Use of Sensor Systems with Spectral Pattern

Recognition for Food Authentication

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Outline

- Overview of food authentication
 - Methods
 - Challenge
- Research problems and aims
- Spectral pattern recognition
 - Classification
 - Model interpretation
- Sensor systems
 - Near-infrared spectroscopy
 - Diffraction grating
 - Computer vision (video based)
- Conclusion
- Future work

1. Overview

- Food adulteration and fraudulent labelling
 - Damage public health
 - Reduce consumer confidence
 - Ruin brand reputation
 - Examples:
 - *"Foreign beef 'is sold as British," BBC News, 2008.*
 - *"Germany investigates possible organic egg fraud," Reuters, 2013.*
 - *"Meat testing: A fifth of samples reveal unspecified animals' DNA," BBC News, 2018.*

1. Overview

- Food authentication is a process which verifies the food compliance with its label description.
 - Origin (species, geographical or genetic)
 - Production method (conventional, organic, traditional procedures, free range)
 - Processing technologies (irradiation, freezing, microwave heating).
- Conventional authentication methods
 - Sensory analysis → five organs perception → expensive, subjective and inconsistent
 - Laboratory-based instrumentation → wet chemistry and chromatography → time-consuming, require complex sample preparation and technical knowledge

1. Overview

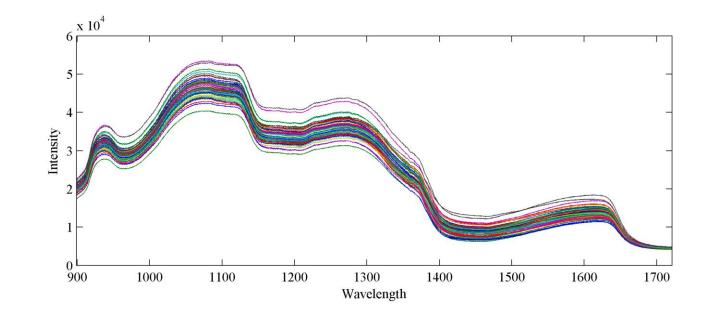
- Challenge: seek and develop efficient and low-cost methods for food authentication
 - Accurate determination
 - Fast and non-destructive
 - Minimal or no sample preparation and reagent consumption
- Novel methods for real-time food authentication methods
 - Optical measuring technologies, such as NIR spectroscopy, hyperspectral imaging and computer vision
 - Pattern recognition algorithms

2. Research problems and aims

- Problems:
 - Low-cost and portable sensors
 - Variable sampling conditions and instrumental limitations
 - Lower fingerprint data quality
 - Pose a serious challenge to pattern recognition methods
 - Nonlinear conditions
 - Caused by instrumental and experimental artefacts
 - Classical methods (PLS) often degrade in performance
- Aims:
 - Extract useful fingerprint data from noisy field data
 - Assist low-cost spectral-based sensors in obtaining the required level of performance compared to high-resolution spectrometers
 - Develop efficient and low-cost sensor systems

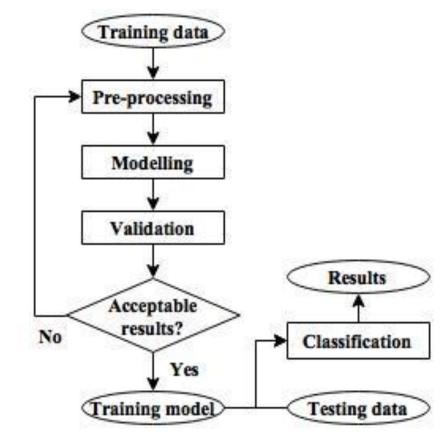
3. Spectral pattern recognition

- An interdisciplinary science of using mathematical, statistical and machine learning methods to identify regularities in spectral data
 - Regularities \rightarrow chemical compositions and physical properties
 - Data presentation \rightarrow radiation intensity versus wavelengths or frequencies
- Essential characteristics
 - High-dimensionality
 - High-collinearity
 - Non-linearity



3. Spectral pattern recognition: framework

- Pre-processing removes physical artefacts in spectra and improves the performance and robustness of classification model
- Modelling discovers the relationship between spectral data and qualitative/quantitative information
- Parameter optimization
- New input data prediction



3. Spectral pattern recognition: partial least squares (PLS)

- PLS is standard chemometric method for processing a wide spectrum of chemical data problems.
- Basic assumption: the investigated system or process is driven by a set of underlying latent variables (LVs).
- PLS searches for linear combinations of independent variables that maximize the covariance between the LV and the response:

max $w^T X^T Y c$, s.t. $w^T w = c^T c = 1$.

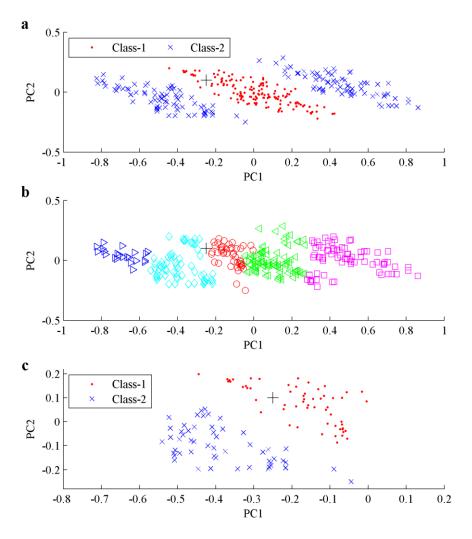
where **X** is the matrix of independent variables, **Y** is the matrix of response, **w** and **c** is the weight vector of **X** and **Y**, respectively.

3. Spectral pattern recognition: partial least squares (PLS)

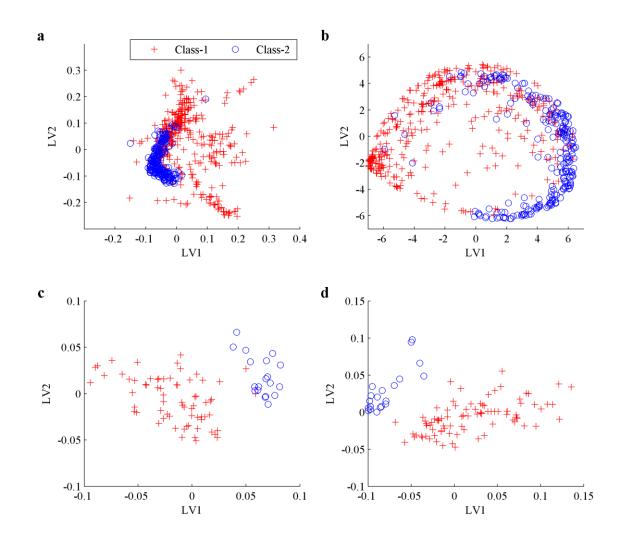
- PLS classification: dummy matrix coding transforms category information into numerical responses.
- Advantages
 - Stably estimate regression coefficients from low-dimensional LVs
 - Efficiently handle some ill-conditioned problems
 - Small sample size
 - High-dimensionality
 - High-collinearity
 - Model interpretation: PLS is good at showing significant variables via loadings or weights compared to SVM and LDA.
- Performance degradation in nonlinear, class imbalance and multiclass conditions

- Motivations
 - PLS is practically suitable for high-dimensionality and multicollinearity
 - Local models reduce global nonlinearity
 - Use weighting schemes based on the distance between query and training samples
- The proposed methods
 - Local PLS for classification
 - Nearest neighbors
 - Nearest clusters
 - Locally weighted
 - Representation classification with PLS regression
 - Model interpretation

- Example 1: nearest clusters PLS-DA
 - Generate multimodal PCA scores
 - Simulate orthogonal combination of Gaussian peaks and reference spectrum can produce simulated data
- The black-cross (+) sample is wrongly classified by PLS-DA
- Local PLS approaches shows simplified and distinctive structure which is approximately linear separable.



 Training sample (a real-world spectral data) projections in the latent variable space of the PLS-DA and kernel PLS-DA model (a & b). Local training sample projections in the latent variable space of the local PLS-DA models (c & d).



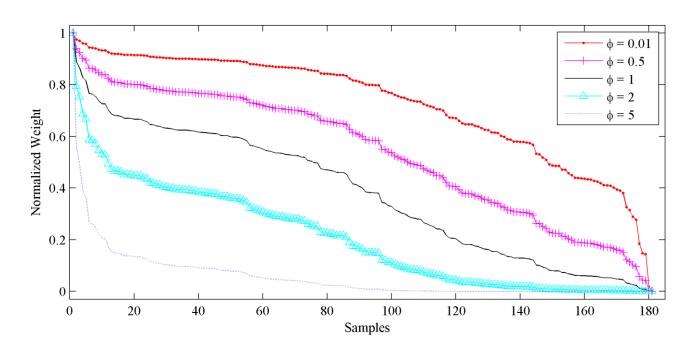
- Example 2: LW-PLS classification
- Weighting scheme ω_n

$$\omega_n = \exp\left(-\frac{\varphi d_n}{\sigma_d}\right)$$

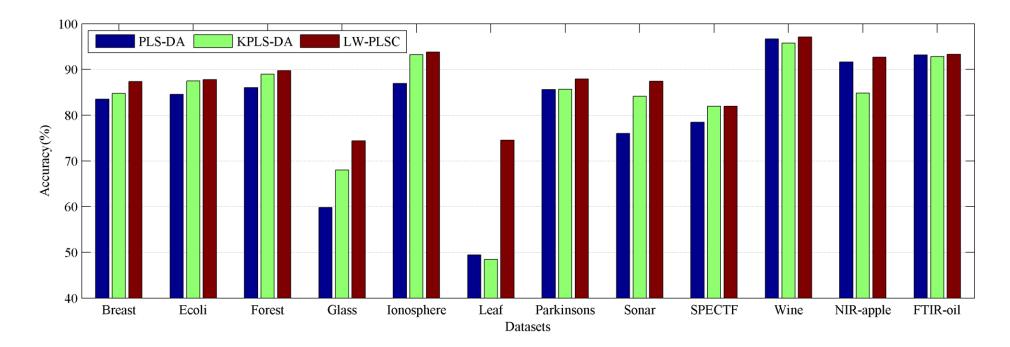
where φ is localization parameter, d_n is Euclidean distance between query and training samples, σ_d is a standard deviation of $\{d_n\}$.

- For a given query, the weighting scheme respectively enlarges and lessens the influence of neighboring and remote samples towards a PLS-DA model.
- Two parameters localization parameter φ and LVs controls sample weights and model complexity, respectively.

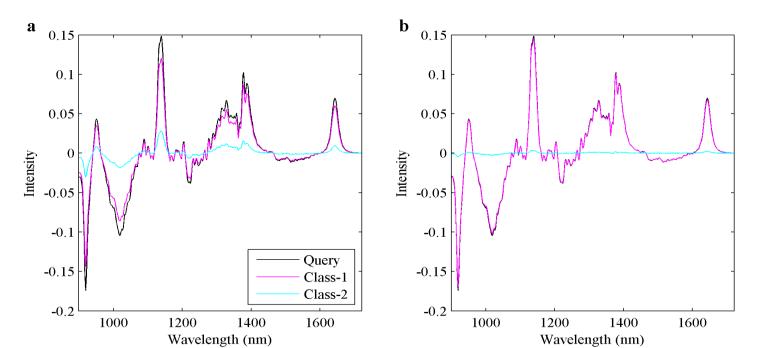
- Graphical representation of different ϕ values with respect to sample weights for a query sample
 - Small ϕ value: LW-PLSC becomes to PLS-DA
 - Large ϕ value: enlarged influence of neighboring samples



- Classification accuracy of PLS-based methods on UCI and spectral datasets.
- LW-PLSC > Kernel PLS-DA (RBF) > PLS-DA



- Example 3: representation classification with weighted PLS regression
 - Use a weighted linear combination of training samples to represent a query
 - Attribute the query to the class which yields the least PLS approximation error
- Classification model interpretation (comparison)



4. Sensor systems

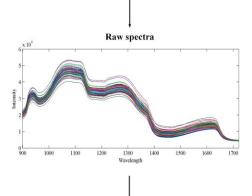
- Near-infrared spectroscopy (NIRS)
 - Organic and conventional apples
- Diffraction grating
 - Apple varieties
 - Organic and conventional apples
- Computer vision system (CVS)
 - Olive oil adulteration
 - Milk fat content (whole, skimmed and semi-skimmed)
 - Milk powder

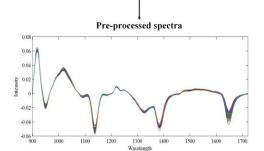


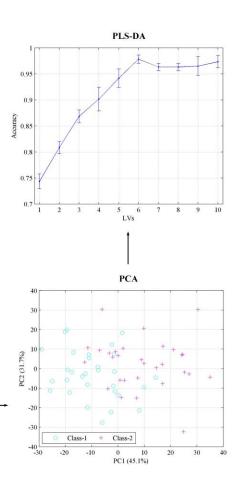
4. Sensor systems: NIRS

Apple samples





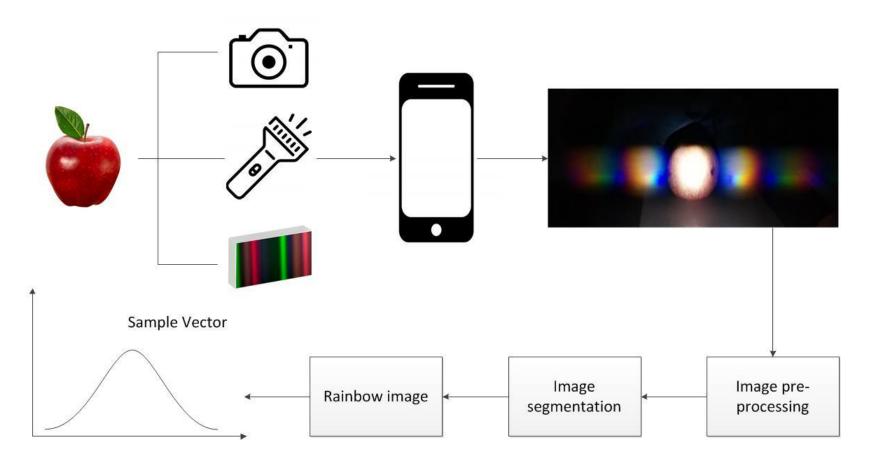




- Differentiation of organic and conventional apples
- Accuracy:
 - LOOCV: 95% (LW-PLSC)
 - Classification: 93% (LW-PLSC)

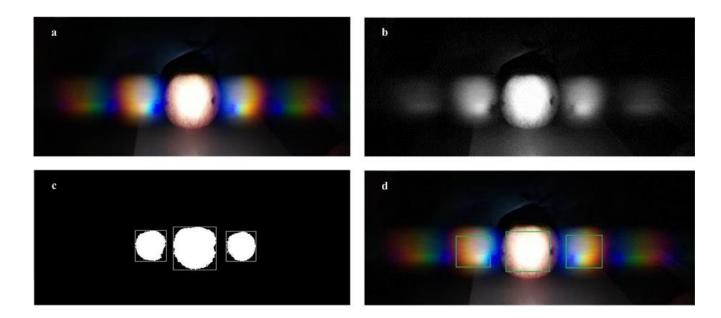
4. Sensor systems: diffraction grating

• Framework



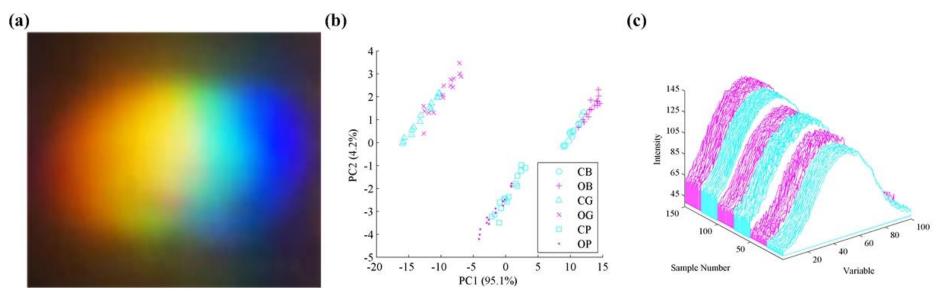
4. Sensor systems: diffraction grating

- a) Rainbow images
- b) Grayscale processing
- c) Mathematical morphology
- d) OSTU for image extraction



4. Sensor systems: diffraction grating

- Rainbow image (a) \rightarrow numerical values (c) \rightarrow PCA scores (b)
- Results
 - Over 93% accuracy
 - LW-PLSC, SVM and LS-SVM outperforms other 9 baseline classifiers
 - Comparable to portable NIR spectrometers



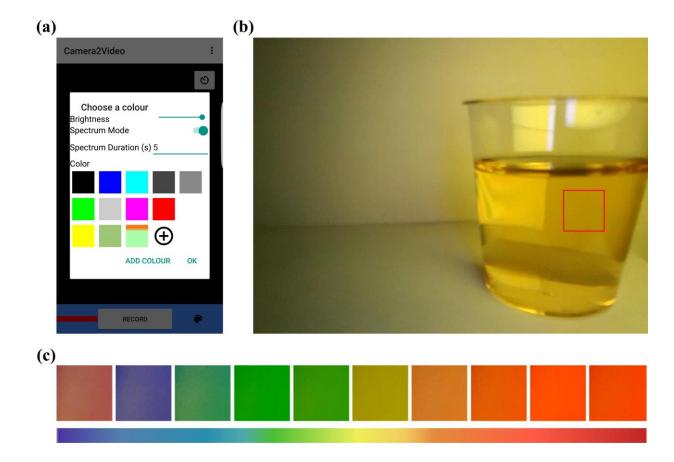
4. Sensor systems: computer vision system

- CVS aims to replace human visual system by artificial sensor and automatically gain high-level understanding from digital images.
- It extracts useful food external information, such as colour, size and shape.
- Procedures: image acquisition, processing and analysis
- Hardware: illumination, camera and computer
- Common applications:
 - content estimation
 - freshness assessment
 - defect detection

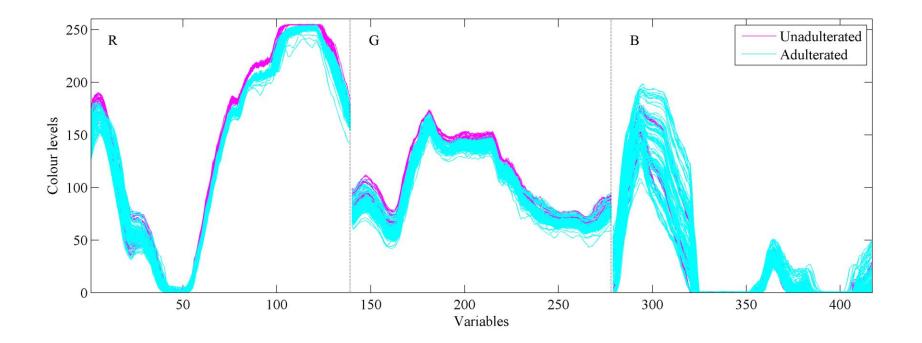
4. Sensor systems: computer vision system

- Limitations of conventional CVS
 - Less practical for consumers
 - Properly designed illumination
 - Careful setting of camera
 - Varying sampling conditions
 - External camera and computer software
- Motivations
 - A feasible alternative to external camera: smartphone
 - Use CVS to capture spectral information (video)

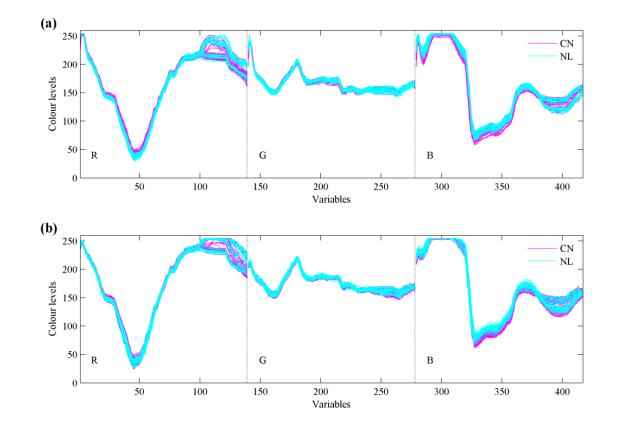
- a) The user interface of Camera2Video app;
- b) Image (960 × 720 pixels) of oil sample illuminated by yellow light. The selected ROI is marked by a red box with 100 × 100 pixels;
- c) Images of ROI illuminated by lights with a sequence of spectral colours.



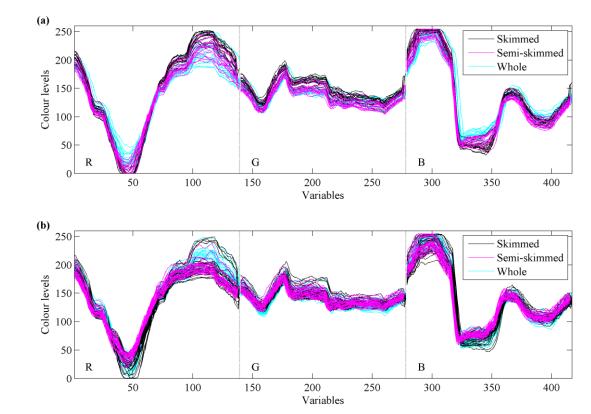
- Video data of unadulterated and adulterated olive oil.
- Distinction of unadulterated and adulterated 80 samples in red colour channel variables 85-125.



- Identification of milk powder origin (CN and NL)
- Two sampling sessions, 168 samples
- Results
 - LOOCV: 86.6% (LW-PLSC)
 - Classification: 89.3% (SVM)



- Classification of skimmed, semi-skimmed and whole milk
- Two sampling sessions, 138 samples
- Results
 - LOOCV: 97.8% (PLS-DA and LW-PLSC)
 - Classification: 100% (PLS-DA and LW-PLSC)



5. Conclusion

- The proposed methods improve the modelling performance and simplicity in classifying nonlinear spectral data.
- They outperform baseline methods in most of the time.
- Low-cost sensor yields comparable results to commercial spectrometer with the aid of state of the art methods, such as LW-PLSC.
- The use of phone videos coupled with pattern recognition has great potential for efficient and low-cost food authentication.

6. Future work

- Model interpretation
 - A comparison between machine learning and chemometrics variable selection.
- Data representation
 - Small sample size
 - 'Variable' weighted regression
 - Between class regularization
- Big data and deep learning
 - Sampling
 - Modelling
 - App development

Publications

- W. Song, H. Wang, P. Maguire, O. Nibouche, Differentiation of organic and non-organic apples using near infrared reflectance spectroscopy — A pattern recognition approach, in: SENSORS, 2016 IEEE, IEEE, 2016.
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- W. Song, H. Wang, P. Maguire, O. Nibouche, Nearest clusters based partial least squares discriminant analysis for the classification of spectral data, Anal. Chim. Acta. 1009 (2018) 27–38.
- W. Song, H. Wang, P. Maguire, O. Nibouche, Collaborative representation based classifier with partial least squares regression for the classification of spectral data, Chemom. Intell. Lab. Syst. 182 (2018) 79-86.
- W. Song, H. Wang, P. Maguire, O. Nibouche, Spectral data classification using locally weighted partial least squares classifier, Data Science and Knowledge Engineering for Sensing Decision Support – Proceedings of the 13th International FLINS Conference (2018) 700-707.
- N. Jiang, W. Song, H. Wang, G. Guo, Y. Liu, Differentiation between organic and non-organic apples using diffraction grating and image processing—A cost-effective approach, Sensors (Switzerland). 18 (2018) 1667.