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Visualizing hyperspectral data with linear and non-linear dimensionality reduction methods

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Introduction

- **Hyperspectral (HS) data** is characterised as high dimensional with a large number of correlated dimensions leading to **a lower intrinsic dimensionality**
- **To visualize**, the HS data is transformed to a **lower dimensionality** explaining the data in terms of clusters
- The **shape of the data manifold** in the higher dimension largely determines the **effectiveness of the visualization method**
- In cases data **manifold is line**ar, classical methods like principal component analysis **(PCA)** and multi-dimensional scaling **(MDS)** can perform well in preserving the structure
- However, when the points in high dimensional space lie very near or in **non-linear manifold**, methods like **PCA and MDS fails** to capture the structure
- This is because the aim of these methods is **to keep distant points as far as possible** and do not utilize information from **neighbouring data points** [1]
- In this case, **non-linear methods utilizing neighbourhood** information can perform better [2].

Objective

- To test the potential of **linear and non-linear data visualisation** technique for visualizing near infrared HS data of tea products.
- Tested techniques: PCA, MDS, Isometric Mapping (ISOMAP) and t-distributed Stochastic Neighbour Embedding (t-SNE)

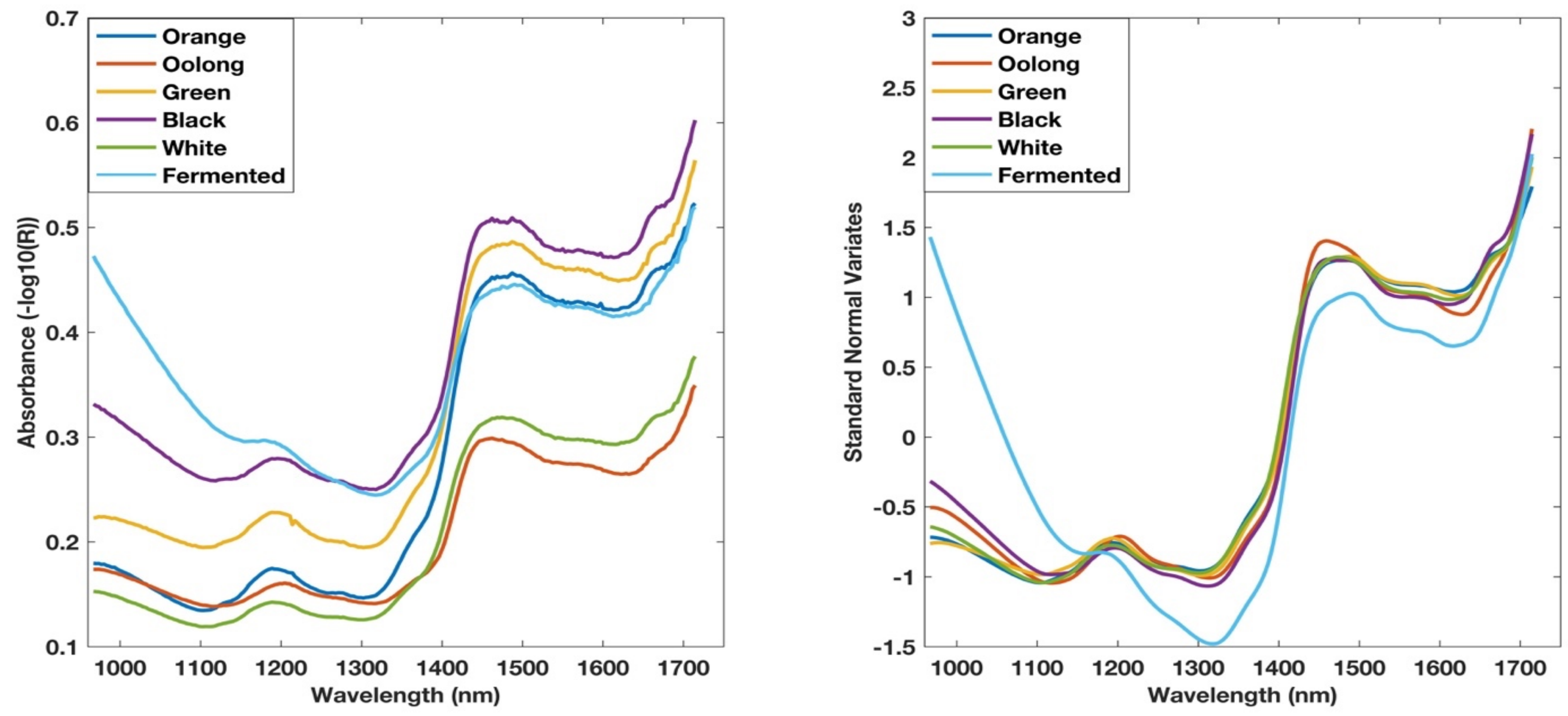
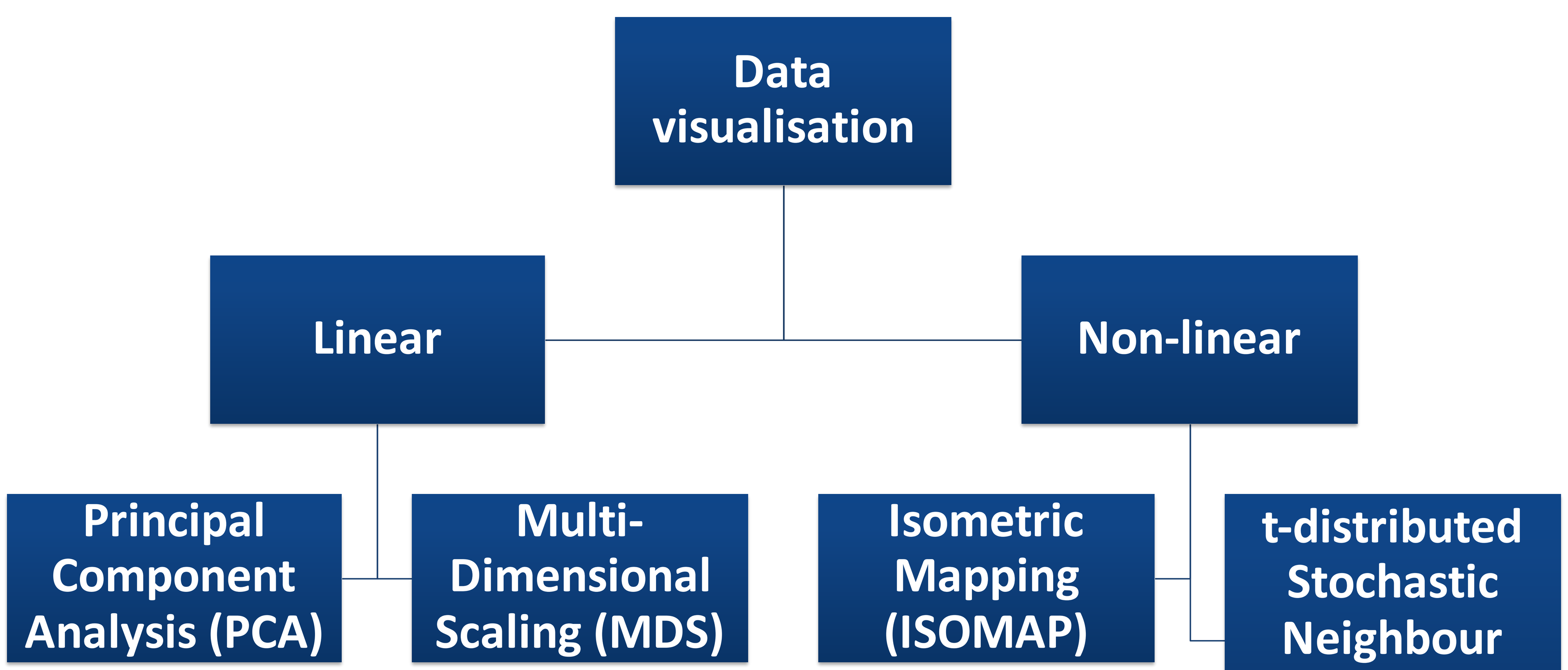


Figure 1: Mean absorbance profile of six different tea samples before and after pre-processing.

Material and methods

- NIRS (950-1750 nm) hyperspectral data of six commercial tea samples (150 spectra each)
    - **Green, Black, Orange, Pu-erh, White and Oolong**
- Data was pre-processed with:
    - Standard Normal Variate
    - Savitzky-Golay smoothing



$min\|TW^T - T_rW_r^T\|^2$

(Score and loadings)

$\min \sum_i \sum_j \|d_{ij} - \hat{d}_{ij}\|^2$

(Euclidean distance)

$\min \sum_i \sum_j \|D_G - D_E\|^2$

(Geodesic distance)

$KL(P\|Q) = \sum_i \sum_j p_{ij} \log \frac{p_{ij}}{q_{ij}}$

(Kullback-leibler)

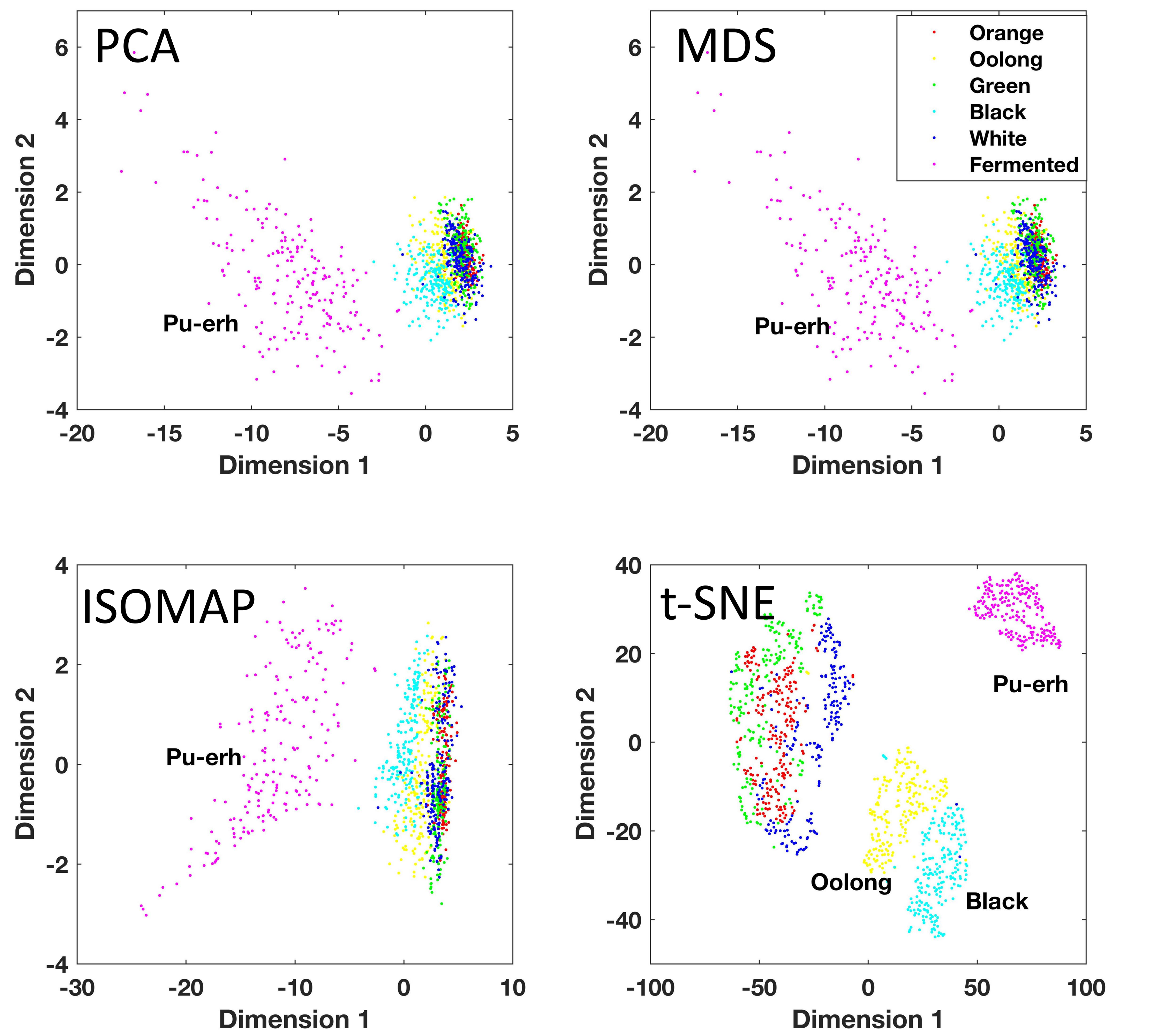


Figure 2: 2D scatter plots for 900 spectra corresponding to six commercial tea samples.

Conclusions

- **Oolong, green, yellow, white, black tea has very similar NIRS profile thus making it difficult for linear methods to separate them**
- PCA, MDS and ISOMAP were able to separate the pu-erh tea from **Oolong, green, yellow, white, black tea**
- t-SNE provided the identification of three different clusters i.e. fermented tea products, oxidised tea products and minimal process tea products.

References

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Mod Life

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