



POTENTIALITIES OF CHEMOMETRICS APPROACH

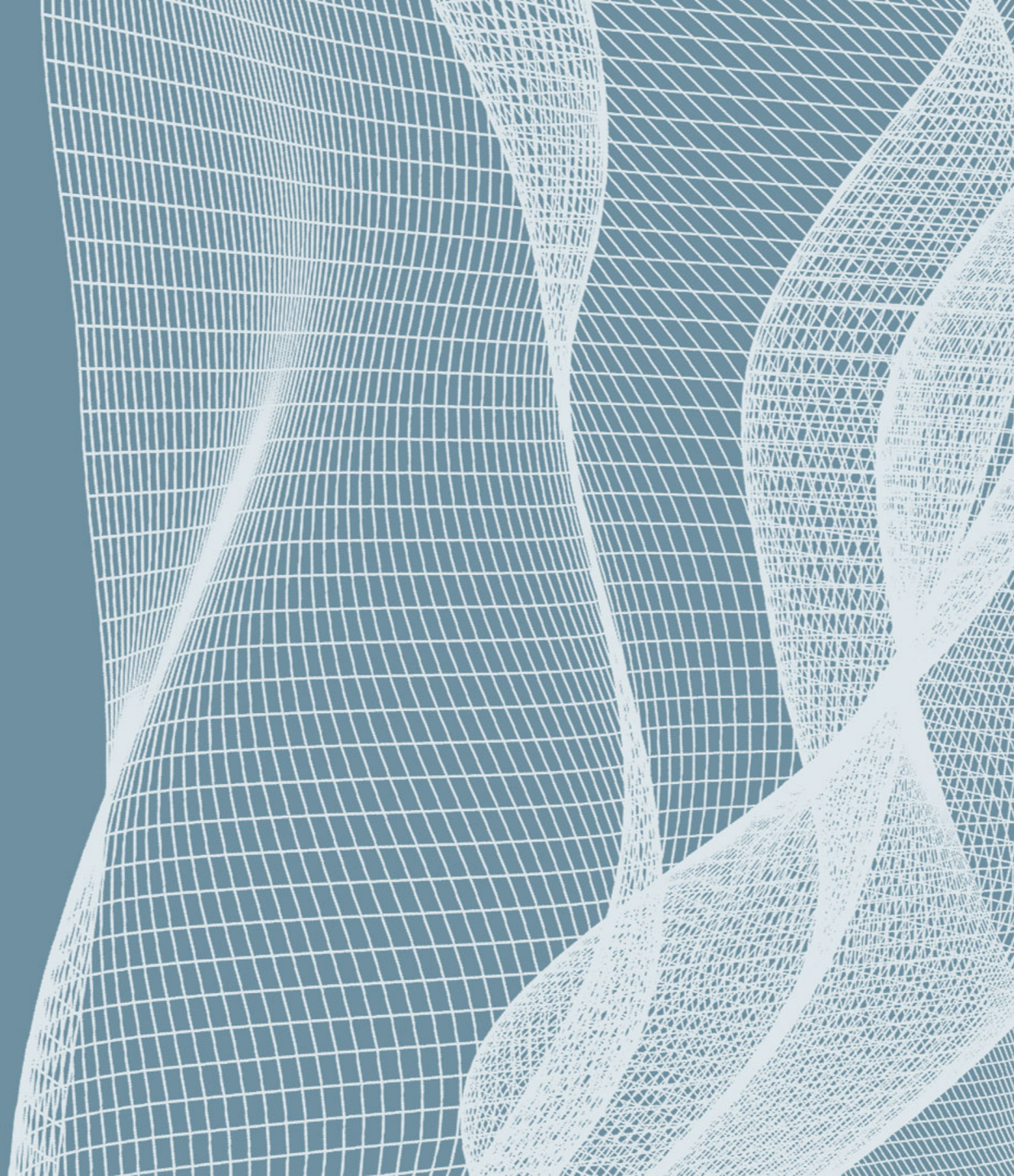
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REACT Webinar

Thursday 29th October, 2020

WHAT IS CHEMOMETRICS?



WHAT IS CHEMOMETRICS?



- Term coined in 1971
- Refers to the use of mathematical models, statistical principles and logic-based methods in the field of chemistry
- Large use in analytical chemistry
- Classic application areas:
 - Calibration, validation and significance testing
 - Optimization of chemical measurements and experimental procedures
 - Extraction of the maximum of chemical information from analytical data

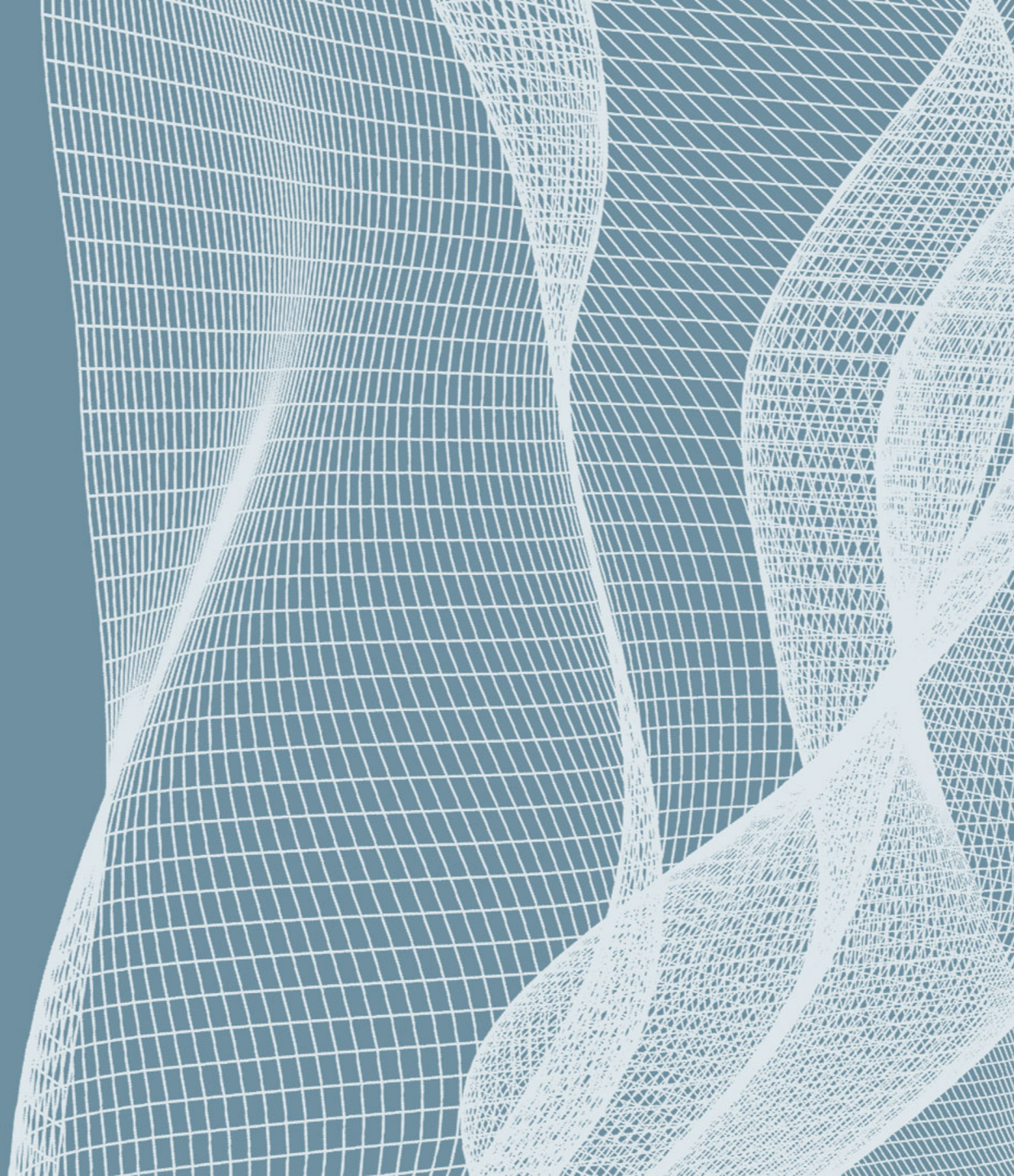
WHAT IS CHEMOMETRICS?



- It is an interdisciplinary field that involves multivariate statistics, mathematical modeling, computer science, and analytical chemistry
- It exploits the potentiality of *multivariate analysis*
 - Treat multiple measurements simultaneously in a data analysis procedures
 - Consider the distribution of multiple variables simultaneously
 - Analyze the correlation between variables
- Can be used not only in chemistry but also in the solving of complex scientific problems

Ref:
P. Gemperline. Practical guide to chemometrics 2nd edition. Taylor & Francis Group, 2006.
R. Todeschini. Introduzione alla chemiometria. Edises, 1998

CHEMOMETRICS FOR TETXTILE



- Application of chemometrics in NIR spectroscopy is finding widespread use
- To monitor identity and quality of raw materials and finished products in different industrial sectors
 - Food
 - Agricultural
 - Polymers
 - Pharmaceutical
 - Organic chemicals

CASE STUDY: Eco Textile for Fashion (ETF Project)

- 2-year project funded by Lombardy region (Italy)
- Aimed to promote a reduction of the environmental impacts due to textile chemical treatment processes
- Through predictive analysis of textile material properties
 - Based on chemometric models from NIR (Near Infra-Red) spectroscopy

CASE STUDY: Eco Textile for Fashion (ETF Project)

- NIR analysis performed on textile samples (linen, cotton)
- Samples were different in
 - Processing step
 - Impurities level
 - Production lot
 - Geographical origin

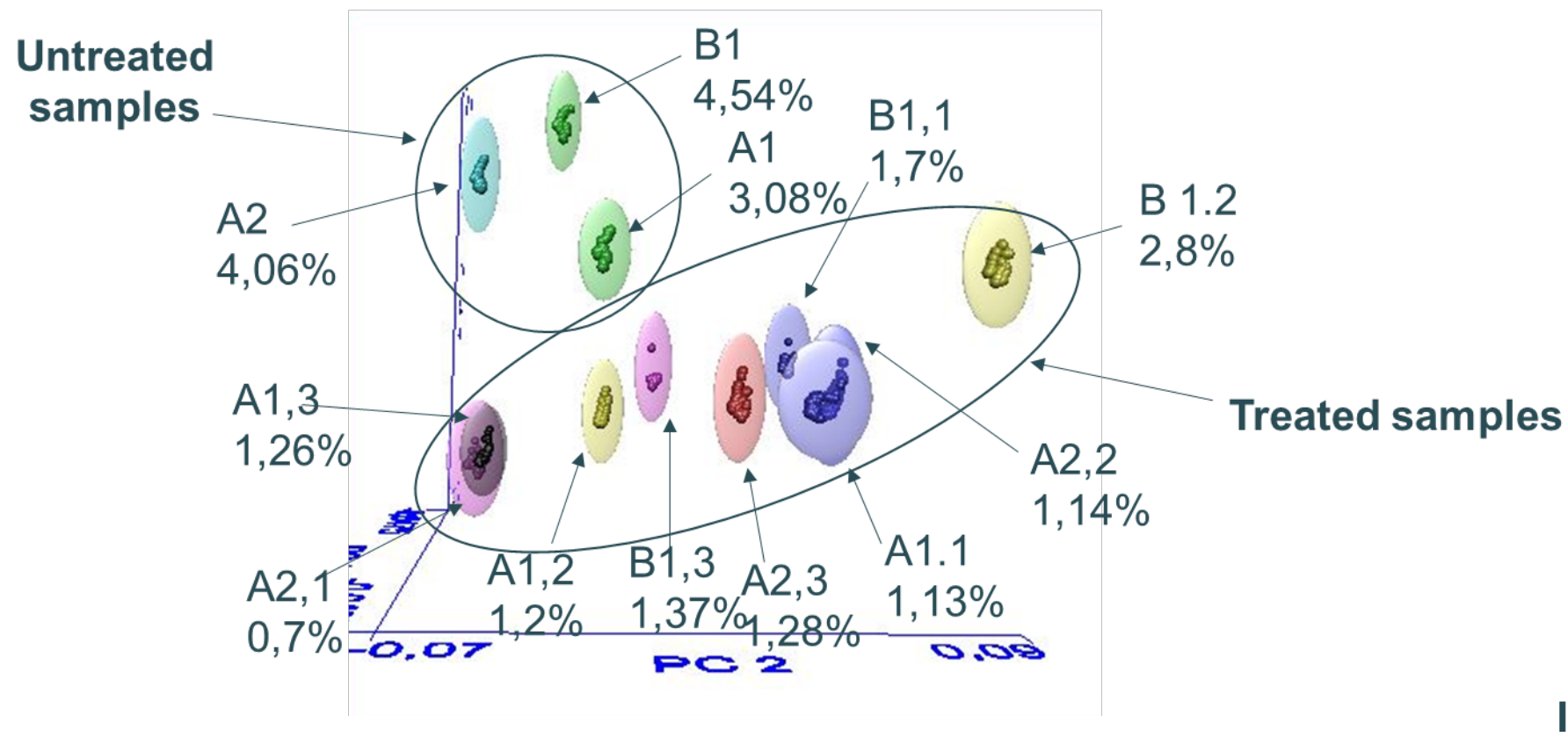


CASE STUDY: Eco Textile for Fashion (ETF Project)

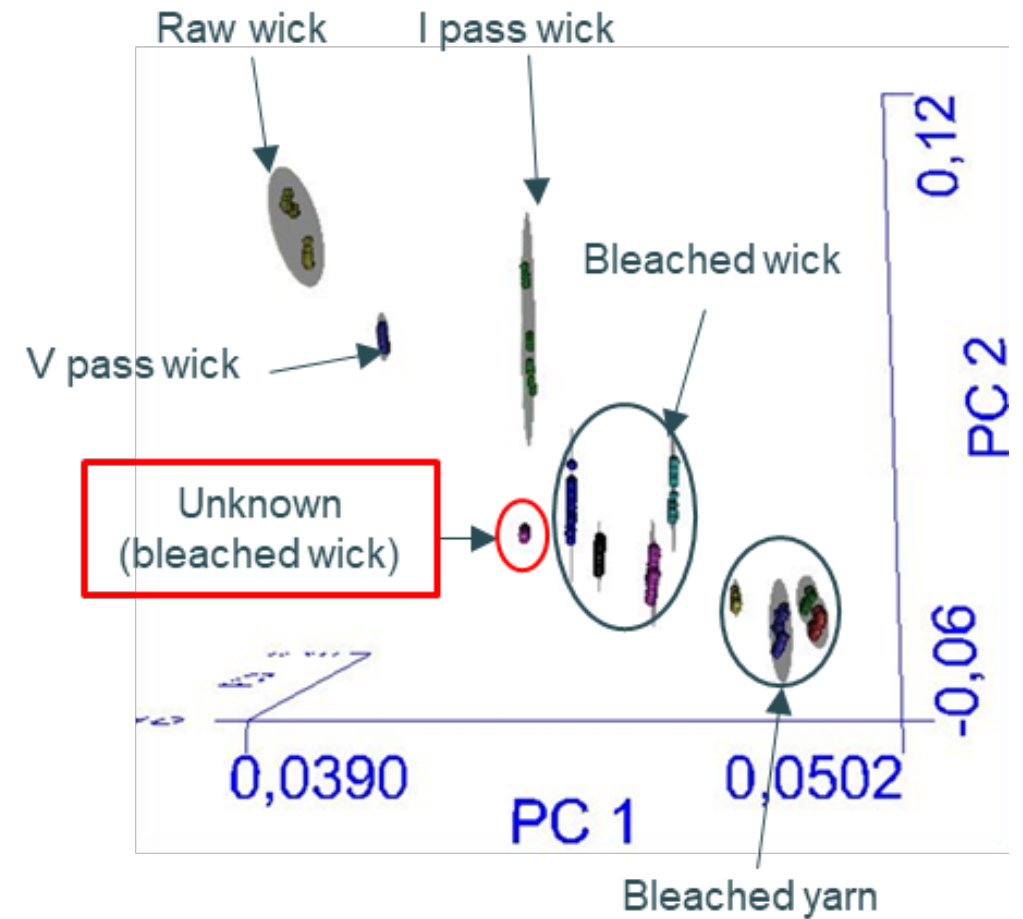
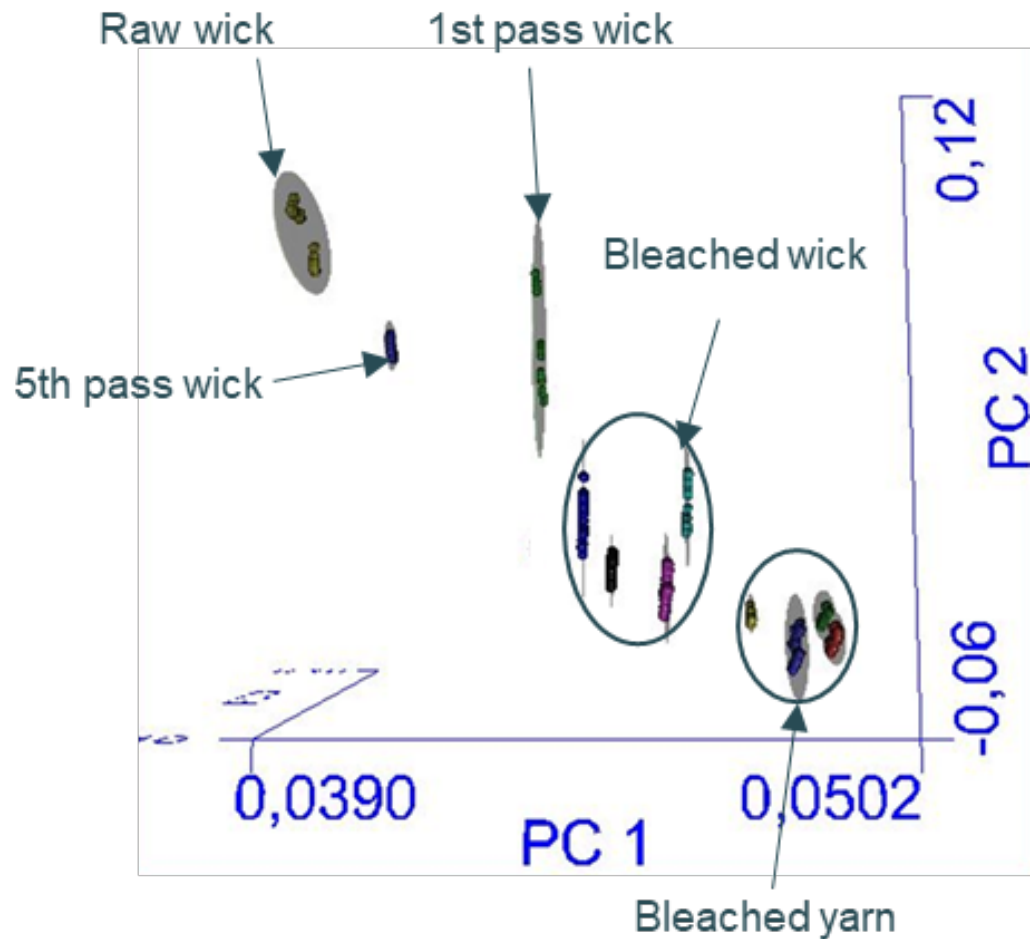
- Traditional chemical analysis for cellulose and impurities levels
- NIR analysis for spectra collection
- Chemometrics analysis



CASE STUDY: Eco Textile for Fashion (ETF Project)



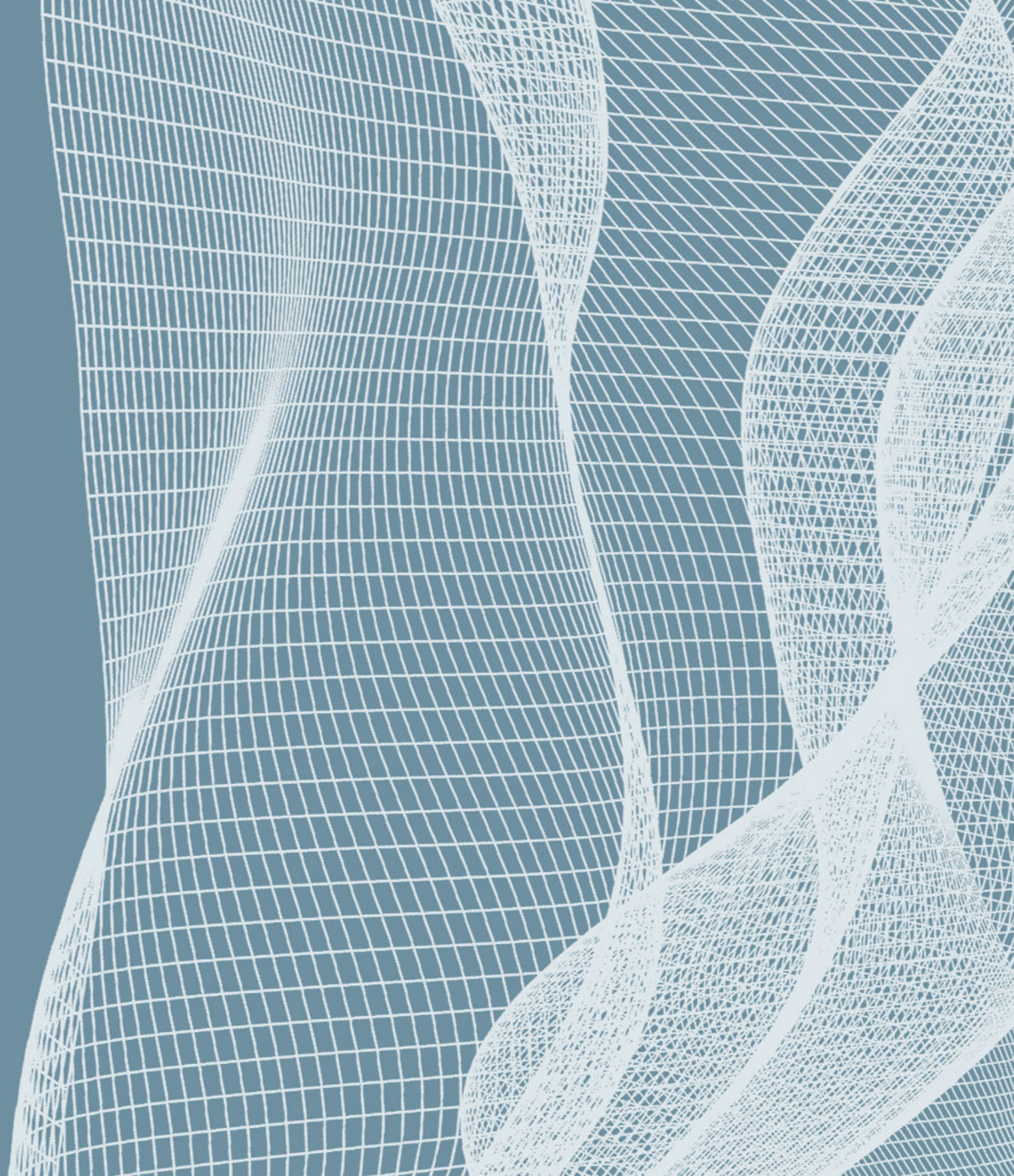
CASE STUDY: Eco Textile for Fashion (ETF Project)



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- Prediction of impurities level of raw textile material
 - No time-consuming and expensive chemical analysis
- Optimization of treatment process according to the predictive analysis results
 - Energy, water and chemicals saving
 - Lower environmental impacts
 - Cheaper
- Traceability (geographical area, lot)
- Quality control (cellulose level)

CONCLUSIONS AND PERSPECTIVES



CHEMOMETRICS POTENTIAL FOR TEXTILE

- Qualitative and quantitative analysis of textiles
 - fibrous composition (e.g. for sorting)
 - presence of chemicals as treatment or contamination (e.g. for sorting and quality control)
 - automatable, fast, non-destructive
- Traceability (production, use, end-of-life)
- Identification of recycled textile material (?)
- ...if there is some chemical (or other) property that you can analyse, you can try chemometrics!



THANK YOU
FOR YOUR
ATTENTION

This project has received funding from the European Union's Horizon 2020
research and innovation programme under grant agreement No 820869

