\text{sim}}}}$
1	1483.90	3024.00	2040.90	-	0.14	1.12
STD_i					± 0.0007	± 0.3815
θ_i					± 0.0016	± 0.9339
2	4288.30	2185.62	1500.68	-	0.09	433.78
STD_i					± 0.0001	± 0.5171
θ_i					± 0.0003	± 1.2657
3	2601.10	1584.34	1015.54	-	0.00	558.46
STD_i					± 0.0000	± 0.8163
θ_i					± 0.0000	± 1.8467
4	1263.50	3216.00	2916.06	-	0.32	0.00
STD_i					± 0.0006	± 0.0000
θ_i					± 0.0014	± 0.0000
5	1609.30	2592.00	1661.44	-	0.10	212.12
STD_i					± 0.0004	± 0.5370
θ_i					± 0.0010	± 1.3143

Table 7.3: Demand parameters of the scenario 1.9_1.6 that minimizes the multi-product error A_Dis given $\alpha^{\text{shift}} = 1$ as well as standard deviations (STD) and boundaries for the 95%-confidence region of $\lambda_{\text{GDP}}^{\phi_{p,r,t^{\text{sim}}}}$ and $\lambda_{\text{IndPro}}^{\phi_{p,r,t^{\text{sim}}}}$

product is modeled separately. Therefore, we simulate prices and sales quantities based on different factors α^{mq} and α^{mp} as indicated in table 7.5. Indeed, using these demand parameters, the multi-product average distance A_Dis = 318.201, P_{out} is smaller compared to the results of table 7.2. Moreover, the results for each single product coincide with the minimum errors in table 7.4.[5] In other words, this simulation does not generate even better results for each single product, but it improves the overall market simulation. Note that A_Dis represents the absolute distance. For this reason, the specific results for each product cannot be compared with each other, i.e., the results do not reveal if prices and sales quantities can be more effectively simulated for one product than for the others.

Subsequently, we change our settings by assuming $\alpha^{\text{shift}} = 0.6$ and solve our supply-demand trade network optimization problem with $P_{out} = \{1, 2, 3, 4, 5\}$, $R = \{A\}$, $T = \{t^{\text{sim}}\}$, $T_0 = \{t^{\text{sim}} - 7, \dots, t^{\text{sim}} - 1\}$, $T_t = \{t - 4, \dots, t - 1\}$ for all $t \in T_0 \cup T$, and $J = 1$ for each scenario again. The multi-product errors are outlined in the table 7.6. The minimum $\text{MSE}_{\text{Price}}$, P_{out} is achieved at 1.9_1.2, whereas scenario 1.3_1.2 provides the best results concerning $\text{MSE}_{\text{Quantity}}$, P_{out} and A_Dis, P_{out}. For this reason, the corresponding demand parameters of 1.3_1.2 (together with standard deviation and boundaries of the 95%-confidence region) are outlined in table 7.7.

[5] This indicates that the capacities are not exhausted, i.e., the optimal prices and sales quantities are interior solutions.

Scenario	A_Dis $P = \{1\}$	A_Dis $P = \{2\}$	A_Dis $P = \{3\}$	A_Dis $P = \{4\}$	A_Dis $P = \{5\}$
1.3_1.2	90.66	799.95	675.41	679.62	426.80
1.3_1.4	111.67	328.39	798.54	874.56	315.57
1.3_1.6	295.87	306.32	393.16	1077.76	407.54
1.3_1.8	490.42	512.07	493.00	1285.45	581.67
1.5_1.2	154.48	799.57	787.07	627.93	427.42
1.5_1.4	73.71	384.39	819.73	819.05	334.83
1.5_1.6	248.56	281.94	421.15	1020.09	367.08
1.5_1.8	438.36	489.72	503.10	1224.81	534.00
1.7_1.2	202.33	799.41	864.67	592.68	427.17
1.7_1.4	57.97	422.65	830.90	784.75	357.47
1.7_1.6	221.34	268.42	435.48	986.15	344.77
1.7_1.8	409.10	476.09	508.74	1190.02	506.52
1.9_1.2	239.73	799.34	916.03	566.54	426.40
1.9_1.4	55.60	450.21	837.97	761.55	377.24
1.9_1.6	203.62	260.14	443.66	963.89	331.16
1.9_1.8	390.32	467.00	512.19	1167.58	488.79

Table 7.4: Single-product error statistics A_Dis of the prices and sales quantities simulations given $\alpha^{\text{shift}} = 1$

As above, we also compare the respective single-product average distance for each product summarized in table 7.8. In accordance with the multi-product results, scenario 1.3_1.2 minimizes the single-product average distance A_Dis, $P = \{3\}$. Combination 1.3_1.4 is most suitable for product 1 and 1.9_1.2 achieves the best result for product 4. The respective distance errors of product 2 and product 5 are minimal for combination 1.9_1.4. Table 7.9 shows the corresponding demand parameters for each product based on the different results of the single-product average distance. Remarkably, the influencing of the economic factors is given by $\lambda_{\text{GDP}}^{\phi_{p,r,t^{\text{sim}}}}$ since $\lambda_{\text{IndPro}}^{\phi_{p,r,t^{\text{sim}}}} = 0$ for all $p \in P_{out}$. However, this estimation results does not occur in every scenario simulation. To conclude, we also simulate optimal prices and sales quantities on the basis of these demand parameters. The resulting average distance A_Dis $= 271.611$ is lower than the minimum multi-product average distance. Notably, the minimum single-product average distances of this simulation are equal to those listed in table 7.8. Thus, allowing different combinations for the products $p \in P_{out}$ leads to a better market simulation.

p	$\lambda_1^{\phi_{p,r,t}\text{sim}}$	$\lambda_2^{\phi_{p,r,t}\text{sim}}$	$\lambda_3^{\phi_{p,r,t}\text{sim}}$	$\lambda_4^{\phi_{p,r,t}\text{sim}}$	$\lambda_{\text{GDP}}^{\phi_{p,r,t}\text{sim}}$	$\lambda_{\text{IndPro}}^{\phi_{p,r,t}\text{sim}}$
1 (1.9_1.4)	1483.90	2646.00	1394.79	-	0.13	0.00
STD_i					±0.0005	±0.0000
θ_i					±0.0010	±0.0000
2 (1.9_1.6)	4288.30	2185.62	1500.68	-	0.09	433.78
STD_i					±0.0001	±0.5171
θ_i					±0.0003	±1.2657
3 (1.3_1.6)	1779.70	1584.34	583.37	-	0.00	333.22
STD_i					±0.0000	±0.5229
θ_i					±0.0000	±1.1828
4 (1.9_1.2)	1263.50	2412.00	1541.79	-	0.35	0.00
STD_i					±0.0003	±0.0000
θ_i					±0.0006	±0.0000
5 (1.3_1.4)	1101.10	2268.00	636.27	-	0.13	163.96
STD_i					±0.0004	±0.3907
θ_i					±0.0009	±0.9562

Table 7.5: Demand parameters of the respective scenario that minimizes the single-product error A_Dis given $\alpha^{\text{shift}} = 1$ as well as standard deviations (STD) and boundaries for the 95%-confidence region of $\lambda_{\text{GDP}}^{\phi_{p,r,t}\text{sim}}$ and $\lambda_{\text{IndPro}}^{\phi_{p,r,t}\text{sim}}$

Remark 7.1. Comparing the results with each other, the lower average distance is achieved with $\alpha^{\text{shift}} = 0.6$. Namely, combination 1.3_1.2 achieves as minimum average distance A_Dis = 335.391, P_{out}, whereas combination 1.9_1.6 with $\alpha^{\text{shift}} = 1$ results in A_Dis = 440.492, P_{out}. Likewise, simulating prices and sales quantities on the basis of different factors α^{mq} and α^{mp} the average distance is lower for $\alpha^{\text{shift}} = 0.6$ than for $\alpha^{\text{shift}} = 1$. Consequently, our results reveal that further simulations with different factors α^{mq} and α^{mp} as well as different shifting factors might be beneficial. Note that considering the single-product average distance results, lower values are achieved for products 1, 2, 4, and 5 with $\alpha^{\text{shift}} = 0.6$ and for product 3 with $\alpha^{\text{shift}} = 1$. Figures 7.2 to 7.6 show the corresponding demand functions together with the auxiliary demand function and historical data. Notably, the demand function imply considerably high consumption for low prices, but if price increases demand strongly decreases.

Scenario	$\text{MSE}_{\text{Price}}$ P_{out}	$\text{MSE}_{\text{Quantity}}$ P_{out}	A_Dis P_{out}
1.3_1.2	0.038	0.038	335.39
1.3_1.4	0.062	0.056	382.90
1.3_1.6	0.093	0.073	446.85
1.3_1.8	0.143	0.077	544.160
1.5_1.2	0.035	0.061	394.49
1.5_1.4	0.051	0.061	368.93
1.5_1.6	0.081	0.071	450.17
1.5_1.8	0.124	0.082	513.66
1.7_1.2	0.033	0.090	453.09
1.7_1.4	0.045	0.066	361.34
1.7_1.6	0.074	0.077	451.72
1.7_1.8	0.122	0.100	586.42
1.9_1.2	0.031	0.121	502.41
1.9_1.4	0.0410	0.070	356.63
1.9_1.6	0.070	0.079	442.33
1.9_1.8	0.117	0.103	581.14

Table 7.6: Multi-product error statistics A_Dis of the price and sales quantities simulations given $\alpha^{\text{shift}} = 0.6$

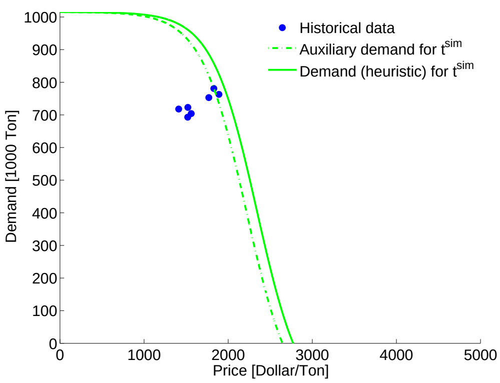

Figure 7.2: Demand function for product 1 at t^{sim}: result of the heuristic approach

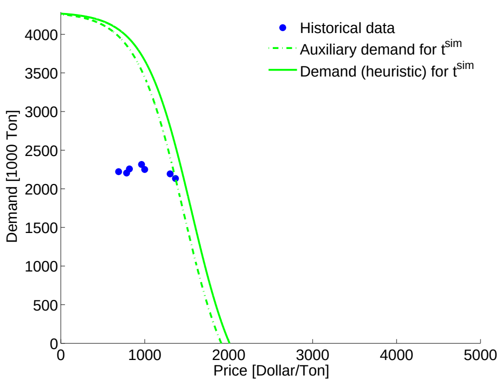

Figure 7.3: Demand function for product 2 at t^{sim}: result of the heuristic approach

7.2.2.2 Forecast of Future Demand

As above, we set $P_{out} = \{1, 2, 3, 4, 5\}$, $R = \{A\}$, $J = 1$, $T_0 = \{t^{\text{sim}} - 7, \dots, t^{\text{sim}} - 1\}$, and $T_t = \{t - 4, \dots, t - 1\}$ for all $t \in T_0 \cup T$, where, in contrast, $T = \{t^{\text{sim}} - 1\}$. We simulate optimal prices and sales quantities by solving the supply-demand trade network optimization problem for $\alpha^{\text{shift}} \in \{0.6, 1\}$. Here, we do not specify all results of

p	$\lambda_1^{\phi_{p,r,t^{\text{sim}}}}$	$\lambda_2^{\phi_{p,r,t^{\text{sim}}}}$	$\lambda_3^{\phi_{p,r,t^{\text{sim}}}}$	$\lambda_4^{\phi_{p,r,t^{\text{sim}}}}$	$\lambda_{\text{GDP}}^{\phi_{p,r,t^{\text{sim}}}}$	$\lambda_{\text{IndPro}}^{\phi_{p,r,t^{\text{sim}}}}$
1	609.18	2036.46	287.73	406.12	0.16	0.00
STD$_i$					±0.0003	±0.0000
θ_i					±0.0008	±0.0000
2	1760.46	1484.03	192.85	1173.64	0.15	0.00
STD$_i$					±0.0000	±0.0000
θ_i					±0.0001	±0.0000
3	1067.82	1083.56	130.10	711.88	0.16	0.00
STD$_i$					±0.0002	±0.0000
θ_i					±0.0003	±0.0000
4	518.70	1935.17	592.54	345.80	0.39	0.00
STD$_i$					±0.0003	±0.0000
θ_i					±0.0008	±0.0000
5	660.66	1772.72	212.84	440.44	0.27	0.00
STD$_i$					±0.0004	±0.0000
θ_i					±0.0008	±0.0000

Table 7.7: Demand parameters of the scenario 1.3_1.2 that minimizes the multi-product error A_Dis given $\alpha^{\text{shift}} = 0.6$ as well as standard deviations (STD) and boundaries for the 95%-confidence region of $\lambda_{\text{GDP}}^{\phi_{p,r,t^{\text{sim}}}}$ and $\lambda_{\text{IndPro}}^{\phi_{p,r,t^{\text{sim}}}}$

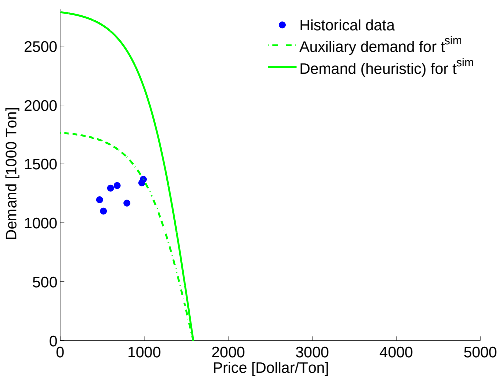

Figure 7.4: Demand function for product 3 at t^{sim}: result of the heuristic approach

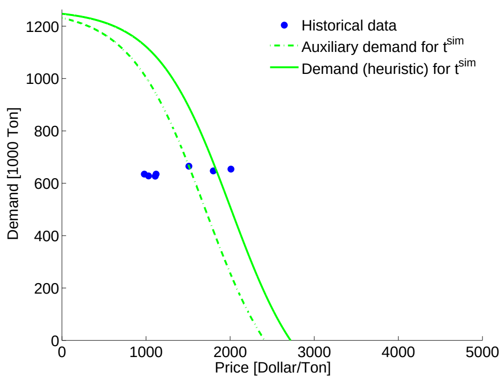

Figure 7.5: Demand function for product 4 at t^{sim}: result of the heuristic approach

A_Dis as above, but only give the result of comparing the minimum distances in table 7.10. Notably, the forecasted demand parameters for product 2 and 4 are identical to the results in section 7.2.2.1. The corresponding demand parameters are indicated in table 7.11 together with standard deviation and approximated boundaries for the 95%-confidence region.
In the course of this section, we will test the predictive value of this approach and compare

Scenario	A_Dis $P = \{1\}$	A_Dis $P = \{2\}$	A_Dis $P = \{3\}$	A_Dis $P = \{4\}$	A_Dis $P = \{5\}$
1.3_1.2	143.07	205.14	565.65	575.25	187.85
1.3_1.4	44.46	234.50	679.13	729.70	226.68
1.3_1.6	159.81	172.52	757.95	894.72	249.27
1.3_1.8	310.99	243.51	779.02	1065.71	321.56
1.5_1.2	233.55	354.93	635.83	546.58	201.56
1.5_1.4	79.86	195.66	733.48	669.74	165.93
1.5_1.6	103.43	358.06	725.92	829.79	233.68
1.5_1.8	261.27	243.38	804.55	1005.73	253.38
1.7_1.2	308.10	478.37	696.39	531.62	250.95
1.7_1.4	118.69	168.66	770.78	631.14	117.45
1.7_1.6	77.52	390.97	744.02	794.71	251.35
1.7_1.8	225.83	576.09	772.59	968.56	389.01
1.9_1.2	370.79	577.34	749.01	513.72	301.18
1.9_1.4	148.41	150.73	796.27	604.22	83.50
1.9_1.6	65.32	386.24	756.71	773.12	230.29
1.9_1.8	208.72	578.45	782.51	950.21	385.82

Table 7.8: Single-product error statistics A_Dis of the price and sales quantities simulations given $\alpha^{\text{shift}} = 0.6$

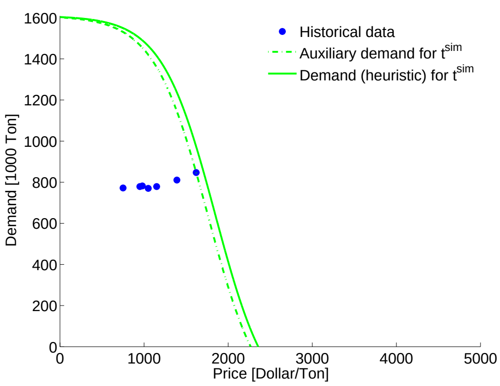

Figure 7.6: Demand function for product 5 at t^{sim}: result of the heuristic approach

the simulation results for t^{sim} with forecasts provided by the parameter identification problem presented in section 7.3.

p	$\lambda_1^{\phi_{p,r,t^{\text{sim}}}}$	$\lambda_2^{\phi_{p,r,t^{\text{sim}}}}$	$\lambda_3^{\phi_{p,r,t^{\text{sim}}}}$	$\lambda_4^{\phi_{p,r,t^{\text{sim}}}}$	$\lambda_{\text{GDP}}^{\phi_{p,r,t^{\text{sim}}}}$	$\lambda_{\text{IndPro}}^{\phi_{p,r,t^{\text{sim}}}}$
1 (1.3_1.4)	609.18	2214.63	536.05	406.12	0.15	0.00
STD_i					±0.0005	±0.0000
θ_i					±0.0012	±0.0000
2 (1.9_1.4)	2572.98	1458.60	563.94	1715.32	0.12	0.00
STD_i					±0.0001	±0.0000
θ_i					±0.0002	±0.0000
3 (1.3_1.2)	1067.82	1083.56	130.10	711.88	0.16	0.00
STD_i					±0.0002	±0.0000
θ_i					±0.0003	±0.0000
4 (1.9_1.2)	758.10	1699.29	885.67	505.40	0.36	0.00
STD_i					±0.0002	±0.0000
θ_i					±0.0005	±0.0000
5 (1.9_1.4)	965.58	1755.98	636.27	643.72	0.11	0.00
STD_i					±0.0003	±0.0000
θ_i					±0.0007	±0.0000

Table 7.9: Demand parameters of the respective scenario that minimizes the single-product error A_Dis given $\alpha^{\text{shift}} = 0.6$ as well as standard deviations (STD) and boundaries for the 95%-confidence region of $\lambda_{\text{GDP}}^{\phi_{p,r,t^{\text{sim}}}}$ and $\lambda_{\text{IndPro}}^{\phi_{p,r,t^{\text{sim}}}}$

Minimum A_Dis	P_{out}	$P = \{1\}$	$P = \{2\}$	$P = \{3\}$	$P = \{4\}$	$P = \{5\}$
Shift	0.6	0.6	0.6	0.6	0.6	1
Scenario	1.3_1.2	1.5_1.4	1.9_1.4	1.5_1.2	1.9_1.2	1.3_1.4

Table 7.10: Overview of scenarios that minimize A_Dis, P_{out} and A_Dis, $P = \{p\}$ for all $p \in P_{out}$ at time $t^{\text{sim}} - 1$ in order to forecast demand at time t^{sim}

7.2.3 Discussion

The structure of this method is rather elaborate and, in addition, the examples presented above reveal that it is not geared to providing a parameter identification that is widely accepted, since there are too many factors and additional assumptions that have to be made prior to the identification process. In addition, we only search for optimal parameters over a discrete set of factors $\alpha_{p,r,t}^{mq}$, $\alpha_{p,r,t}^{mp}$, and α^{shift}. Moreover, since this approach includes the assumption that closeness of the simulations to the historical values is a good indicator for the most appropriate demand function, complete data of all regions is needed to accurately model the price formation in the whole market. Therefore, we only refer to the results of this identification approach as approximation.
Here, the results are obtained by optimizing prices and sales quantities of a single region. Extending the optimization model to multiple regions gives rise to additional influencing

p	$\lambda_1^{\phi_{p,r,t^{\text{sim}}}}$	$\lambda_2^{\phi_{p,r,t^{\text{sim}}}}$	$\lambda_3^{\phi_{p,r,t^{\text{sim}}}}$	$\lambda_4^{\phi_{p,r,t^{\text{sim}}}}$	$\lambda_{\text{GDP}}^{\phi_{p,r,t^{\text{sim}}}}$	$\lambda_{\text{IndPro}}^{\phi_{p,r,t^{\text{sim}}}}$
1 (1.5_1.4/0.6)	702.90	2133.98	636.27	468.60	0.14	0.00
STD_i					±0.0004	±0.0000
θ_i					±0.0009	±0.0000
2 (1.9_1.4/0.6)	2572.98	1458.60	563.94	1715.32	0.12	0.00
STD_i					±0.0001	±0.0000
θ_i					±0.0002	±0.0000
3 (1.5_1.2/0.6)	1232.10	1063.99	154.42	821.40	0.15	0.00
STD_i					±0.0001	±0.0000
θ_i					±0.0002	±0.0000
4 (1.9_1.2/0.6)	758.10	1699.29	885.67	505.40	0.36	0.00
STD_i					±0.0002	±0.0000
θ_i					±0.0005	±0.0000
5 (1.3_1.4/1)	1101.10	2268.00	636.27	-	0.13	163.96
STD_i					±0.0004	±0.3907
θ_i					±0.0009	±0.9562

Table 7.11: Demand parameters of scenarios that minimize A_Dis, $P = \{p\}$ for all $p \in P_{out}$ at time $t^{\text{sim}} - 1$ in order to forecast demand at time t^{sim}

factors on demand. For example, trade between these regions might also have crucial influence on the simulation results and, hence, also on the determination of the demand functions according to this scheme.
However, this method provides some benefits. First, this method is able to yield reasonable demand function approximations that provide a lot of information for further studies. Moreover, it allows to test additional assumptions and conduct further scenario simulations to analyze the effects of input factors (e.g., the effect of changes in the economic parameters or the production settings) on optimal prices and sales quantities, but also on the market model in general. Nevertheless, as more simulations have to be made, the more time-consuming this method is. This motivates us to look for an alternative method still having in mind the conclusions we can draw from the presented heuristic approach. For example, the historical prices and sales quantities show a different structure for each product that is also reflected in the parameter estimates. Consequently, the results of this procedure reveal the importance of estimating the demand function of each product separately. Therefore, in the next step, we investigate a parameter identification method reduced to the product-specific data.

7.3 Development of an Optimization Model to Identify Demand Parameters

In this section, we set up a least-squares optimization problem to identify the parameters of the *tanh-demand model* (7.1). As mentioned above, further assumptions are necessary to compensate the insufficiency of data regarding the demand in low or high price ranges. In the following, we summarize the additional assumptions that are required to enable an efficient parameter identification and present our resulting parameter identification problem. As above, we test this approach using data from a small subsystem of the petrochemical network and illustrate the results below.

7.3.1 Parameter Identification Problem (PIP)

The least-squares method described in section 5.3 is an appropriate tool for various parameter estimation problems. Likewise, our objective is to identify parameters using this approach. Before setting up the parameter identification based on least-squares estimation, further assumptions are required (cf. section 7.1).

Assumptions 7.5. *Assumptions regarding the optimization problem*

1. *As specified in section 6.2,* $\lambda_i^{\phi_{p,r,t}} \geq 0,\ i = 1, 2, 4,\ \lambda_3^{\phi_{p,r,t}} > 0$ *and* $\lambda_k^{\phi_{p,r,t}} \geq 0,\ k \in \{GDP, IndPro\}$.

2. *Suppose we aim to identify the parameters at time* t_0*. Given a data set* T_{t_0} *consisting of prices and sales quantities of selected past years that are supposed to influence the situation at time* t_0*, we suggest that it is more likely that recent data satisfies the demand function at time* t_0 *than older data.*[6] *To integrate this assumption we add weighting factors to each residual in the least-squares functional, where we attach greater weight to more recent data and smaller weight to older data. In particular, we define*
$$w_t = \lambda \cdot (1-\lambda)^{t-1} \quad t = 1, \ldots, T_{t_0}, \tag{7.23}$$
where $0 < \lambda < 1$*. In other words, we assume that the variance of the errors* $\left(a^q_{p,r,t} - \phi^{eco}_{p,r,t_0}\left(a^\pi_{p,r,t}\right)\right),\ t \in T_{t_0}$ *is time-dependent and increases if* $t_0 - t$ *increases.*

3. *We assume that our data is located in the second price range. In other words, we suggest that the demand function is strictly decreasing at historical prices* $a^\pi_{p,r,t},\ t \in T_{t_0}$*, given the economic situation, i.e.,*
$$\begin{aligned}&\frac{\partial \phi^{eco}_{p,r,t_0}}{\partial x^\pi_{p,r,t_0}}(a^\pi_{p,r,t})\\ &= -\frac{\lambda_1^{\phi_{p,r,t_0}} + \lambda_{\text{IndPro}}^{\phi_{p,r,t_0}} \cdot \Delta a^{\text{IndPro}}_{r,t_0,J}}{\lambda_3^{\phi_{p,r,t_0}}} \cdot \text{sech}^2\left(\frac{\lambda_2^{\phi_{p,r,t_0}} + \lambda_{\text{GDP}}^{\phi_{p,r,t_0}} \cdot \Delta a^{\text{GDP}}_{r,t_0,J} - a^\pi_{p,r,t}}{\lambda_3^{\phi_{p,r,t_0}}}\right) \leq s,\end{aligned} \tag{7.24}$$

[6] Compare assumption 7.1 and 7.2 in the heuristic approach: under the assumption of no change in the economic situation from time $t_0 - 1$ to t_0 the data of $t_0 - 1$ satisfies the demand function at time t_0.

where $s < 0$.

4. *In addition, we assume that in the first price range, the demand function is almost constant, i.e., we assume that the derivative w.r.t.* $x^{\pi}_{p,r,t}$ *at* $a^{\pi}_{p,r,t} = 0$ *is approximately zero:*

$$0 > \frac{\partial \phi^{eco}_{p,r,t_0}}{\partial x^{\pi}_{p,r,t_0}}(0) \geq a, \tag{7.25}$$

where $a \gg -1$*. That means, we assume that*

$$-\frac{\lambda_1^{\phi_{p,r,t_0}} + \lambda_{\text{IndPro}}^{\phi_{p,r,t_0}} \cdot \Delta a^{\text{IndPro}}_{r,t_0,J}}{\lambda_3^{\phi_{p,r,t_0}}} \cdot \operatorname{sech}^2\left(\frac{\lambda_2^{\phi_{p,r,t_0}} + \lambda_{\text{GDP}}^{\phi_{p,r,t_0}} \cdot \Delta a^{\text{GDP}}_{r,t_0,J}}{\lambda_3^{\phi_{p,r,t_0}}}\right) \geq a, \tag{7.26}$$

where $0 > a > s$.

To include those assumptions in the parameter identification, we gain from the characteristics of the sech-function. In addition, we establish the following notation: $\overline{a}^{\pi}_{p,r,t_0}$ is the maximum price for all $t_0 \in T_{t_0}$ and $\underline{a}^{\pi}_{p,r,t_0}$ is the minimum price for all $t \in T_{t_0}$. Regarding inequality (7.24), if

$$\lambda_2^{\phi_{p,r,t_0}} + \lambda_5^{\phi_{p,r,t_0}} \cdot \Delta a^{\text{GDP}}_{r,t_0,J} - \overline{a}^{\pi}_{p,r,t_0} \geq 0, \tag{7.27}$$

we obtain

$$\begin{aligned} 0 \leq \operatorname{sech}^2\left(\frac{\lambda_2^{\phi_{p,r,t_0}} + \lambda_{\text{GDP}}^{\phi_{p,r,t_0}} \cdot \Delta a^{\text{GDP}}_{r,t_0,J} - \overline{a}^{\pi}_{p,r,t_0}}{\lambda_3^{\phi_{p,r,t_0}}}\right) & \\ \leq \operatorname{sech}^2\left(\frac{\lambda_2^{\phi_{p,r,t_0}} + \lambda_{\text{GDP}}^{\phi_{p,r,t_0}} \cdot \Delta a^{\text{GDP}}_{r,t_0,J} - a^{\pi}_{p,r,t_0}}{\lambda_3^{\phi_{p,r,t_0}}}\right) & \\ \leq \operatorname{sech}^2\left(\frac{\lambda_2^{\phi_{p,r,t_0}} + \lambda_{\text{GDP}}^{\phi_{p,r,t_0}} \cdot \Delta a^{\text{GDP}}_{r,t_0,J} - \underline{a}^{\pi}_{p,r,t_0}}{\lambda_3^{\phi_{p,r,t_0}}}\right) & \end{aligned} \tag{7.28}$$

for all $t \in T_{t_0}$. Therefore, it suffices to require that the inequality (7.24) holds at the historical minimum price instead of including this inequality for all prices $a^{\pi}_{p,r,t}$, $t \in \{t_0 - 1, \ldots, t_0 - J\}$.
Next, we investigate which values $\Delta a^{\text{GDP}}_{r,t}$ and $\Delta a^{\text{IndPro}}_{r,t}$, $t \in T_{t_0}$ have the most adverse effect to the derivative with respect to the price of the demand function. In other words, we determine the worst-case scenario of the historical values, since we have no information about the real development of the economic situation at time t_0, i.e., $\Delta a^{\text{GDP}}_{r,t_0,J}$ and $\Delta a^{\text{IndPro}}_{r,t_0,J}$. If inequality (7.24) is also satisfied for these values, it is supposed to hold under more moderate conditions. Obviously, the absolute value of the derivative is smallest for minimum change in the index of industrial production $\underline{\Delta a}^{\text{IndPro}}_{r,t_0,J}$. Furthermore, if

$$\lambda_2^{\phi_{p,r,t_0}} + \lambda_{\text{GDP}}^{\phi_{p,r,t_0}} \cdot \underline{\Delta a}^{\text{GDP}}_{r,t_0,J} - \overline{a}^{\pi}_{p,r,t_0} \geq 0, \tag{7.29}$$

i.e.,

$$\operatorname{sech}\left(\frac{\lambda_2^{\phi_{p,r,t_0}} + \lambda_{\text{GDP}}^{\phi_{p,r,t_0}} \cdot \underline{\Delta} a_{r,t_0,J}^{\text{GDP}} - \overline{a}_{p,r,t_0}^{\pi}}{\lambda_3^{\phi_{p,r,t_0}}}\right) \geq 0, \tag{7.30}$$

the derivative with respect to the price is closest to zero for the maximum change of the gross domestic product $\overline{\Delta} a_{r,t}^{\text{GDP}}$ (cf. equation (7.28)). Thus, it suffices to require

$$-\frac{\lambda_1^{\phi_{p,r,t_0}} + \lambda_{\text{IndPro}}^{\phi_{p,r,t_0}} \cdot \underline{\Delta} a_{r,t_0,J}^{\text{IndPro}}}{\lambda_3^{\phi_{p,r,t_0}}} \cdot \operatorname{sech}^2\left(\frac{\lambda_2^{\phi_{p,r,t_0}} + \lambda_{\text{GDP}}^{\phi_{p,r,t_0}} \cdot \overline{\Delta} a_{r,t_0,J}^{\text{GDP}} - \underline{a}_{p,r,t_0}^{\pi}}{\lambda_3^{\phi_{p,r,t_0}}}\right) \leq s \tag{7.31}$$

and

$$\lambda_2^{\phi_{p,r,t_0}} + \lambda_{\text{GDP}}^{\phi_{p,r,t_0}} \cdot \underline{\Delta} a_{r,t_0,J}^{\text{GDP}} - \overline{a}_{p,r,t_0}^{\pi} \geq 0 \tag{7.32}$$

in the parameter identification problem. Likewise, we can reduce the number of inequalities expressing the saturation quantity at price zero to one. Contrary to above, we determine the worst-case-scenario such that there is an upper bound on the derivative. Restricted to the historical data, the derivative is at its maximum for maximum change of the index of industrial production, $\overline{\Delta} a_{r,t_0,J}^{\text{IndPro}}$, and for minimum change of the GDP, $\underline{\Delta} a_{r,t_0,J}^{\text{GDP}}$, provided that $\lambda_2^{\phi_{p,r,t_0}} + \lambda_{\text{GDP}}^{\phi_{p,r,t_0}} \cdot \underline{\Delta} a_{r,t_0,J}^{\text{GDP}} - \overline{a}_{p,r,t_0}^{\pi} \geq 0$. Thus, by including

$$-\frac{\lambda_1^{\phi_{p,r,t_0}} + \lambda_{\text{IndPro}}^{\phi_{p,r,t_0}} \cdot \overline{\Delta} a_{r,t_0,J}^{\text{IndPro}}}{\lambda_3^{\phi_{p,r,t_0}}} \cdot \operatorname{sech}^2\left(\frac{\lambda_2^{\phi_{p,r,t_0}} + \lambda_{\text{GDP}}^{\phi_{p,r,t_0}} \cdot \underline{\Delta} a_{r,t_0,J}^{\text{GDP}}}{\lambda_3^{\phi_{p,r,t_0}}}\right) \geq a, \tag{7.33}$$

we ensure that inequality (7.25) is satisfied if the change in the economic situation does not exceed the presumed worst case.[7]

Including these inequalities leads to a constrained weighted least-squares problem, which will be presented and explained in the following. In contrast to our heuristic approach, we do not predetermine some parameters, but estimate all six parameters simultaneously. The parameter identification problem (PIP) is then given by

$$\min_{\substack{\lambda_1^{\phi_{p,r,t_0}},\, \lambda_2^{\phi_{p,r,t_0}},\, \lambda_3^{\phi_{p,r,t_0}},\\ \lambda_4^{\phi_{p,r,t_0}},\, \lambda_{\text{GDP}}^{\phi_{p,r,t_0}},\, \lambda_{\text{IndPro}}^{\phi_{p,r,t_0}}}} \sum_{t \in T_{t_0}} \left(w_t \cdot \left(a_{p,r,t}^{q} - \phi_{p,r,t_0}^{eco}\left(a_{p,r,t}^{\pi}\right)\right)\right)^2 \tag{7.34a}$$

subject to

$$0 \leq \lambda_1^{\phi_{p,r,t_0}} + \lambda_{\text{IndPro}}^{\phi_{p,r,t_0}} \cdot \underline{\Delta} a_{r,t_0,J}^{\text{IndPro}} - \lambda_4^{\phi_{p,r,t_0}}, \tag{7.34b}$$

$$0 \leq \lambda_2^{\phi_{p,r,t_0}} + \lambda_{\text{GDP}}^{\phi_{p,r,t_0}} \cdot \underline{\Delta} a_{r,t_0,J}^{\text{GDP}} - \overline{a}_{p,r,t_0}^{\pi}, \tag{7.34c}$$

$$s^{pos} \leq \lambda_3^{\phi_{p,r,t_0}}, \tag{7.34d}$$

[7] Note that our resulting restrictions are sufficient but not necessary for the assumptions to hold. Moreover, in general, the change of GDP and the change of the index for industrial production is not supposed to be extremely reverse, i.e., if one of the indices heavily decreases, the other one does not heavily increase at the same time.

$$0 \leq \lambda_4^{\phi_{p,r,t_0}}, \tag{7.34e}$$

$$0 \leq \lambda_k^{\phi_{p,r,t_0}} \quad k \in \{GDP, IndPro\}, \tag{7.34f}$$

$$0 \leq \frac{\lambda_1^{\phi_{p,r,t_0}} + \lambda_{\text{IndPro}}^{\phi_{p,r,t_0}} \cdot \underline{\Delta} a_{r,t_0,J}^{\text{IndPro}}}{\lambda_3^{\phi_{p,r,t_0}}} \cdot \text{sech}^2 \left(\frac{\lambda_2^{\phi_{p,r,t_0}} + \lambda_{\text{GDP}}^{\phi_{p,r,t_0}} \cdot \overline{\Delta} a_{r,t_0,J}^{\text{GDP}} - \underline{a}_{p,r,t_0}^{\pi}}{\lambda_3^{\phi_{p,r,t_0}}} \right) + s, \tag{7.34g}$$

and

$$0 \leq -\frac{\lambda_1^{\phi_{p,r,t_0}} + \lambda_{\text{IndPro}}^{\phi_{p,r,t_0}} \cdot \overline{\Delta} a_{r,t_0,J}^{\text{IndPro}}}{\lambda_3^{\phi_{p,r,t_0}}} \cdot \text{sech}^2 \left(\frac{\lambda_2^{\phi_{p,r,t_0}} + \lambda_{\text{GDP}}^{\phi_{p,r,t_0}} \cdot \underline{\Delta} a_{r,t_0,J}^{\text{GDP}}}{\lambda_3^{\phi_{p,r,t_0}}} \right) - a. \tag{7.34h}$$

Constraints (7.34b) to (7.34f) are due to theorem 6.2 in section 6.2.2. Note that the factor $s^{pos} > 0$ is inserted in equation (7.34d) to ensure $\lambda_3^{\phi_{p,r,t_0}} > 0$.[8] Additionally, we include the constraints (7.34g) and (7.34h) mentioned above that reflect our assumptions concerning the shape the demand function.
In the subsequent section, we apply this parameter identification approach to the subsystem of the petrochemical network that was already used to test the first method in section 7.2.

7.3.2 Forecast of Future Demand

We implemented the generalized Gauss-Newton algorithm described in section 5.3.3 in MATLAB using active set methods to solve the quadratic subproblems. To test our method, we solve the parameter identification problem (PIP) for the five products with external demand $P_{out} = \{1, 2, 3, 4, 5\}$ of the subsystem that we already considered in section 6.3 and 7.2.2. We set $J = 1$ to compute the change in the economic situation (cf. section 3.3) and $T_{t^{\text{sim}}} = \{t^{\text{sim}} - 10, \ldots, t^{\text{sim}} - 1\}$. We include the exponential weighting factors with $\lambda = 0.4$. Moreover, we select $s = -0.03$, $a = -0.01$, and $s^{pos} = 1$ and set the initial values equal to the respective best results of our heuristic approach. The algorithm converges to a local solution for all products except products 3 and 4.[9] Therefore, we start with solving a subproblem by reducing the number of data $\{t^{\text{sim}} - 10, \ldots, t^{\text{sim}} - 5\}$. Then, we use these solutions as initial values in order to solve the PIP based on the whole range of data, which leads to a solution on this occasion. The resulting demand parameters for t^{sim} are presented in table 7.12. Likewise, we calculate the standard deviation (STD_i) and approximated boundaries for the 95%-confidence region θ_i for all parameters $\lambda_i^{\phi_{p,r,t^{\text{sim}}}}$, $i = \{1, 2, 3, 4, GDP, IndPro\}$. If the estimated parameters are equal to zero (e.g., $\lambda_4^{\phi_{p,r,t^{\text{sim}}}}$ and $\lambda_{\text{GDP}}^{\phi_{p,r,t^{\text{sim}}}}$ for $p = 1$), the corresponding constraints are active (e.g.,

[8] Note that $\lambda_3^{\phi_{p,r,t_0}}$ controls the rapidness of the negative hyperbolic tangent to decrease. The bigger $\lambda_3^{\phi_{p,r,t_0}}$, the smaller $\tanh((\lambda_2^{\phi_{p,r,t_0}} + \lambda_{\text{GDP}}^{\phi_{p,r,t_0}} \cdot \Delta a_{r,t_0,J}^{\text{GDP}} - x_{p,r,t}^{\pi})/\lambda_3^{\phi_{p,r,t_0}})$ given $x_{p,r,t}^{\pi} \leq \lambda_2^{\phi_{p,r,t_0}}$, $t \in T_{t_0}$, i.e., the smaller the price $a_{p,r,t}^{\pi}$ for which $\tanh((\lambda_2^{\phi_{p,r,t_0}} + \lambda_{\text{GDP}}^{\phi_{p,r,t_0}} \cdot \Delta a_{r,t_0,J}^{\text{GDP}} - x_{p,r,t}^{\pi})/\lambda_3^{\phi_{p,r,t_0}}) \approx 0$.

[9] The algorithm stops if $\|(\lambda_1^{\phi_{p,r,t_0}}, \lambda_2^{\phi_{p,r,t_0}}, \lambda_3^{\phi_{p,r,t_0}}, \lambda_4^{\phi_{p,r,t_0}}, \lambda_{\text{GDP}}^{\phi_{p,r,t_0}}, \lambda_{\text{IndPro}}^{\phi_{p,r,t_0}})'\|_2 \leq 10^{-7}$.

p		$\lambda_1^{\phi_{p,r,t^{\text{sim}}}}$	$\lambda_2^{\phi_{p,r,t^{\text{sim}}}}$	$\lambda_3^{\phi_{p,r,t^{\text{sim}}}}$	$\lambda_4^{\phi_{p,r,t^{\text{sim}}}}$	$\lambda_{\text{GDP}}^{\phi_{p,r,t^{\text{sim}}}}$	$\lambda_{\text{IndPro}}^{\phi_{p,r,t^{\text{sim}}}}$	Iter.
1		817.29	5925.00	2400.30	0.00	0.00	7.54	8
	STD_i	±3.51	±63.49	±39.78	±0.00	±0.00	±3.19	
	θ_i	±10.49	±189.59	±118.79	±0.00	±0.00	±9.53	
2		2271.70	2205.70	502.41	0.00	0.04	6.81	14
	STD_i	±5.32	±82.04	±50.17	±0.00	±0.03	±5.29	
	θ_i	±22.65	±349.36	±213.65	±0.00	±0.12	±22.55	
3		696.32	2179.10	733.30	702.45	0.00	1.50	12
	STD_i	±7.93	±36.82	±16.18	±6.04	±0.00	±3.37	
	θ_i	±23.67	±109.95	±48.31	±18.05	±0.00	±10.07	
4		702.27	4123.10	1558.80	0.00	0.00	19.16	10
	STD_i	±3.34	±55.83	±32.11	±0.00	±0.00	±3.79	
	θ_i	±9.98	±166.73	±95.88	±0.00	±0.00	±11.31	
5		445.37	3242.20	1327.60	445.37	0.00	0.00	8
	STD_i	±1.00	±1.68	±0.08	±1.00	±0.00	±0.00	
	θ_i	±2.27	±3.80	±0.19	±2.27	±0.00	±0.00	

Table 7.12: Demand parameter results of the PIP for t^{sim}

constraint (7.34e) and (7.34f) for $k = GDP$ and $p = 1$). In this case, the standard deviation is also zero, which indicates that the parameters can be neglected for the product under consideration at time t^{sim}.
In addition to these active inequalities, the choice of s and a provokes that the corresponding constraints (7.34g) and (7.34h) are also active at the solution for all $p \in P_{out}$. Thus, additional assumptions in this manner are necessary in order to get a reliable parameter identification. Selecting values for s and a that are closer to zero can provoke that the generalized Gauss-Newton algorithm does not converge.[10] To conclude, figures 7.7 to 7.11 show the resulting demand functions together with the historical data. Notably, the consumption for price zero is in the price range of the historical data, and the demand function slowly decreases if price rises so that the customer's willingness to buy is high. In chapter 7.4, we return to these results by simulating prices and sales quantities integrating the demand functions in the supply-demand trade network optimization problem.

7.3.3 Discussion

Because of the insufficient data available, applying the method of least-squares to estimate demand parameters of the *tanh-demand model eco* relies on additional assumptions that can change the result considerably. Therefore, the additional components have to be selected carefully such that the assumptions 7.5 are well integrated. These are the set

[10] In the subsequent section, we discuss an alternative approach to include additional assumptions in the PIP. However, these are more restrictive than the constraints (7.34g) and (7.34h).

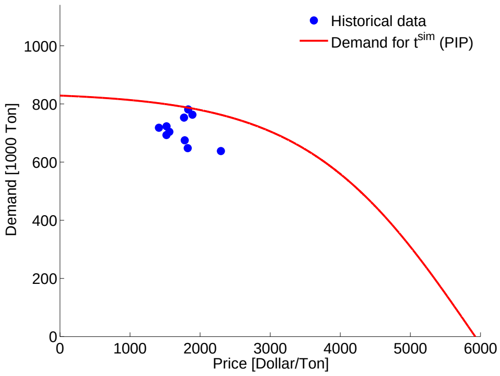

Figure 7.7: Demand function for product 1 at t^{sim}: optimal solution of the PIP

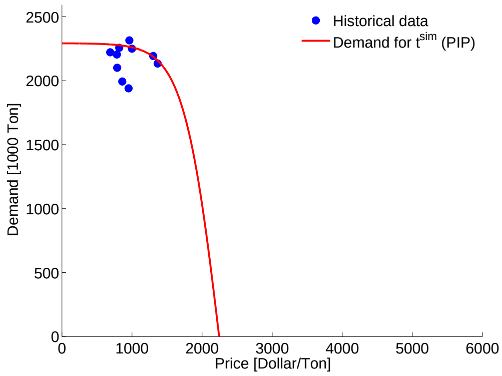

Figure 7.8: Demand function for product 2 at t^{sim}: optimal solution of the PIP

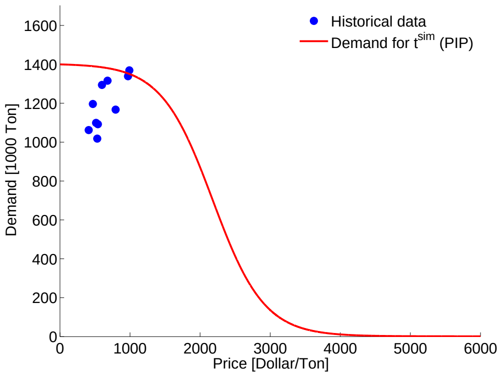

Figure 7.9: Demand function for product 3 at t^{sim}: optimal solution of the PIP

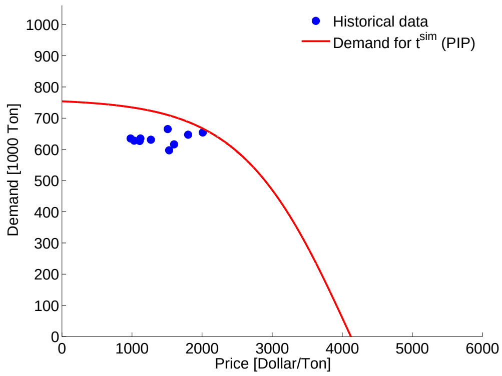

Figure 7.10: Demand function for product 4 at t^{sim}: optimal solution of the PIP

T_{t_0}, the weighting factors w_t, $t \in T_{t_0}$, and the factors s, a, and s^{pos}. Most important, appropriate initial values are essential to ensure local convergence. Here, the results of the heuristic approach serve as appropriate initial values so that the algorithm converges to a local solution. If they are not available, globalization techniques become necessary (cf. standard optimization textbooks, e.g., [NW06]).

Supplementary, suppose that reliable prognoses exist about the behavior of the customer in the high price range $\tilde{a}^{\pi,k}_{p,r,t_0} > \max(a^{\pi}_{p,r,t})_{t \in T_{t_0}}$ or the low price range $\tilde{a}^{\pi,k}_{p,r,t_0} < \min(a^{\pi}_{p,r,t})_{t \in T_{t_0}}$, respectively. We can take advantage of this information by including it in the least-squares estimation as follows.

Given auxiliary prognoses $\left(\tilde{a}^{\pi,k}_{p,r,t_0}, \tilde{a}^{q,k}_{p,r,t_0}, \Delta a^{GDP,k}_{r,T_{t_0}}, \Delta a^{IndPro,k}_{r,T_{t_0}}\right)$, $k = 1, \ldots, K$, where

$$\tilde{a}^{q,k}_{p,r,t_0} - \phi^{eco}_{p,r,t_0}\left(\tilde{a}^{\pi,k}_{p,r,t_0}\right) \sim \mathcal{N}\left(0, \tilde{\sigma}^2_k\right), \tag{7.35}$$

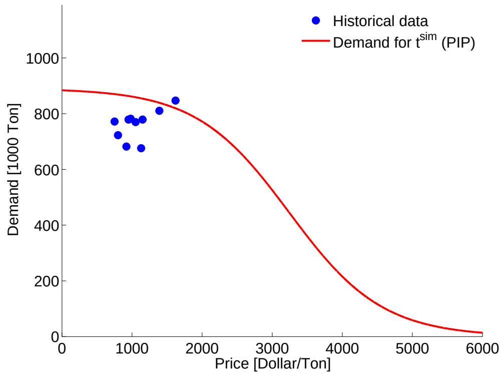

Figure 7.11: Demand function for product 5 at t^{sim}: optimal solution of the PIP

we add

$$\sum_{k=1}^{K} \left(\frac{1}{\tilde{\sigma}_k} \left(\tilde{a}^{q,k}_{p,r,t_0} - \phi^{eco}_{p,r,t_0} \left(\tilde{a}^{\pi,k}_{p,r,t_0} \right) \right) \right)^2 \tag{7.36}$$

to the objective function of the PIP (7.34a) (cf. section 5.3.1) . As a result, the constraints (7.34g) and (7.34h) can become redundant because the additional information determines the shape of the demand function instead. This concept, however, implies stronger assumption on the behavior of the customer in low and high price ranges. Therefore, adding notional data need to be based on reliable scenario analysis.

7.4 Comparison, Discussion, and Outlook

In this section, we compare and discuss the results of the heuristic approach and our parameter identification problem (PIP). Therefore, in section 7.4.1, to compare the effects of their distinct results in our supply-demand trade network optimization problem (4.3) defined in section 4.2, we will simulate prices and sales quantities at t^{sim} by means of the respective forecasted demand functions for time t^{sim} (see section 7.2.2.2 for the heuristic approach and section 7.3.2 for the PIP). Afterwards, we discuss the differences, the respective advantages, and the open problems of both methods.

7.4.1 Including the Estimated Demand Models in the Supply-Demand Trade Network Optimization Model

Having integrated the demand parameters from the respective forecast for t^{sim} in the supply-demand trade network optimization problem, we simulate prices and sales quantities at time t^{sim}. For this purpose, we assume that the change in the economic situation at this time is known.[11] The results are summarized in table 7.13 and 7.14. Moreover, figures 7.12 to 7.16 illustrate the optimal solution on the corresponding demand function as well as the real data at t^{sim}.

Method	Product 1	Product 2	Product 3	Product 4	Product 5
Heuristic	1960.33	1524.25	1200.07	1882.08	1858.86
PIP	3987.40	2190.66	2180.66	2872.69	3242.20
PIP + assump. 7.6	2737.12	2004.50	1655.25	2396.59	2663.85

Table 7.13: Comparison of the price simulations in \$/t at t^{sim} obtained by integrating the respective demand models in the supply-demand trade network optimization model

Method	Product 1	Product 2	Product 3	Product 4	Product 5
Heuristic	767.55	1865.18	764.40	611.00	1079.05
PIP	561.61	239.64	700.96	506.69	445.37
PIP + assump. 7.6	618.57	1231.53	895.96	536.79	595.01

Table 7.14: Comparison of the sales quantities simulations in $1000t$ at t^{sim} obtained by integrating the respective demand models in the supply-demand trade network optimization model

The resulting demand functions display distinct behavior over the whole price range. In general, the heuristic approach indicates higher consumption for lower prices than the PIP method. Note that the heuristic approach does not need to get along with the

[11] For a true forecast, changes in the economic factors also need to be forecasted. This, however, is beyond the scope of this thesis.

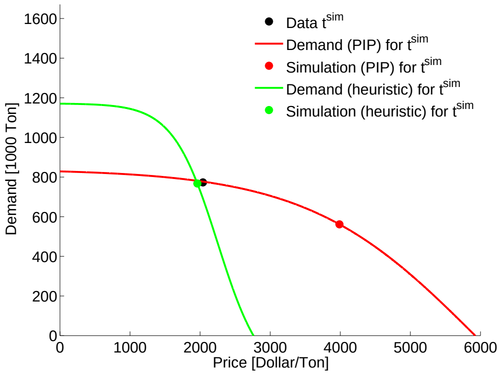

Figure 7.12: Comparison of the optimal solution for product 1 at t^{sim} obtained by integrating the respective demand models in the network optimization model (4.3)

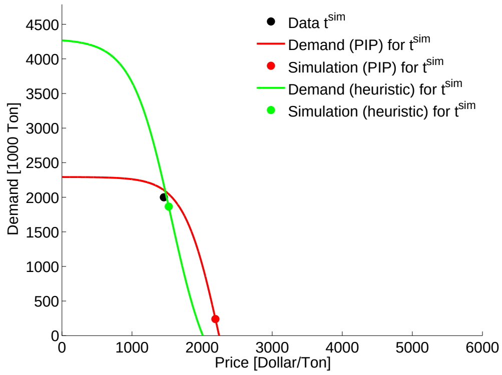

Figure 7.13: Comparison of the optimal solution for product 2 at t^{sim} obtained by integrating the respective demand models in the network optimization model (4.3)

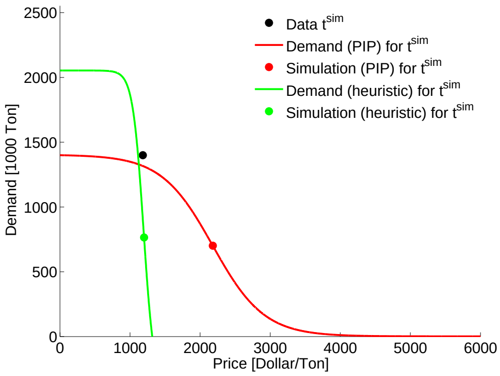

Figure 7.14: Comparison of the optimal solution for product 3 at t^{sim} obtained by integrating the respective demand models in the network optimization model (4.3)

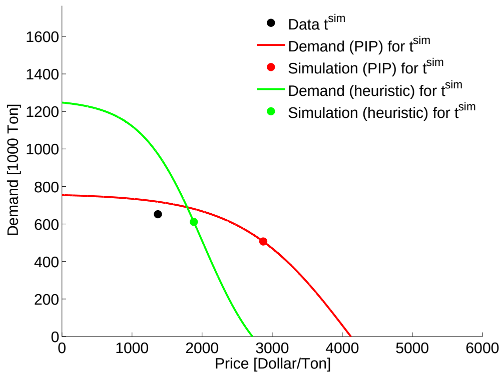

Figure 7.15: Comparison of the optimal solution for product 4 at t^{sim} obtained by integrating the respective demand models in the network optimization model (4.3)

additional assumption in case the price is zero (inequality (7.25)). On the other hand, the results of the PIP do not give any hint to the real maximum price or maximum consumption. Whereas the heuristic method approximates an upper bound on the maximum consumption and indicates an maximum price, this is not true for the PIP.

The solutions of the network optimization problem (4.3) with demand parameters estimated by the PIP consistently results in higher prices and lower quantities. The results obtained from the heuristic forecast achieve a better simulation of prices and sales quantities. These results are not surprising because the heuristic approach takes all production processes and available market information into account, whereas the PIP methodology

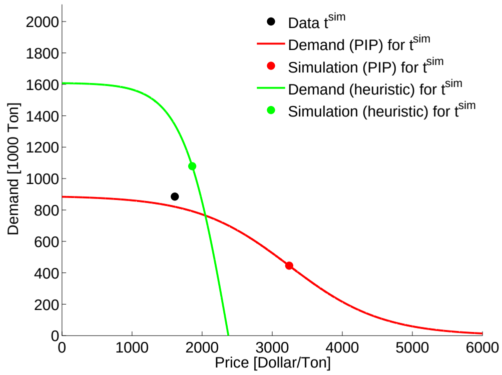

Figure 7.16: Comparison of the optimal solution for product 5 at t^{sim} obtained by integrating the respective demand models in the network optimization model (4.3)

is only built on exogenous information. Basically, the second approach has the advantage of identifying the demand parameters independent of the market model, but is in need of more information about the consumer behavior, especially for high prices (cf. section 7.3.3). If knowledge about the consumer's maximum willingness to pay is provided, we expect that the PIP methodology achieves better results.
To support this statement, we again identify the demand parameters for all $p \in P_{out} = \{1, 2, 3, 4, 5\}$ of the subsystem as in section 7.3.2 (i.e., $J = 1$, $T_{t^{\text{sim}}} = \{t^{\text{sim}} - 10, \dots, t^{\text{sim}} - 1\}$, $\lambda = 0.4$, $s = -0.03$, $a = -0.01$, $s^{pos} = 1$, and the initial values are set equal to the respective best results of our heuristic approach (see section 7.2.2.2)) by adding further assumptions to the PIP (7.34).

Assumptions 7.6. *Assuming that there is information available in order to add one scenario, i.e., K=1 in equation (7.35) and (7.36), to the database used in section 7.3.2 to solve the PIP (7.34) let*

$$\left(\tilde{a}^{\pi,1}_{p,r,t^{\text{sim}}}, \tilde{a}^{q,1}_{p,r,t^{\text{sim}}}, \Delta a^{\text{GDP},1}_{r,T_{t^{\text{sim}}}}, \Delta a^{\text{IndPro},1}_{r,T_{t^{\text{sim}}}}\right) = \left(2 \cdot a^{\pi}_{p,r,t^{\text{sim}}-1}, 0, \Delta a^{\text{GDP}}_{r,t^{\text{sim}}-1,1}, \Delta a^{\text{IndPro}}_{r,t^{\text{sim}}-1,1}\right), \quad (7.37)$$

where

$$\phi^{eco}_{p,r,t^{\text{sim}}}\left(\tilde{a}^{\pi,1}_{p,r,t^{\text{sim}}}\right) \sim \mathcal{N}\left(\tilde{a}^{q,1}_{p,r,t^{\text{sim}}}, \tilde{\sigma}^2_1\right), \quad (7.38)$$

with $\tilde{\sigma}_1 = 60.97$ *so that*

$$P\left(\phi^{eco}_{p,r,t^{\text{sim}}}\left(\tilde{a}^{\pi,1}_{p,r,t^{\text{sim}}}\right) \in \left[\tilde{a}^{q,1}_{p,r,t^{\text{sim}}} - 100, \tilde{a}^{q,1}_{p,r,t^{\text{sim}}} + 100\right]\right) = 0.9. \quad (7.39)$$

Remark 7.2. Adding this assumptions to the PIP has the purpose to show that this approach is able to deliver better results if more information about the consumer behavior is available. However, the assumptions 7.6 represent an exemplary scenario and do not reflect prognoses about the real behavior. Consequently, further information about the consumer's maximum willingness to pay is necessary, which, for example, can be obtained from consumer questioning.

The corresponding demand parameters for each product $p \in P_{out}$ obtained by the PIP (7.34) together with the assumptions 7.6 are summarized in table 7.15 and the corresponding simulation results of the network optimization problem (4.3) are given in the tables 7.13 and 7.14. The resulting demand functions together with the results obtained from the heuristic approach, which were already presented above, are illustrated in the figures 7.17 to 7.21. Notably, using the extended PIP provides better simulations of the prices and sales quantities.

p		$\lambda_1^{\phi_{p,r,t^{\text{sim}}}}$	$\lambda_2^{\phi_{p,r,t^{\text{sim}}}}$	$\lambda_3^{\phi_{p,r,t^{\text{sim}}}}$	$\lambda_4^{\phi_{p,r,t^{\text{sim}}}}$	$\lambda_{\text{GDP}}^{\phi_{p,r,t^{\text{sim}}}}$	$\lambda_{\text{IndPro}}^{\phi_{p,r,t^{\text{sim}}}}$	Iter.
1		798.40	3676.10	970.01	0.00	0.00	9.28	10
	STD_i	±3.10	±74.11	±40.51	±0.00	±0.00	±3.12	
	θ_i	±10.83	±258.85	±141.47	±0.00	±0.00	±10.88	
2		1209.90	2034.70	498.98	1061.90	0.05	6.98	13
	STD_i	±58.83	±75.30	±48.93	±60.74	±0.03	±5.37	
	θ_i	±275.55	±352.67	±229.16	±284.50	±0.13	±25.14	
3		1399.70	2078.60	579.03	0.00	0.00	11.84	11
	STD_i	±3.24	±27.37	±11.57	±0.00	±0.00	±3.10	
	θ_i	±11.30	±95.59	±40.41	±0.00	±0.00	±10.83	
4		707.25	3233.60	1117.10	0.00	0.09	28.46	16
	STD_i	±3.71	±109.55	±52.56	±0.00	±0.01	±4.08	
	θ_i	±12.96	±382.61	±183.58	±0.00	±0.04	±14.24	
5		891.08	3747.70	1344.90	0.00	0.00	0.22	9
	STD_i	±2.81	±38.83	±20.38	±0.00	±0.00	±2.96	
	θ_i	±8.19	±113.29	±59.45	±0.00	±0.00	±8.63	

Table 7.15: Demand parameter results of the extended PIP for t^{sim}: assumptions 7.6 were added to the PIP

7.4.2 Concluding Remarks

Both approaches are applicable to varying historical data time series as exemplarily shown in sections 7.2.2 and 7.3.2 and provide demand parameters. They consider different minimization problems: whereas the heuristic approach seeks for the demand function so that corresponding price and sales simulations are close to the historical values, the PIP determines the demand parameters such that historical values are approximated. Equally, the real historical value is also located near the demand function determined by the PIP. However, regarding the simulation results of the network optimization model

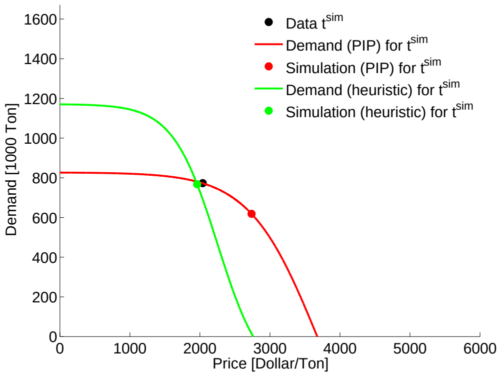

Figure 7.17: Comparison of the optimal solution for product 1 at t^{sim} obtained by integrating the respective demand models, where assumptions 7.6 were added to the PIP, in the network optimization model (4.3)

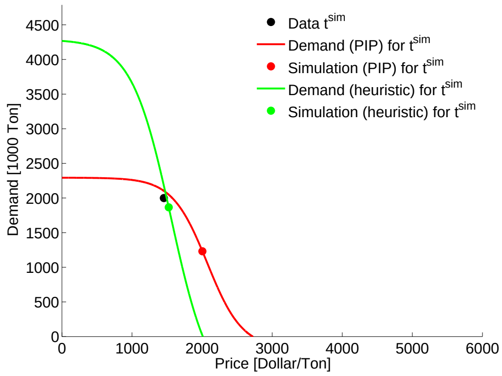

Figure 7.18: Comparison of the optimal solution for product 2 at t^{sim} obtained by integrating the respective demand models, where assumptions 7.6 were added to the PIP, in the network optimization model (4.3)

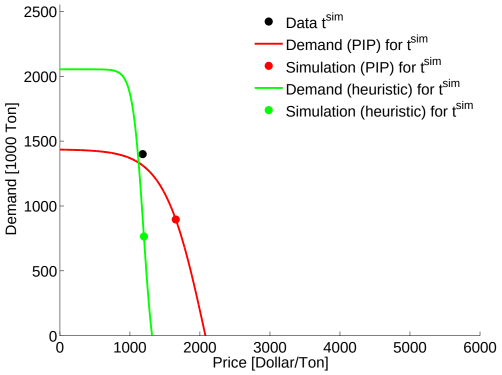

Figure 7.19: Comparison of the optimal solution for product 3 at t^{sim} obtained by integrating the respective demand models, where assumptions 7.6 were added to the PIP, in the network optimization model (4.3)

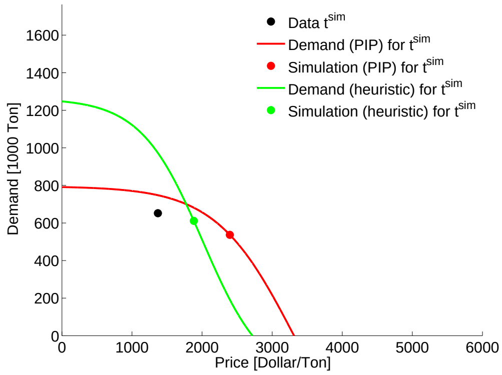

Figure 7.20: Comparison of the optimal solution for product 4 at t^{sim} obtained by integrating the respective demand models, where assumptions 7.6 were added to the PIP, in the network optimization model (4.3)

(4.3), its shape induces a higher price as optimal solution than the demand function resulting from the heuristic approach.
Both methods are in need of numerous a-priori assumptions that also risk to falsify the simulations by misinterpreting the current market situation.[12] Therefore, we content

[12]Certainly, reducing the parameter identification to the intermediate interval simplifies the estimation

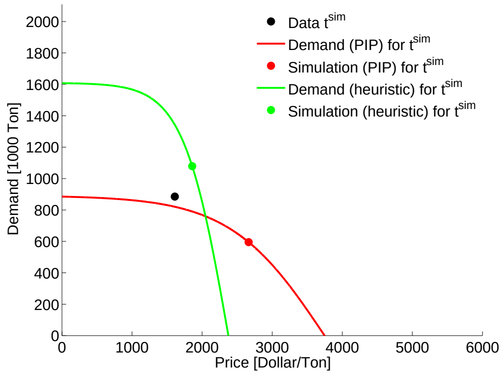

Figure 7.21: Comparison of the optimal solution for product 5 at t^{sim} obtained by integrating the respective demand models, where assumptions 7.6 were added to the PIP, in the network optimization model (4.3)

ourselves with giving some examples and do not claim to obtain an overall solution. Nevertheless, the parameter identification process is applicable to a wide product range differing in historical time series. Moreover, using the concept of exponentially smoothing the historical values results in time-varying demand functions.
However, as said before, both techniques require additional information to deliver reliable results, and if this is not available, auxiliary assumptions are necessary. As a consequence, the solutions have quite different features. More precisely, the first approach provides a rather high maximum consumption at price zero with a strict decline and a maximum price, which is close to the historical data. The second method provokes that the maximum consumption at price zero is in the price range of the historical prices, and consumption shows a flat decline implying a large price range. Although the simulation results of the heuristic approach are closer to real data, there is no reason to prefer this approach in every aspect. In general, the PIP methodology preferably provides a exogenous solution without using market data, but needs more information than currently available. Given assessments of the consumer's maximum willingness to pay the PIP is expected to give better results (cf. the results because of assumptions 7.6). To conclude, we emphasize that more information is necessary to establish a unique demand model with reliable parameter estimations.

process. Since we aim to apply our demand model in the optimization model to simulate prices and sales quantities, it is necessary to estimate the parameters of the demand model in the whole domain by means of historical data.

8 Conclusion

This thesis has established a general approach to modeling aggregated demand for commodities, which takes into account all essential influencing factors. On this basis, explicit demand models were studied and applied to our case study of the petrochemical market. We decided on a phenomenological approach instead of modeling the utility function of the customers, because quantifying the customers' preferences requires more extensive assumptions about their decision-making.

Thus, our first question was to collect and analyze essential influencing factors of demand in order to transfer the characteristics of demand and its crucial impacts into a mathematical framework. In addition to the own price of the product in demand, these included market parameters such as economic indices quantifying the changes in the economic situation, prices of substitutes and complements, and also specific characteristics of the customers. So far, however, we have assumed that all customers in the market act independently, but have identical behavior and can be considered as one customer by aggregating their demand. Consequently, our approach was restricted to the case of a homogeneous population of customers.

Regarding the influences of prices of substitutes, we analyzed the effects of different possibilities to switch production processes as reason for substitution on demand. To cope with this emerging complexity we aggregated all substitution possibilities and proposed a demand model including substitution because of gradual switching. This model includes a moderate price region for which the substitutable demand that can be satisfied by all substitutes is split up according to the respective price ratio. If one of the products becomes considerably cheaper, the whole demand is absorbed by it.

In conjunction with the market optimization problem including the supply-demand interactions that we developed in cooperation with Kramer [Kra13] to simulate prices and sales quantities in a multi-commodity market, we aimed to integrate demand models that were based on our phenomenological approach. Therefore, we were aware of computational practicality in solving the optimization problem by giving preference to smooth model functions.

For this purpose, this thesis provided an explicit demand model for the petrochemical market that reflects the nonlinear relationship between demand and price. Moreover, we presented model extensions including the impacts of other products' prices and the change of the economic situation and proved that these models satisfy the assumptions stated in chapter 3 to the greatest extent. In the case of substitutes, finding a suitable model turned out to be more complex and the model function was not differentiable. In addition, the choice of parameterization enabled a simple interpretation of the values. They provided an upper bound for the consumption at price zero and indicated at which price demand is zero.

To integrate these demand models in the network optimization problem in order to determine optimal pricing and production strategies, their parameters needed to be identified. However, it was a challenge to estimate demand parameters if only incomplete information on the customer's behavior is available. By means of additional assumptions, we came up with two approaches. Firstly, the heuristic approach determined appropriate values by simulating prices and sales quantities. In the second approach, we solved a constrained weighted least-squares problem. Both approaches succeeded in providing demand parameters. Since these differ, further information is necessary to accomplish our case study. Nevertheless, our methods to identify parameters reveal some benefits. Taking into account the temporal effect, techniques resembling the moving average filter are applied in both parameter identification methods. Consequently, we are able to provide parameter estimations for each product in each region each year.
There are several possibilities to extend this work:

- So far, our approach of modeling demand is simplified by aggregating the customers' demand under the assumption that all customers act independently and have the same consumption behavior. Provided that information is available that enables us to break down the complex effects of interacting customers, multi-agent models might be appropriate to investigate the influences of a structured population of consumers on aggregated demand.

- Including uncertainty in the demand model gives rise to more sophisticated approaches. In addition to modeling the change of the economic situation or various characteristics of the consumer as random variable, setting up a stochastic optimization model that represents the decision process of the consumer might be especially convenient with regard to the complexity of substitution processes.

- Assuming that the multi-commodity market under consideration is an oligopoly the concept of game theory may serve as an appropriate tool to model price formation in case multiple market participants are involved. Therefore, interactions between producers and customers have to be explicitly modeled.

- All in all, reseachers need a database that provides information to break down the complex decision processes of customers, and their influence on the aggregated demand-price relationship. In addition, more information about the behavior in low or high price ranges is crucial with regard to parameter identification. This is because so far it has only been possible to estimate parameters by including additional assumptions. It would be desirable to uniquely identify demand parameters using only historical data.

Notation

The following lists contain the notation used to present the general approach to modeling demand in chapter 3, to establish the explicit *tanh-demand model* in chapter 6, and to discuss methods to identify demand parameters in chapter 7.

Variables

$\boldsymbol{x}^{\pi}_{r,t}$	Price vector in region r at time t	section 3.1

Parameters

$a^{\zeta_i}_{r,t}$	Absolute value of an economic index ζ_i in region r at time t	section 3.3
$\Delta a^{\zeta_i}_{r,t(,J)}$	Change of the value of an economic index ζ_i from previous times to t. J is the number of previous times to be included in the computation	section 3.3
$a^{E\zeta_i}_{r,t,t+1}$	Forecast of absolute value of an economic index ζ_i at time t for $t+1$	section 3.3
$\Delta a^{E\zeta_i}_{r,t,t+1(,J)}$	Change of the forecasted value of an economic index ζ_i at time t for $t+1$. J is the number of previous times to be included in the computation	section 3.3
w_j	Factor to weight historical data from time $t-j$ by determining influencing factors of demand $\phi_{p,r,t}(\cdot)$	section 3.3
$\boldsymbol{\alpha}^{\text{consumer}}_{r,t}$	Vector containing the characteristics of the consumer in region r at time t.	section 3.1
$\alpha^{\text{min\_quant}}_{p,r,t}$	Minimum quantity of product p the consumer need to produce to fulfill his commitments at time t	section 3.4
$\alpha^{\text{max\_quant}}_{p,r,t}$	Maximum quantity of product p the consumer can reprocess or store at time t, i.e., this quantity can also be considered as maximum capacity	section 3.4
$\alpha^{b1}_{p,r,t}$	First price barrier: if $x^{\pi}_{p,r,t} \leq a^{b1}_{p,r,t}$ the potential demand will be fulfilled because of exceptionally low prices	section 3.4

$\alpha^{b2}_{p,r,t}$	Second price barrier: if $\alpha^{b1}_{p,r,t} \leq x^{\pi}_{p,r,t} \leq \alpha^{b2}_{p,r,t}$, demand is strictly decreasing	section 3.4
$\alpha^{b3}_{p,r,t}$	Third price barrier: if $\alpha^{b2}_{p,r,t} \leq x^{\pi}_{p,r,t} \leq \alpha^{b3}_{p,r,t}$, demand is reduced to a minimum level. If $\alpha^{b3}_{p,r,t} \leq x^{\pi}_{p,r,t}$, then demand is zero.	section 3.4
$\alpha^{\text{max\_price}}_{p,r,t}$	Maximum price for product p in region r at time t the consumer is willing to pay.	section 3.4
$\alpha^{b}_{r,t}$	Available budget of the consumer in region r at time t	section 3.4
$\alpha^{E\pi}_{p,r,t+z}$	Integer parameter to express consumer's expectation of price change for product p for time $t+z$ at time t	section 3.4
$\alpha^{\text{con}}_{p,r,t}$	Binary parameter indicating whether there is a contract between producer and consumer for product p in region r at time t	section 3.4
$\alpha^{q\_\text{con}}_{p,r,t}$	Contract quantity the customer purchases of product p in region r at time t	section 3.4
$\delta_{p_{i_1},p_{i_2},t}$	Switching barrier for the price ratio $\frac{p_{i_1}}{p_{i_2}}$ at time t	section 3.5
$a^{sc}_{p_{i_1},p_{i_2},t}$	Additional costs for switching from p_{i_1} to p_{i_2} at time t	section 3.5
$a^{\text{com}}_{p_{i_j},p_{i_k},t}$	Ratio of products p_{i_j} and p_{i_k} required for reprocessing	section 3.6
$a^{\text{com}}_{p_{i_j},\mathcal{C}_i,t}$	Weight proportion of product p_{i_j} in the basket of products of $\mathcal{C}_i$	section 3.6
$\lambda_1^{\phi_{p,r,t}}$, $\lambda_2^{\phi_{p,r,t}}$, $\lambda_3^{\phi_{p,r,t}}$, $\lambda_4^{\phi_{p,r,t}}$	Demand parameters for product p in region r at time t in the *tanh-demand model*	section 6.2
$\lambda_{GDP}^{\phi_{p,r,t}}$, $\lambda_{IndPro}^{\phi_{p,r,t}}$	Demand parameters for product p in region r at time t in the *tanh-demand model eco*	section 6.2
$\underline{a}^{\pi}_{p,r,t}$	Historical minimum price of the time interval T_t	section 7.3
$\overline{a}^{\pi}_{p,r,t}$	Historical maximum price of the time interval T_t	section 7.3
$\underline{\Delta} a^{\text{GDP}}_{r,t,J}$	Historical minimum change in the GDP of time interval T_t. J is the number of previous times to be included in the computation	section 7.3
$\overline{\Delta} a^{\text{GDP}}_{r,t,J}$	Historical maximum change in the GDP of time interval T_t. J is the number of previous times to be included in the computation	section 7.3
$\underline{\Delta} a^{\text{IndPro}}_{r,t,J}$	Historical minimum change in the index for industrial production of time interval T_t. J is the number of previous times to be included in the computation	section 7.3

$\overline{\Delta} a^{\text{IndPro}}_{r,t,J}$	Historical maximum change in the index for industrial production of time interval T_t. J is the number of previous times to be included in the computation	section 7.3
$\tilde{a}^{\pi,k}_{p,r,t_0}$, $\tilde{a}^{q,k}_{p,r,t_0}$, $\Delta a^{GDP,k}_{r,T_{t_0}}$, $\Delta a^{IndPro,k}_{r,T_{t_0}}$	Data for scenario k in region r at time t_0	section 7.3

Functions

$\phi_{p,r,t}(\cdot)$	Demand function for product p in region r at time t $\phi_{p,r,t}\colon (\mathbb{R}_0^+)^{\lvert P\rvert} \times \mathbb{R} \times \mathbb{R}^I \times \mathbb{R}^I \times \mathbb{R}^C \to \mathbb{R}_0^+$	section 3.1
$\varphi_{p,r,t}(\cdot)$	Demand function restricted to the price range $[\alpha^{b1}_{p,r,t}, \alpha^{b2}_{p,r,t})$ in which the demand strictly decreases $\varphi_{p,r,t}\colon (\mathbb{R}_0^+)^{\lvert P\rvert} \times \mathbb{R} \times \mathbb{R}^I \times \mathbb{R}^I \times \mathbb{R}^C \to \mathbb{R}_0^+$	section 3.4
$\phi^{q\_add}_{p,r,t}(\cdot)$	Demand function for product p in region r at time t capturing the additional quantity the customer orders because he expects the price to rise in the future $\phi^{q\_add}_{p,r,t}\colon (\mathbb{R}_0^+)^{\lvert P\rvert} \times \mathbb{R} \times \mathbb{R}^I \times \mathbb{R}^I \times \mathbb{R}^C \to \mathbb{R}_0^+$	section 3.4
$\phi^{E\pi}_{p,r,t}(\cdot)$	Demand function for product p in region r at time t including the consumer's expectation on price changes $\phi^{E\pi}_{p,r,t}\colon (\mathbb{R}_0^+)^{\lvert P\rvert} \times \mathbb{R} \times \mathbb{R}^I \times \mathbb{R}^I \times \mathbb{R}^C \to \mathbb{R}_0^+$	section 3.4
$\phi^{con}_{p,r,t}(\cdot)$	Demand function for product p in region r at time t including the possibilities for contracts $\phi^{con}_{p,r,t}\colon (\mathbb{R}_0^+)^{\lvert P\rvert} \times \mathbb{R} \times \mathbb{R}^I \times \mathbb{R}^I \times \mathbb{R}^C \to \mathbb{R}_0^+$	section 3.4
$\phi^{b}_{p,r,t}(\cdot)$	Demand function for product p in region r at time t capturing the basis demand to be satisfied by p $\phi^{b}_{p,r,t}\colon (\mathbb{R}^+)^{\lvert P\rvert} \times \mathbb{R} \times \mathbb{R}^I \times \mathbb{R}^I \times \mathbb{R}^C \to \mathbb{R}_0^+$	section 3.5
$\rho_{p_{i_1}}(\cdot)$	Splitting function determining the share of the substitutable demand for product p_{i_1} w.r.t. $x^{\pi}_{p_{i_1},r,t}/x^{\pi}_{p_{i_2},r,t}$ $\rho_{p_{i_1},p_{i_2}}\colon \mathbb{R}^+ \to [0,1]$	section 3.5/ section 6.2
$\phi^{a}_{\mathcal{P}_i,r,t}(\cdot)$	Demand function in region r at time t capturing the substitutable demand for application a to be satisfied by all products $p_i \in \mathcal{P}_i$ $\phi^{a}_{\mathcal{P}_i,r,t}\colon (\mathbb{R}^+)^{\lvert P\rvert} \times \mathbb{R} \times \mathbb{R}^I \times \mathbb{R}^I \times \mathbb{R}^C \to \mathbb{R}_0^+$	section 3.5
$\phi^{a,b}_{p,r,t}(\cdot)$	Demand function for product p in region r at time t including the sum of the share of $\phi^{a}_{p_i,r,t}(\cdot)$ and $\phi^{b}_{p_i,r,t}(\cdot)$ for $p_i \in \mathcal{P}_i$ $\phi^{a,b}_{p,r,t}\colon (\mathbb{R}^+)^{\lvert P\rvert} \times \mathbb{R} \times \mathbb{R}^I \times \mathbb{R}^I \times \mathbb{R}^C \to \mathbb{R}_0^+$	section 3.5

$\phi^{\text{agg}}_{\mathcal{P}_i,r,t}(\cdot)$	Aggregated demand function for product p in region r at time t capturing the substitutable demand to be satisfied by all products $p_i \in \mathcal{P}_i$ $\phi^{\text{agg}}_{\mathcal{P}_i,r,t}\colon (\mathbb{R}^+)^{\lvert P\rvert} \times \mathbb{R} \times \mathbb{R}^I \times \mathbb{R}^I \times \mathbb{R}^C \to \mathbb{R}^+_0$	section 3.5
$\phi_{\mathcal{P}_i,r,t}(\cdot)$	Approximation of aggregated demand function $\phi^{\text{agg}}_{\mathcal{P}_i,r,t}(\cdot)$ for product p in region r at time t capturing the substitutable demand to be satisfied by all products $p_i \in \mathcal{P}_i$ $\phi_{\mathcal{P}_i,r,t}\colon (\mathbb{R}^+)^{\lvert P\rvert} \times \mathbb{R} \times \mathbb{R}^I \times \mathbb{R}^I \times \mathbb{R}^C \to \mathbb{R}^+_0$	section 3.5/ section 6.2
$\phi^{\text{sub}}_{p,r,t}(\cdot)$	Demand function capturing the influence of substitutable products for product p in region r at time t $\phi^{\text{sub}}_{p,r,t}\colon (\mathbb{R}^+)^{\lvert P\rvert} \times \mathbb{R} \times \mathbb{R}^I \times \mathbb{R}^I \times \mathbb{R}^C \to \mathbb{R}^+_0$	section 3.5/ section 6.2
$\phi^{\text{com}}_{p,r,t}(\cdot)$	Demand function capturing the influence of complementary products for product p in region r at time t $\phi^{\text{com}}_{p,r,t}\colon (\mathbb{R}^+_0)^{\lvert P\rvert} \times \mathbb{R} \times \mathbb{R}^I \times \mathbb{R}^I \times \mathbb{R}^C \to \mathbb{R}^+_0$	section 3.6/ section 6.2
$\phi_{\mathcal{C}_i,r,t}(\cdot)$	Demand function for the basket of $p \in \mathcal{C}_i$ weighted by their respective factors $a^{\text{com}}_{p,\mathcal{C}_i,t},\ p \in \mathcal{C}_i$ in region r at time t $\phi_{\mathcal{C}_i,r,t}\colon (\mathbb{R}^+_0)^{\lvert P\rvert} \times \mathbb{R} \times \mathbb{R}^I \times \mathbb{R}^I \times \mathbb{R}^C \to \mathbb{R}^+_0$	section 3.6/ section 6.2
$\phi^{\text{bundle}}_{\mathcal{C}_i,r,t}(\cdot)$	Demand function for the basket of $p \in \mathcal{C}_i$ weighted by their respective factors $a^{\text{com}}_{p,\mathcal{C}_i,t},\ p \in \mathcal{C}_i$ in region r at time t $\phi^{\text{bundle}}_{\mathcal{C}_i,r,t}\colon (\mathbb{R}^+_0) \times \mathbb{R} \times \mathbb{R}^I \times \mathbb{R}^I \times \mathbb{R}^C \to \mathbb{R}^+_0$	section 3.6
$\Psi_{\mathcal{C}_i,r,t}(\cdot)$	Cost function of the basket of $p \in \mathcal{C}_i$ weighted by their respective factors $a^{\text{com}}_{p,\mathcal{C}_i,t},\ p \in \mathcal{C}_i$ $\Psi_{\mathcal{C}_i,r,t}\colon (\mathbb{R}^+_0)^{\lvert P\rvert} \to \mathbb{R}^+_0$	section 3.6
$\phi^{\text{eco}}_{p,r,t}(\cdot)$	Demand function capturing the influence of the economic situation for product p in region r at time t $\phi^{\text{eco}}_{p,r,t}\colon (\mathbb{R}^+_0)^{\lvert P\rvert} \times \mathbb{R} \times \mathbb{R}^I \times \mathbb{R}^I \times \mathbb{R}^C \to \mathbb{R}^+_0$	section 6.2

Time Sets

$\{t-1, \ldots, t-J\}$	Set of data points for which we assume that they influence the economic situation at time t	section 3.3
T_t	Set of data points for which we assume that they influence the demand parameters at time t	section 7.2/ section 7.3
T_0	Set of data points for which we assume that the market situation is comparable	section 7.2
T	Set of data points used to simulate prices and sales quantities in the heuristic approach to identifying parameters	section 7.2

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