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[^{18}F]FET-PET brain image segmentation using *k*-means: Evaluation of five cluster validity indices

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Dynamic brain [^{18}F]fluoro-ethyl-L-tyrosine positron emission tomography ([^{18}F]FET-PET) images could be used to accurately, reproducibly and precisely define the spatial distribution for tumor regions and adjacent healthy tissues for radiotherapy treatment planning. However, image segmentation is a pre-required step in order to delineate the tumor regions. Commonly, drawing regions-of-interest (ROIs) directly on PET images is performed by the physicians to identify different functional structures in dynamic PET images. This approach is a time-consuming, effort-demanding task and operator dependent. Furthermore, it is a challenge due to the inability of the operator to integrate the full time activity curves (TACs) of the voxels in the evaluation and because of the noise in PET images.
An alternative solution is the automated segmentation of dynamic PET images using k-means cluster analysis, which is not only time-saving and highly reproducible, but also takes into consideration the full TACs. This algorithm requires determination of the optimal number of clusters in advance. To resolve this issue, cluster validity indices can be used to validate the goodness of partitions after clustering. The validity indices however are affected by data characteristics, like noise or the dimensionality of the data. To evaluate which cluster validity indices can be used for the noisy and high-dimensional [^{18}F]FET-PET data sets, general requirements were developed during this study. These requirements are that the number of clusters suggested by the index should result in a physiologically reasonable segmentation, not depend on the number of the investigated voxels and be highly reproducible. Additionally, the index should have a clear single extremum to have a unique solution and the computation time should be reasonable for use in a clinical setting.
In this study, the Akaike information criterion (AIC), WB, *I*, modified Dunn's and Silhouette validity indices were implemented and compared with respect to the pre-mentioned requirements to find the appropriate number of clusters for dynamic brain [^{18}F]FET-PET data.
The results showed that the suggested optimal numbers of clusters by WB, *I*, modified Dunn's and Silhouette validity indices were not affected by the number of the investigated voxels. In addition, the optimal number of clusters given by modified Dunn's and Silhouette indices was 2 or 3 leading to a very poor segmentation. WB and *I* indices suggested in median 5, [range 4-6] and 4, [range 3-6] clusters, respectively. Moreover, WB-index showed a single global maximum, whereas the other indices showed also local extrema.
In conclusion, within all indices, the WB-index performed best for automated determination of the relevant number of (*k*-means) clusters for [^{18}F]FET-PET brain images as it allows better differentiation of different tissues with suggesting higher number of clusters. WB cluster validity index is simple, reproducible and has an unique global minimum.