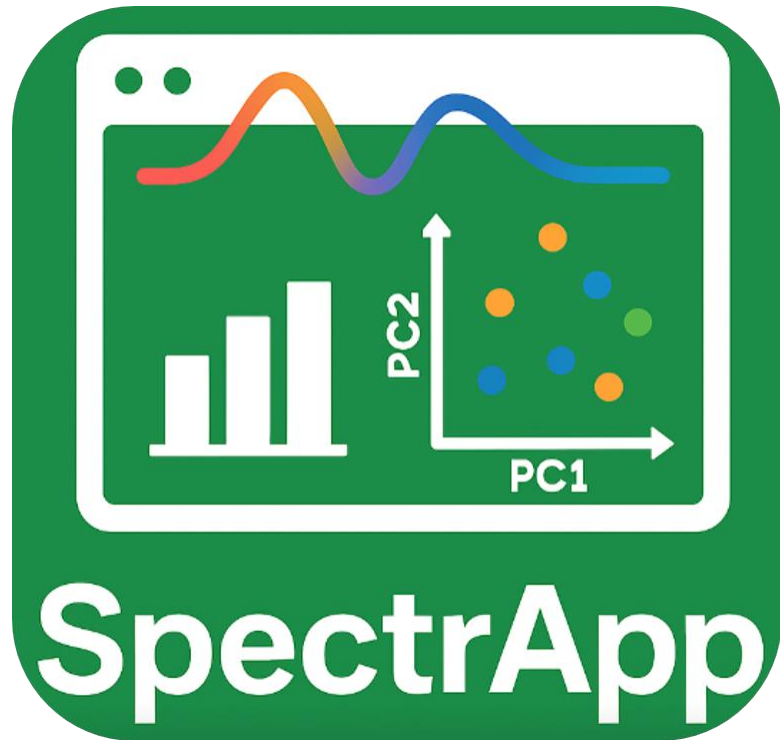


SpectrApp



Applications that facilitates to perform statistical analysis.

It aims to be an alternative to paid solutions (e.g., Matlab, STATA,...) providing a user-friendly interface of R routines for many common tasks.





 **Login**
SpectrApp

Username

Enter your username

Password

Enter your password

 **Login**

Username: *eafs*

Password: *2025*



Department of Chemistry

DATA BLOOM
UNIVERSITY OF TURIN



DataBloom
Let your data flourish

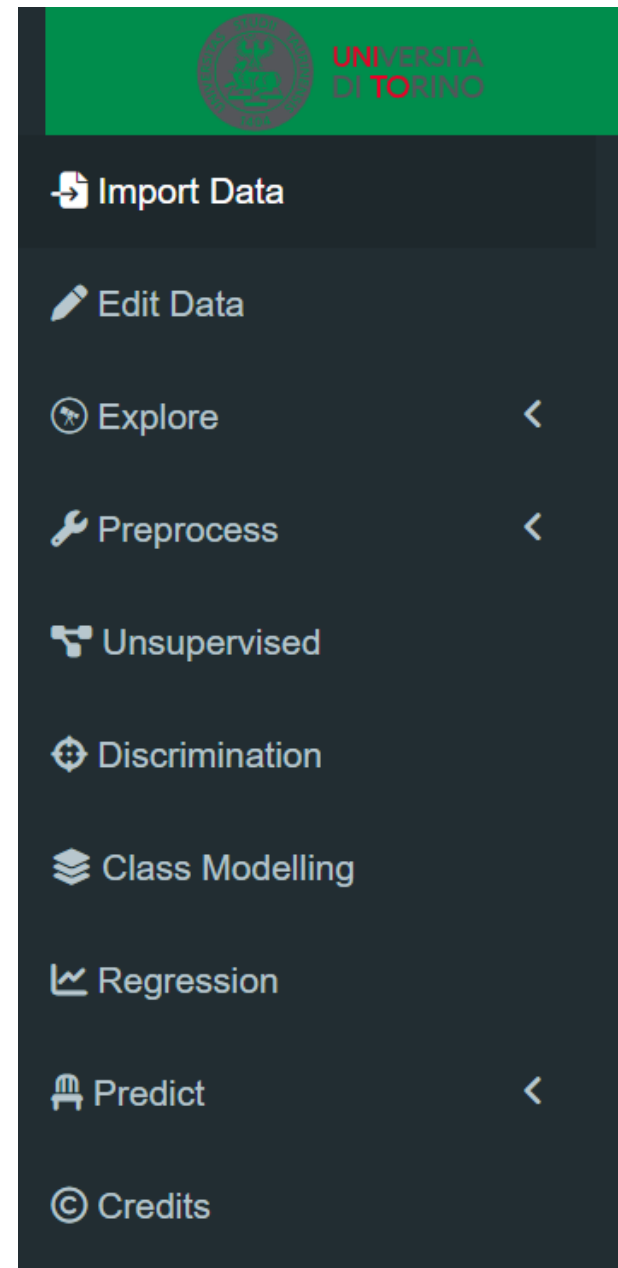
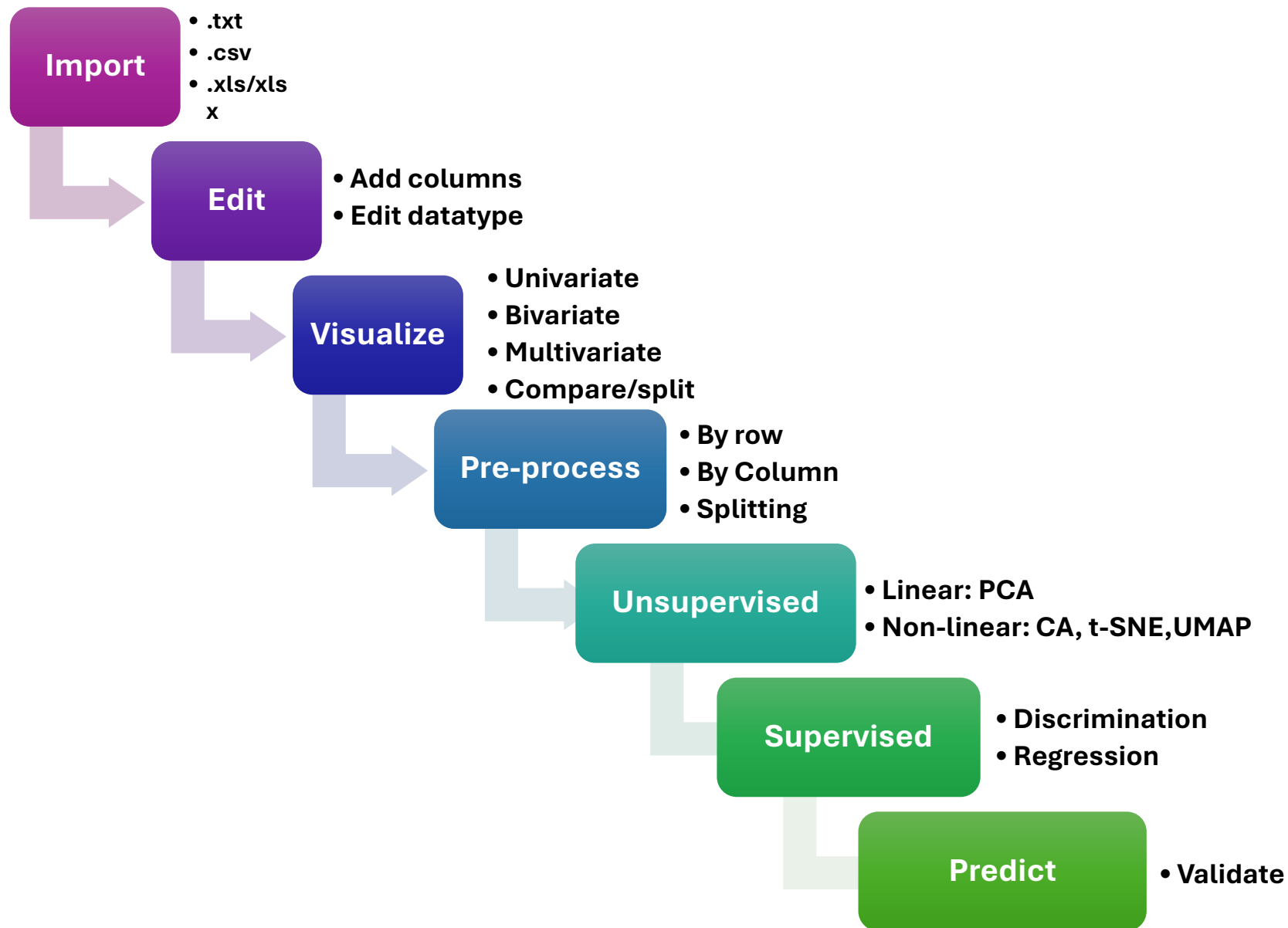


© Spectrapp - Developed by the Department of Chemistry of the University of Turin and DataBloom Srl



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SpectrApp pipeline



Import data

The screenshot shows the 'Import Data' interface of a software application. On the left is a dark sidebar with navigation options: 'Import Data' (selected), 'Edit Data', 'Explore', and 'Preprocess'. The main area has a green header bar with the 'UNIVERSITA DI TORINO' logo and a hamburger menu icon. Below the header, the interface is divided into sections. The 'Type of file:' section contains a blue dropdown menu currently set to '.csv'. A red callout box labeled 'Define data format' with an upward-pointing arrow is positioned below this dropdown. The 'Data:' section shows an upload progress bar for a file named 'eafs2025_blood.csv', with the status 'Upload complete'. To the right of the file name is a blue button with a gear icon and a dropdown arrow. A red callout box labeled 'Edit import settings' with an upward-pointing arrow is positioned below this button. On the far right of the main area is a green 'Import' button with a cloud and upload icon. The top right corner of the application window features a dark green bar with a sun icon and a red circular refresh button.

UNIVERSITA DI TORINO

Import Data

Edit Data

Explore

Preprocess

Type of file:

.csv

Define data format

Data:

Upload... eafs2025_blood.csv

Upload complete

Edit import settings

Import

Import data

Type of file:

.csv

Data:

Upload...eafs2025_blood.csv

Upload complete

30
Rows

602
Columns

→ Next step → Edit

Once imported, click on "Next step"

Search:

ID	Blood_source	700	701	702	703	704	705	706	707	708
	All	All	All	All	All	All	All	All	All	All
S_1	Blood_1	0.839248598	0.83859545	0.8373409510000001	0.836078405	0.835126758	0.834991634	0.835918605	0.837677121	0.840327

Edit data

- Edit Data
- Explore
- Preprocess
- Unsupervised
- Discrimination
- Class Modelling
- Regression
- Predict
- Credits

Remove variables / samples

Variables to exclude:
Nothing selected

Samples to exclude:
Nothing selected

Remove

Define numeric / categorical variables

Remove samples/variables

Numeric variables:
700, 701, 702, 703, 704, 705, 706, 707, 708, 709, 710, 711, 712, ...

Factor variables:
Blood_source

Check numeric vars.

Check categorical vars

⚙️

✓ Approve dataset

Once checked, click on "Approve"

Data pre-processing

Import Data

Edit Data

Explore

Preprocess

Numeric

Chemicals

Data

Unsupervised

Discrimination

Class Modelling

Regression

Spectra / Time / Numeric Variables

☐ Select ranges

All data selected.

Choose pre-processing technique(s):

Background (row)

Baseline

Continuum Removal

Row Scaling

Standard Normal Variate (SNV)

SNV + Detrend

Extended Multiplicative Signal Correction (EMSC)

With spectra,
select the
variable range

Select one or more pre-
processing from the list (N.B.
the order is significant)

Data pre-processing

Spectra / Time / Numeric Variables

☐ Select ranges

All data selected.

Choose pre-processing technique(s):

Extended Multiplicative Signal Correction (EMSC) ×

Preprocessing Settings

↔ Range scaling

☰ Smoothing

▣ Binning

🖌 Background / Baseline

📊 Row scaling & EMSC

Edit settings *ad hoc* for specific pre-processing

⚙ Preprocess

→ Next step →
Chemicals

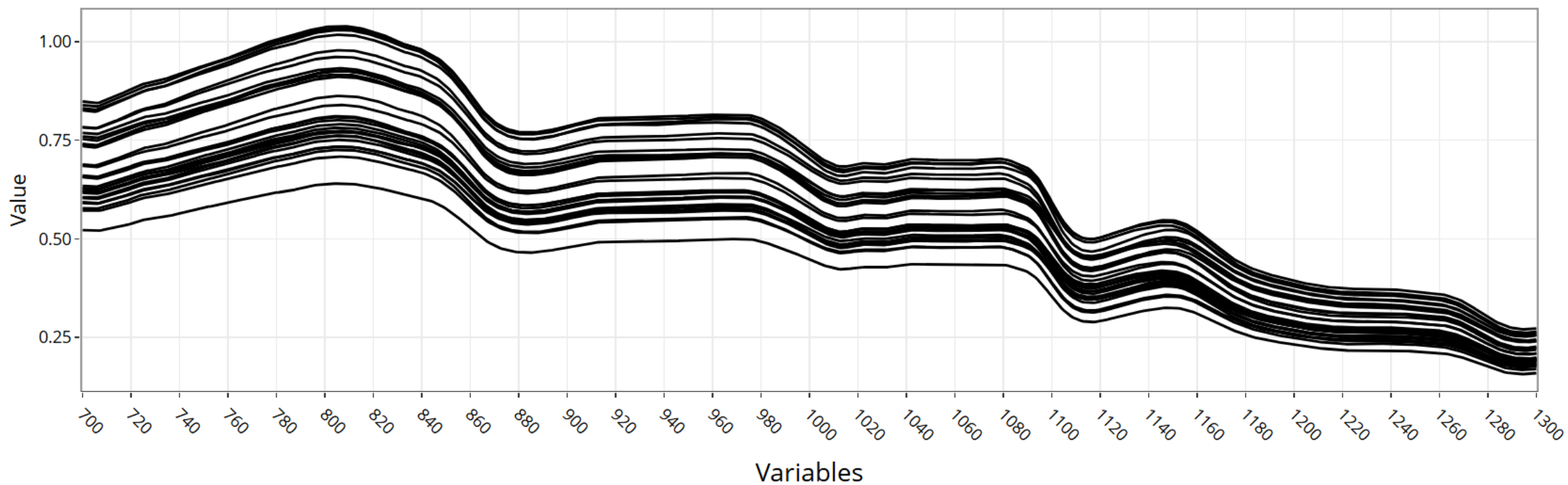
Data pre-processing

Compare raw and
pre-processed

Original data



Click to enter Plot title



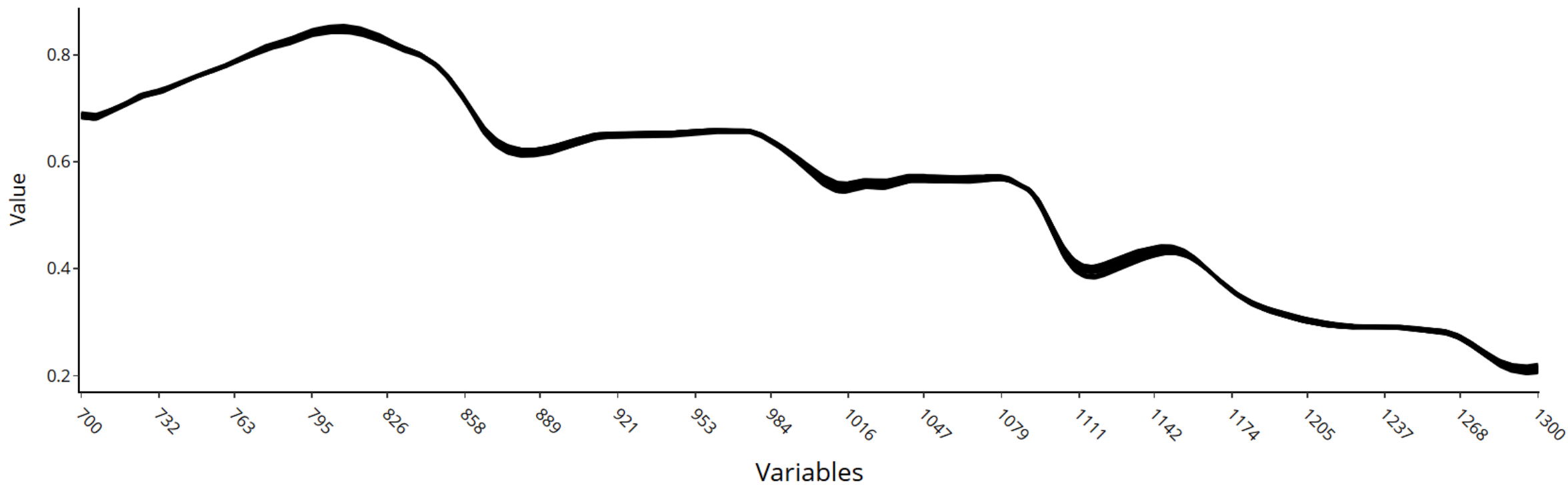
Data pre-processing

Compare raw and
pre-processed

Pre-processed data



Click to enter Plot title



Data pre-processing

Edit graphs
settings

erage (if factor variable):

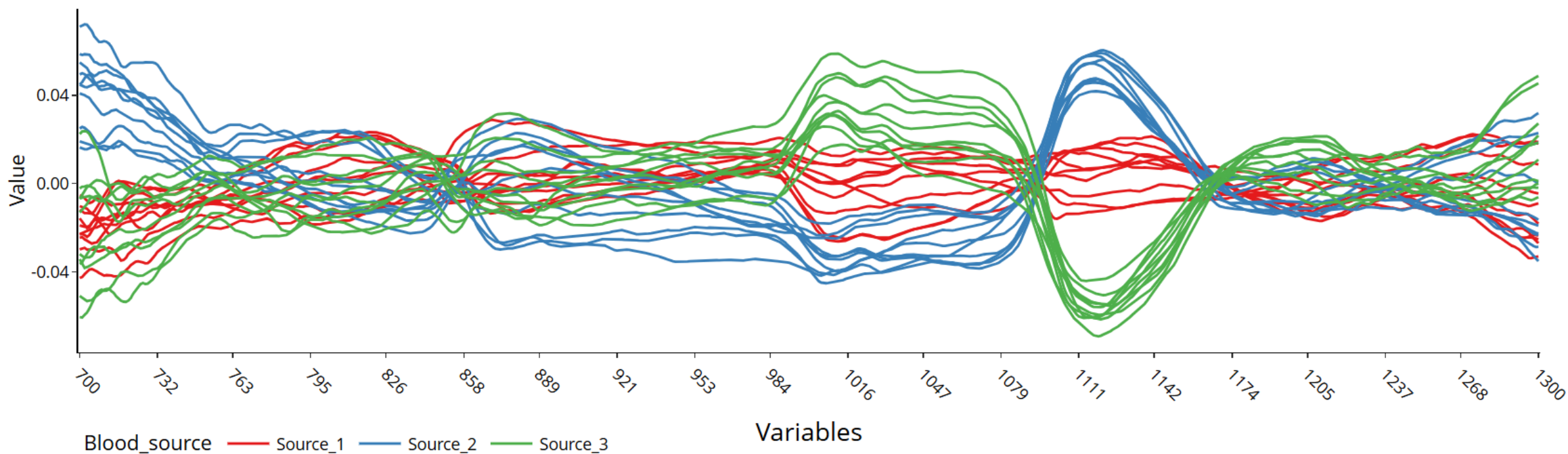
Original data



Pre-processed data



Click to enter Plot title



Data pre-processing

Pre-processed data

Show10entries

Search:

	Blood_source	Instrument	700	701	702	703	704	705	706	707	708	709	710	711	712	713	714	715	716	717	718	719	720
S_1	Source_1	A	-0.024	-0.024	-0.025	-0.026	-0.027	-0.027	-0.027	-0.027	-0.025	-0.024	-0.022	-0.021	-0.019	-0.018	-0.016	-0.016	-0.015	-0.014	-0.013	-0.014	-0.015
S_2	Source_1	B	-0.010	-0.011	-0.011	-0.011	-0.013	-0.014	-0.014	-0.015	-0.016	-0.017	-0.016	-0.016	-0.015	-0.014	-0.014	-0.014	-0.014	-0.015	-0.014	-0.014	-0.014
S_3	Source_1	A	-0.005	-0.006	-0.007	-0.008	-0.009	-0.008	-0.008	-0.007	-0.007	-0.007	-0.008	-0.009	-0.009	-0.010	-0.009	-0.009	-0.009	-0.009	-0.009	-0.007	-0.007
S_4	Source_1	B	-0.030	-0.030	-0.029	-0.030	-0.030	-0.030	-0.030	-0.031	-0.031	-0.030	-0.030	-0.030	-0.029	-0.029	-0.030	-0.032	-0.034	-0.035	-0.035	-0.034	-0.032
S_5	Source_1	A	-0.012	-0.013	-0.013	-0.013	-0.014	-0.014	-0.013	-0.011	-0.009	-0.007	-0.005	-0.003	-0.002	-0.001	0.000	0.001	0.001	0.001	0.001	0.001	0.001
S_6	Source_1	B	-0.023	-0.023	-0.023	-0.024	-0.023	-0.021	-0.019	-0.017	-0.016	-0.015	-0.016	-0.016	-0.017	-0.017	-0.016	-0.014	-0.013	-0.011	-0.010	-0.009	-0.009
S_7	Source_1	A	-0.016	-0.017	-0.019	-0.020	-0.020	-0.018	-0.016	-0.015	-0.013	-0.010	-0.009	-0.007	-0.005	-0.002	-0.000	0.001	0.001	0.001	0.001	-0.000	-0.001
S_8	Source_1	B	-0.019	-0.019	-0.020	-0.020	-0.019	-0.018	-0.017	-0.016	-0.017	-0.018	-0.020	-0.022	-0.023	-0.023	-0.022	-0.021	-0.020	-0.018	-0.018	-0.018	-0.017
S_9	Source_1	A	-0.043	-0.042	-0.041	-0.040	-0.039	-0.039	-0.039	-0.040	-0.041	-0.041	-0.042	-0.041	-0.041	-0.042	-0.042	-0.042	-0.042	-0.041	-0.040	-0.039	-0.038
S_10	Source_1	B	-0.023	-0.022	-0.022	-0.021	-0.021	-0.021	-0.020	-0.020	-0.019	-0.019	-0.018	-0.019	-0.019	-0.019	-0.019	-0.019	-0.018	-0.017	-0.016	-0.016	-0.015

Showing 1 to 10 of 30 entries

If the pre-process is fine, you can start building the models

Previous

1

2

3

Next

If the pre-process is fine, you can start building the models

30
Samples

2
Factor variables

601
Numeric variables

0
Chemical variables

→ Unsupervised

→ Discrimination

→ Class Modelling

→ Regression

Unsupervised models

Exclude these variables from modeling:

Nothing selected

Remove vars from computation

PCA

HCA

K-means

DBSCAN

t-SNE

UMAP


PCA model

Nr. of PCs for PCA model:

10

Select PCA methodology:

SVD

 Calculate

Unsupervised models

Exclude these variables from modeling:

Nothing selected ▼

PCA HCA K-means DBSCAN t-SNE UMAP

PCA model

Nr. of PCs for PCA model:

10

Select PCA methodology:

SVD ▼

Calculate

Edit model settings

Build the model

Unsupervised models

Exclude these variables from modeling:

Nothing selected

PCA HCA K-means DBSCAN t-SNE UMAP

PCA model

Nr. of PCs for PCA model:

10

Select PCA methodology:

SVD

Calculate

This approach works for both unsupervised and supervised models

Supervised models - discrimination

The image shows a software interface for selecting supervised models for discrimination. At the top, a horizontal bar contains several model names: kNN, LogReg, LDA, QDA, PLS-DA, and RF. The 'kNN' model is highlighted with a red border. A red arrow points from a red box labeled 'Available models' to this bar. Below the model bar, the text 'kNN model' is displayed. The interface includes four main configuration sections, each with a red annotation box below it: 1. 'Select variable (Y):' with a green dropdown menu showing 'Instrument' and a red box labeled 'Select the response' with a calculator icon. 2. 'Select classes:' with a blue dropdown menu showing 'A, B' and a red box labeled 'Select the classes'. 3. 'Select validation:' with an orange dropdown menu showing 'None' and a red box labeled 'CV parameters'. 4. 'k up to:' with a white input field containing the number '7' and a red box labeled 'Model settings'. All red annotation boxes have arrows pointing up to their respective configuration elements.

Available models

kNN LogReg LDA QDA PLS-DA RF

kNN model

Select variable (Y): Instrument

Select classes: A, B

Select validation: None

k up to: 7

Select the response

Select the classes

CV parameters

Model settings

Supervised models - regression

MLR PCR PLS

Available models

PLS model

Select response (Y):


700.00

Nr. of components:

10

Select validation:

None

 Calculate

Credits

Eugenio Alladio, PhD



Eugenio Alladio, PhD

Assistant Professor at the Department of Chemistry, University of Turin.

Alberto Mazzoleni



Alberto Mazzoleni

PhD student at the Department of Chemistry, University of Turin.

Giovanni Solarino



Giovanni Solarino

PhD student at the Department of Chemistry, University of Turin.

Lorenzo Castellino



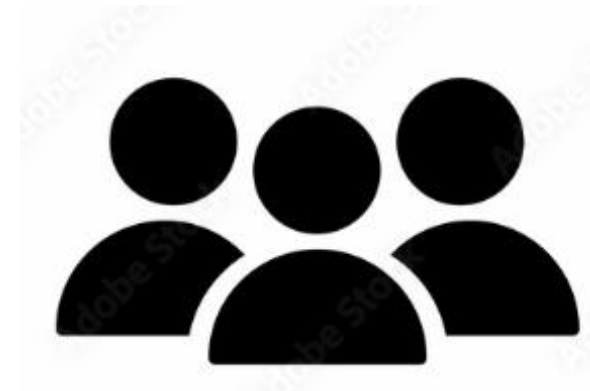
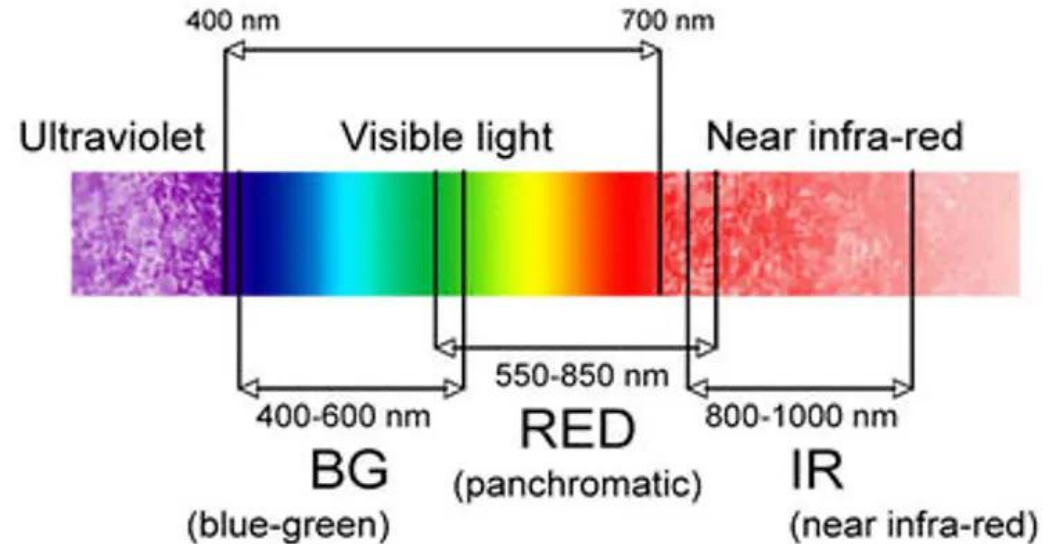
Lorenzo Castellino

PhD student at the Department of Chemistry, University of Turin.

SpectrApp – workshop datasets

eafs2025_full_example.csv

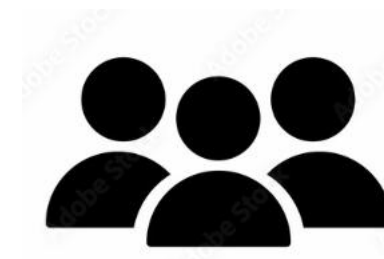
- **Features:** NIR wavelengths + concentration.
- **Classes:** 2 types, 3 operators.
- **Samples:** training + test.



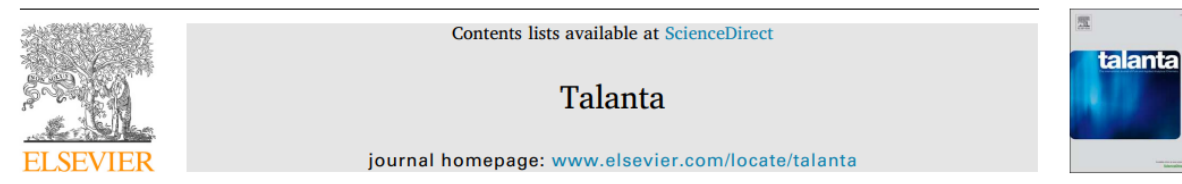
SpectrApp – workshop datasets

eafs2025_blood.csv

- **Features:** 600 NIR wavelengths.
- **Classes:** 3 subjects, 2 instruments.
- **Samples:** 30 samples.



Talanta 209 (2020) 120565



Toward a novel framework for bloodstains dating by Raman spectroscopy:
How to avoid sample photodamage and subsampling errors

Alicja Menżyk^{a,*}, Alessandro Damin^b, Agnieszka Martyna^a, Eugenio Alladio^{b,c}, Marco Vincenti^{b,c},
Gianmario Martra^b, Grzegorz Zadora^{a,d}

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^c Centro Regionale Antidoping e di Tossicologia "A. Bertinaria", Regione Gonzole 10/1, 10043, Orbassano, Torino, Italy

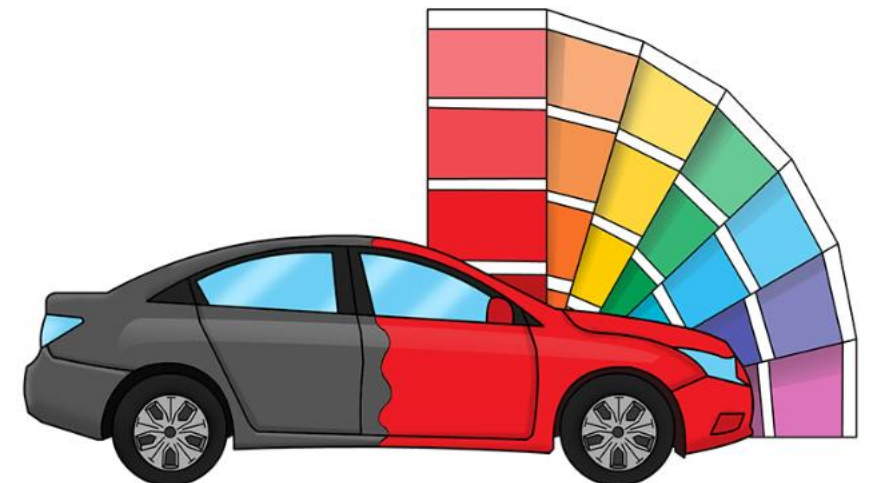
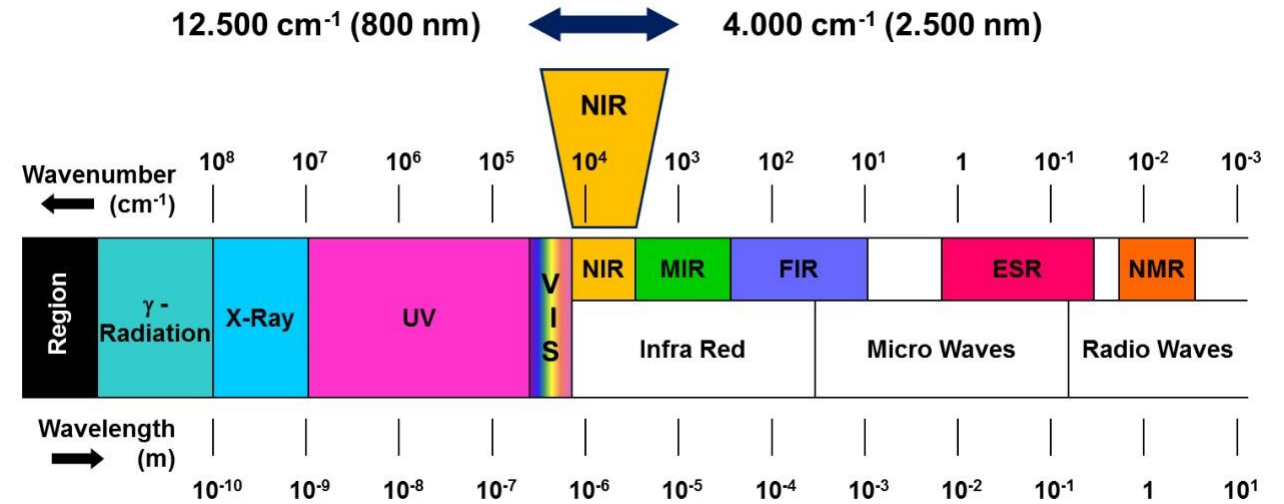
^d Institute of Forensic Research, Westerplatte 9, 31-033, Krakow, Poland



SpectrApp – workshop datasets

eafs2025_carpaints.xlsx

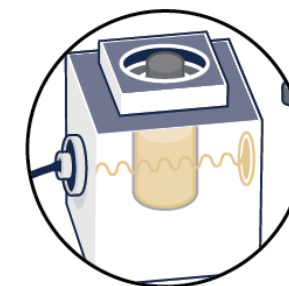
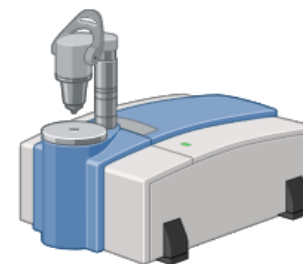
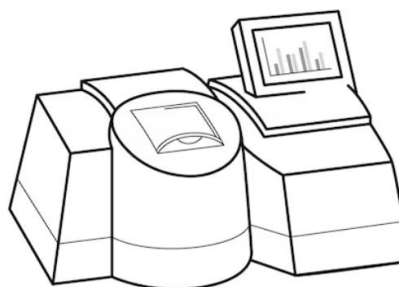
- **Features:** 175 NIR wavelengths.
- **Classes:** 2 classes, 4 replicates
- **Samples:** 48 samples.



SpectrApp – workshop datasets

eafs2025_spraypaints.xlsx

- **Features:** UV-Vis, FTIR and micro-Raman wavelengths (3 spreadsheets).
- **Classes:** Spray brands, fluo vs. non-fluo.
- **Samples:** ~30 samples.



SpectrApp – workshop datasets

eafs2025_gsr.xlsx

- **Features:** SEM/EDX for gunshot residue analysis (elements) concentration.
- **Classes:** stubs and data from hands, barrell, cartridge and hammer.
- **Samples:** ~80 samples.



SpectrApp – workshop datasets

eafs2025_glass.csv

- **Features:** μ -XRF elements composition from glass samples + refraction index
- **Classes:** samples from 3 classes (lightbulb, windows, car).
- **Samples:** 105 samples.



SpectrApp – workshop datasets

eafs2025_ICP_MS.csv

- **Features:** ICP-MS elements composition from glass samples
- **Classes:** samples from 4 classes.
- **Samples:** training and test datasets.



SpectrApp – workshop datasets

eafs2025_gasoline.csv

- **Features:** gasoline samples with known Octane numbers were measured between 900 and 1700 nm using NIR.
- **Response:** Octane number rating.
- **Samples:** 60 samples.



SpectrApp – workshop datasets

eafs2025_wines.csv

- **Features:** set of covariates described in Forina et al. (1986).
- **Class:** 3 Italian wines – Barolo, Barbera, Grignolino.
- **Samples:** 178 samples.



Data

PDF Available

Wines M.Forina, C.Armanino, M.Castino, M.Ubigli,
“Multivariate data analysis as discriminating method of
the origin of wines”, Vitis, 25, 189-201 (1986)

January 1986

DOI:[10.13140/2.1.4312.6560](https://doi.org/10.13140/2.1.4312.6560)

Authors:



Michele Forina

Università degli Studi di Genova

SpectrApp



Cost-effective: As an alternative to paid solutions like Matlab or STATA, SpectrApp offers a cost-effective option for performing statistical analysis, particularly for users or organizations with budget constraints.

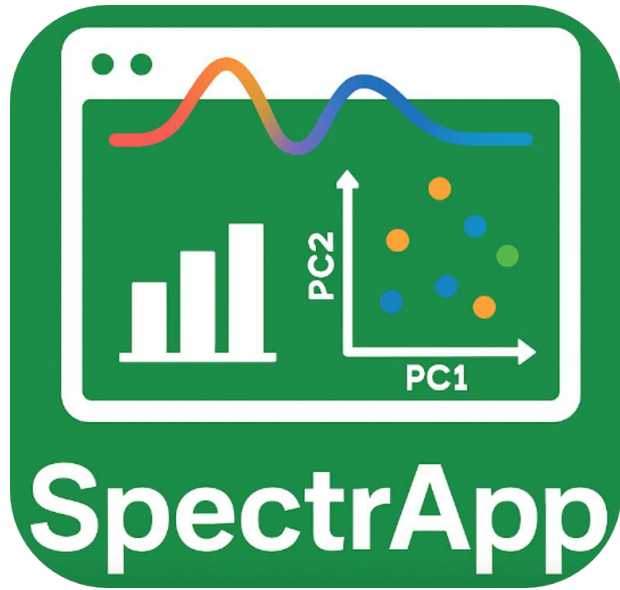
User-friendly interface: SpectrApp provides a user-friendly interface, making statistical analysis accessible to users with varying levels of expertise. This can lower the barrier to entry for individuals or teams who may not have extensive programming skills.

Wide range of analysis techniques: SpectrApp offers a comprehensive set of analysis techniques, including decomposition methods like PCA and PLS, unsupervised models such as clustering, and supervised models like regression (e.g., multivariate regression) and classification (e.g., kNN). This breadth of functionality caters to diverse analytical needs.

Updates and maintenance: SpectrApp's development team must consistently update and maintain the application to ensure compatibility with new R releases, address bugs or security vulnerabilities, and add features or improvements. Failure to do so could lead to usability issues or a stagnant feature set over time.

Learning curve for new users: Despite its user-friendly interface, SpectrApp still requires users to understand statistical concepts and the underlying methodology behind the analysis techniques it offers. New users may need to invest time in learning how to interpret results and make informed decisions based on the outputs generated by the application.

SpectrApp – future perspectives



- **Enhanced integration and compatibility;**
- **Advanced chemometrics modules:** Continuously expanding the repertoire of statistical analysis techniques within SpectrApp can enhance its utility for users across diverse domains.
- **Scalability and performance optimization:** Investing in scalability and performance optimization;
- **Community engagement and support:** an article is in the making with the intention of release to general public shortly after (GitHub code will be available, too)!
- **Cross-platform compatibility;**
- **Continuous improvement and innovation.**

Thank you for your
participation in
our painfully
awkward
conversations.
Let's try not to
do that again.

someecards
user card



Let's Keep in Touch

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