Principal component analysis: examples Introduction to Statistical Modelling

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Examples

- Adulteration of olive oil
- Malavi, Derick, Amin Nikkhah, Katleen Raes, and Sam Van Haute. 2023. "Hyperspectral Imaging and Chemometrics for Authentication of Extra Virgin Olive Oil: A Comparative Approach with FTIR, UV-VIS, Raman, and GC-MS." Foods 12 (3): 429. https://doi.org/10.3390/foods12030429
- 2 Human faces dataset
- https://scikit-learn.org/0.19/datasets/olivetti_faces.html

Adulteration of olive oil

Problem setting

Extra virgin olive oil (EVOO):

- High quality
- Flavorful
- Health benefits
- More expensive (than regular oil)

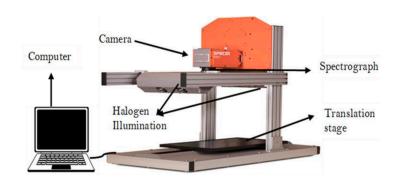
To reduce cost, EVOO is often adulterated with other, cheaper food oils.



Research questions

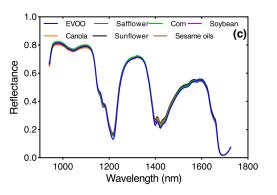
- Classification: Can we detect whether a given EVOO sample has been adulterated?
 - Yes/no answer (categorical)
- **2 Regression:** Can we detect the degree of adulteration?
 - Continuous answer, from 0% (no adulteration) to 100%

Hyperspectral imaging (HSI)



- Measures reflected infrared light (700-1800 nm) off sample
- Provides a non-destructive way of testing sample

Hyperspectral "images" (spectra)



- HSI measures reflectance at 224 wavelengths from 700 to 1800 nm
- Reflectance at given wavelength is determined by molecular features of sample

Experimental setup

Samples to test (61 total):

- 13 different kinds of unadulterated EVOO
- 6 vegetable oils
- 42 adulterated mixtures
 - EVOO + one of 6 vegetable oils at one of 7 different percentages (from 1% to 20%)

Each sample is imaged 3 times: 183 samples

Each sample produces a HSI spectrum of length 224

Data matrix

Data matrix has 183 rows (samples) and 224 columns (spectra).

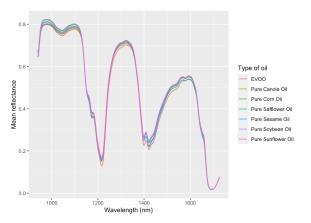
In addition, we have some metadata:

- Name of sample
- Degree of adulteration

	Sample ID/Wavelength	Sample ^	Classification	% Adulteration $^{\circ}$	938.94000200000005	942.45001200000002	945.96002199999998
1	Monini Classico EVOO	1	Olive	0	0.650031	0.655155	0.704436
2	Monini Classico EVOO	2	Olive	0	0.646796	0.651895	0.701250
3	Monini Classico EVOO	3	Olive	0	0.651539	0.656589	0.704596
4	Fontana EVOO	4	Olive	0	0.649832	0.654923	0.703678
5	Fontana EVOO	5	Olive	0	0.645579	0.650628	0.698899
6	Fontana EVOO	6	Olive	0	0.647227	0.652270	0.700465
7	Divella EVOO	7	Olive	0	0.646414	0.651584	0.700632
8	Divella EVOO	8	Olive	0	0.649089	0.653915	0.701284
9	Divella EVOO	9	Olive	0	0.639494	0.645490	0.701185
10	EVOO from Spain	10	Olive	0	0.643378	0.648587	0.699279
11	EVOO from Spain	11	Olive	0	0.646907	0.651400	0.696273
12	EVOO from Spain	12	Olive	0	0.640076	0.645553	0.697743
13	Borges EVOO	13	Olive	0	0.645270	0.650284	0.698843
14	Borges EVOO	14	Olive	0	0.641859	0.646935	0.695553
15	Borges EVOO	15	Olive	0	0.639936	0.645475	0.698057
16	Premium Oil EVOO	16	Olive	0	0.640139	0.645473	0.696361
17	Premium Oil EVOO	17	Olive	0	0.639872	0.645166	0.695145
18	Premium Oil EVOO	18	Olive	0	0.645821	0.650525	0.695868

A first look at the data

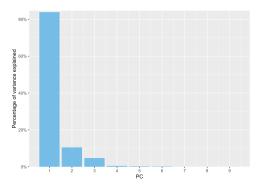
Averaged spectra for each kind of oil (EVOO + 6 others)



Plot shows small differences between spectra: **promising sign** that we will be able to address the research questions.

Principal component analysis: scree plot

Not all 224 wavelengths are equally informative. Much of our dataset is redundant.

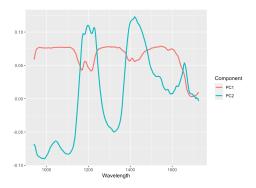


This is confirmed by the scree plot:

- First 2 PCs explain **94% of variance** in the data
- First 3 PCs: almost 100%

Principal component analysis: loadings vectors

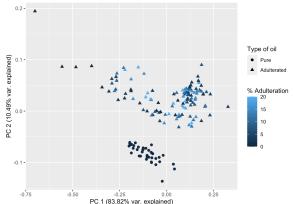
Loadings vectors are linear combinations of features, tell us how features contribute to variability in dataset.



For our example:

- Loadings vector 1: where do spectra differ the most?
- Loadings vector 2: where is next source of variability located?

Principal component analysis: scores



Can we tell pure and adulterated samples apart?

• Yes: clearly different on score plot.

Can we predict the percentage of adulteration?

• **No**: hard to distinguish from first 2 PCs alone.

Predicting the percentage of adulteration

We will need more than 2 PCs to correctly predict percentage of adulteration.

Two different approaches:

- Principal component regression:
 - Compute PCs
 - 2 Do a regression on PCs
- Partial least squares regression:
 - Compute factors that are most variable and most correlated with outcome
 - 2 Do a regression on resulting factors

Both models can be built using the pls package in R.

Dataset

For this example we will use only the 42 adulterated mixtures.

Each mixture is imaged 3 times: $42 \times 3 = 126$ samples

Predictors: 224 wavelengths

Outcome: percentage of adulteration (1%-20%)

Performing a fair assessment: train/test split

Evaluating the model using the same data used to train it leads to an **optimistic** estimate of the model's performance.

To avoid this bias, randomly select and set aside some data for testing, and use the remaining data to develop the model.

Test data (20%) (80%)

Adulteration prediction:

Train dataset: 101 samples

• Test dataset: 25 samples

Can you spot an issue with this?

Performing a fair assessment: data leakage

- Each of the 42 mixtures is imaged 3 times.
- Presumably these replicates are very similar
- If some replicates end up in the test dataset and some in the train dataset: model gains unfair advantage.



Avoiding data leakage: stratified train/test split

Main idea: develop model with some of the mixtures, test performance on different mixtures:

- 1 Randomly select 80% of mixtures
- 2 Put all 3 replicates for those 80% in the training set
- 3 Put the remainder in the test set.



Building the PCR/PLS models

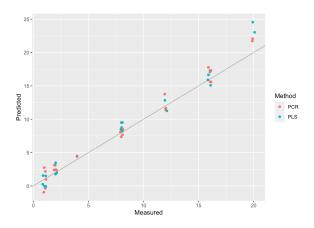
PCR model:

PLS model: replace pcr by plsr.

Arguments:

- scale = FALSE: Don't scale spectra (same units)
- ncomp = 10: Build model with up to 10 components
- validation = "CV": Assess performance of model with i components using cross-validation

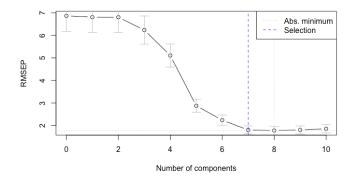
Performance of PCR/PLS models



Both models do well on the test data.

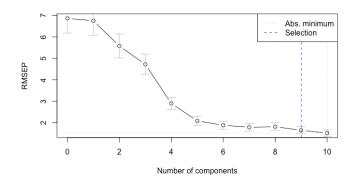
Optimal number of components: PCR

(obtained via selectNcomp(method = "onesigma"))



- Optimal number of components: 7
- RMSEP for 7 components: 1.796

Optimal number of components: PLS



- Optimal number of components: 9
- RMSEP for 9 components: 1.627

Conclusions

Can we detect whether a given EVOO sample has been adulterated?

- Yes: Look at score plot
- More conclusive answer next lecture

Can we detect the degree of adulteration?

Yes: Build PCR or PLS model

Human faces dataset