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Improved Alzheimer disease diagnosis with a machine learning approach and neuroimaging: Case study development. Supplément

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Multimedia Appendix 1: PCA

The PCA computation process with mathematical formulas is explained as follows:

An orthonormal basis vector is generated by the PCA. This vector makes it possible to maximize the dispersion of all projected samples. After the preprocessing steps, the *n* remaining voxels for each subject are rearranged into a vector form. Let $X = (x_{ij})_{n\times m}$ be the sample set of these vectors, where n is the number of samples (patients), m is the number of features and x_{ij} represents the j^{th} feature value of the i^{th} sample, where i =1,2,…,n and j=1,2,…,m. In this research, some gray-scale features are selected as characteristics of the sample. The chosen gray-scale features are: mean, variance, skewness, kurtosis, energy and entropy. The specific steps of PCA are as follows:

1) Standardize the original data by subtracting all samples from the corresponding feature's mean value.

$$\overline{x_j} = \frac{1}{n}\sum_{i=1}^{n} x_{ij} \tag{1.1}$$

2) Calculate the covariance matrix $P = (r_{jk})_{m\times m}$, where r_{jk} represents the correlation between the j^{th} and k^{th} feature.

$$P = \begin{bmatrix} r_{11} & \cdots & r_{1m} \\ \vdots & \ddots & \vdots \\ r_{m1} & \cdots & r_{mm} \end{bmatrix} \tag{1.2}$$

3) Compute the eigenvalue λ_i and the eigenvector e_i of the covariance matrix P:

$$\lambda_i e_i = P e_i \tag{1.3}$$

4) Record the resulting eigenvalues in the order of large to small: $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_k$. Calculate the contribution rate of each principal component.

$$\frac{\lambda_g}{\sum_{g=1}^{k} \lambda_g} \tag{1.4}$$

The higher the contribution rate, the stronger the information about the original variables contained in the principal component.

5) Transform the original sample matrix X into a new matrix $Y = (Y_{ij})_{n\times m_1}$, where $i = 1,2,\dots,n$ and $j = 1,2,\dots,m_1$.

$$Y = X \times [e_1, e_2, \dots e_{m_1}] \tag{1.5}$$

where $[e_1, e_2, \dots e_{m_1}]$ represents a new feature space composed of m_1 feature vectors. m_1 are the principal components extracted by PCA.