CREATION 3D FLUORESCENCE SPECTRA OF WINE

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Abstract: Our research provides for the analysis of different types of Georgian wine based on 3D fluorescence spectroscopy (3DF) using the Black Comet (200-950 nm) spectrometer manufactured by StellarNet. In this method, the 3D fluorescence signal is divided into a fixed number of statistical components. For each type of wine, a 3D database is strictly defined, which we conventionally call references. The etalon describe the excitation/emission spectra in detail. The advantage of the 3DF method compared to other statistical methods, such as peak component analysis (PCA), lies in the uniqueness of the unfolding of the spectra. The fluorescence spectra of the wine will be further analyzed by peak component analysis (PCA). After performing the PCA analysis, in order to reduce the number of tolerant etalon, we used the tolerant etalon sample (TES) comparison analysis, thus determining how tolerant the researched wine sample is to this or that specific etalon.

Keywords: 3D fluorescence spectroscopy, peak component analysis, wine analysis, Georgian wine, Tolerant etalon sample

1. Introduction

The combination of 3D fluorescence spectroscopy (3DF) and peak component analysis (PCA) has been used in various fields, including chemistry, biology, environmental science, and food analysis.

The combination of 3D fluorescence spectroscopy (3DF) and peak component analysis (PCA) presents a powerful tool for quality control and authentication in the wine industry, particularly for Georgian wine.

The algorithm for processing the fluorescence excitation-emission matrix for the classification of Argentine white wine is presented in [1]. The effectiveness of using the TES method in wine classification lies in the fact [2] that the types of molecules (such as polyphenols, vitamins, amino acids) and the amount depend on the specific type and maturity of the wine, as well as the wine technology [3].

The study includes fluorescence spectroscopy excitation/emission matrix (AEM) analysis, peak component analysis (PCA) and tolerance etalon sample (TES) comparison analysis method development and modeling according to wine product variety and origin. About 100 samples of four types of white Georgian wine were taken. The methodology chosen by us is based on the one hand on the hardware complex, which was gradually modernized by our group [4,5,6], on the other hand on the development of new analytical approaches [7] that are quite acceptable to be used in typical laboratory control of food products and beverages.

For analyses 3D spectra it is known techniques that are specifically designed for spectroscopic data analysis, such as Multivariate Curve Resolution (MCR), Parallel Factor Analysis (PARAFAC), or Multivariate Analysis of Variance (MANOVA).

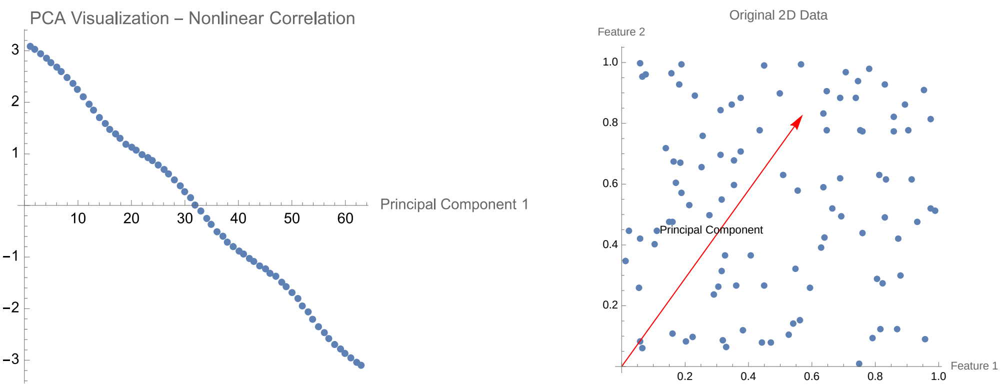
2. Experiment

Fluorescence spectra were recorded using a Black Comet (200-950 nm) spectrometer manufactured by StellarNet. LED lamps of different frequencies were used as light sources. A wine sample of 100 µl is placed in a quartz cuvette and the spectra are recorded at room temperature. The number of scans is determined from the same experimental measurement to exclude drift effects on the sample. At the beginning of each experiment, the standard is calibrated. The excitation wavelength range is between 250-500 nm, and the emission wavelength is between 275-600 nm. Measurements are performed at different excitation wavelengths with a 5 nm bias. The total time to scan a sample is approximately 10 minutes. Measurements were performed over a short period of time (10-15 days), thereby minimizing the influence of atmospheric effects and instrumental fluctuations (eg. lamp intensity fluctuations).

PCA was performed for descriptive analysis of spectral features and TES modeling of analog classes will be used to classify these data. SpectraWiz and LAbView software were used for graphical visualization of the spectra. Data recording and processing were performed in MS Excel and MySQL.

3. Results and Conclusion

With PCA analysis, we will build tables and graphs for the sample of a specific group. Figure 1a shows the generation of 2D data with non-linear correlation and the execution of PCA to reduce the dimensionality to 1D. We visualize data points in a reduced one-dimensional space. Figure 1b shows a 2D plot that visualizes the original 2D data and the first principal component vector obtained from PCA. In Figure 1b visualized the original 2D data as scattered points and plot the first principal component vector obtained from PCA as a red arrow. The arrow represents the direction of maximum variance in the data, which corresponds to the first principal component. The plot also includes a label indicating that it represents the principal component.



a) b)

Fig.1. a) 2D data with non-linear correlation and the execution of PCA to reduce the dimensionality to 1D, b) 2D plot that visualizes the original 2D data and the first principal component vector obtained from PCA

In Figure 2 given 3D plot to visualize the original 3D data, the principal component vectors obtained from PCA, and the data points projected onto the principal component subspace. In this 3D plot, we visualize the original 3D data as scattered points, plot the first two principal component vectors obtained from PCA. The data points projected onto the principal component subspace as green points.

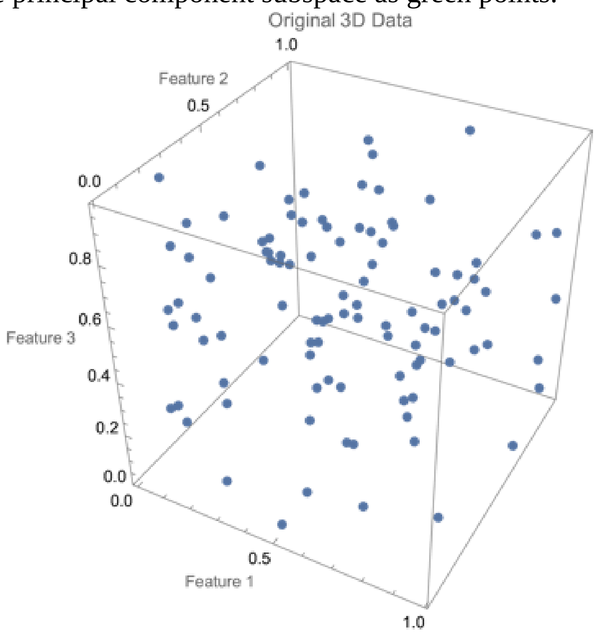


Fig.2 3D plot to visualize the original 3D data, the principal component vectors obtained from PCA

Conclussion:

The combination of 3DF and PCA allows for a detailed assessment of the unique fluorescence patterns present in different types of Georgian wine. This can be used as a reliable method for quality control and authentication, helping to identify any adulteration or counterfeit products in the market. By comparing the fluorescence spectra of a given wine sample with the well-defined references (etalons), we can verify its authenticity and origin.

The fluorescence spectra of wine can be influenced by factors such as grape variety, soil composition, and climate conditions. The 3DF method, combined with PCA and etalon references, can potentially be used to establish a link between the fluorescence patterns and the geographical origin of the wine. This could be valuable for wine producers aiming to protect and promote wines with specific geographical indications.

Different vintages of the same wine type can exhibit variations in their fluorescence properties due to varying environmental conditions and winemaking processes. The 3DF analysis, along with PCA and etalon references, might help discern these subtle differences and aid in distinguishing between wines from different years.

Some wines are known for their unique characteristics and premium quality, which are often reflected in their distinct fluorescence profiles. Utilizing the 3DF method with PCA analysis can help classify wines into different quality grades based on their fluorescence patterns. This information can be valuable for consumers, sommeliers, and wine enthusiasts when making purchasing decisions.

Understanding the fluorescence properties of different wines can provide insights into the chemical composition and structural changes during the winemaking process. This knowledge may assist winemakers in optimizing their production techniques and ensuring consistent quality in the final product.

The 3DF technique can provide a wealth of data on the complex chemical composition of wines. Researchers can use this information to study the presence of various compounds and their interactions, contributing to a deeper understanding of wine chemistry and its influence on wine characteristics.

Overall, the combination of 3DF, PCA, and etalon references in the analysis of Georgian wine offers a powerful and sophisticated approach to gain valuable insights into the unique fluorescence properties of different wine types. As this technology evolves and becomes more established, it has the potential to revolutionize the field of wine analysis and enhance various aspects of the wine industry.

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