Implementation of Hasse Diagram technique in environmental risk assessment

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Benefits of HDT usage

- The results obtained could be used for environmental management with respect to the future monitoring and remediation activities:
  - ✓ Pollutant (quality indicator) prioritization;
  - ✓ Optimization of monitoring scheme: chains, HDT "branches".

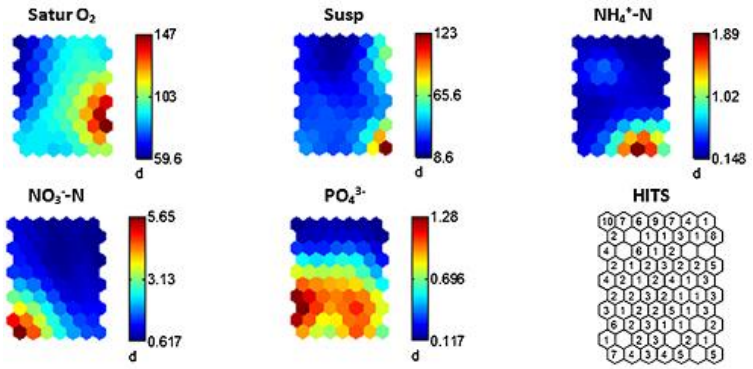
S. Tsakovski, A. Astel and V. Simeonov. Assessment of the water quality of a river catchment by chemometric expertise***. J. Chemomet***., **24** (11-12), 2010, 694-702.

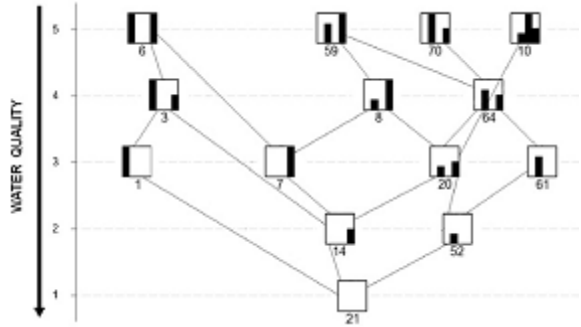
Ts. Voyslavov, S. Tsakovski and V. Simeonov. Surface Water Quality Assessment using Self-organizing Maps and Hasse Diagram Technique. ***Chemom. Intel. Lab. Syst***., **118**, 2012, 280-286.

Backstage work

- ✓ “Proper” set of indicators;
- ✓ Creation of equivalence classes;
- ✓ Introducing of expert and/or legislation information.

- ✓ Rank index ➔ environmental authorities





Environmental monitoring

"Not everything that can be counted counts, and not everything that counts can be counted."
(oft attributed to Albert Einstein)

corollary for environmental monitoring

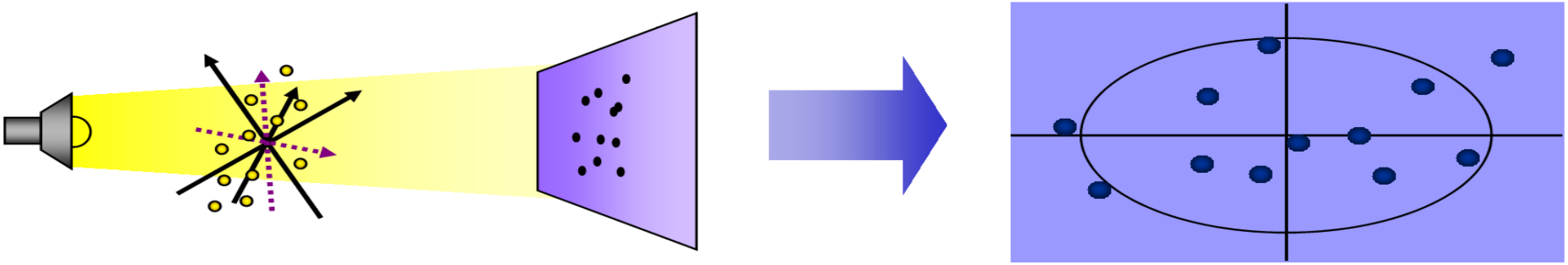
Not everything that can be measured is worth measuring, and not everything worth measuring is measurable.

Environmental monitoring data

- Much more than 6 variables (K);
- Observations: sampling points, sampling situations, objects etc. (N);
- Most of the phenomena are characterized by 2 to 6 factors;
- Source apportioning – receptor modeling.

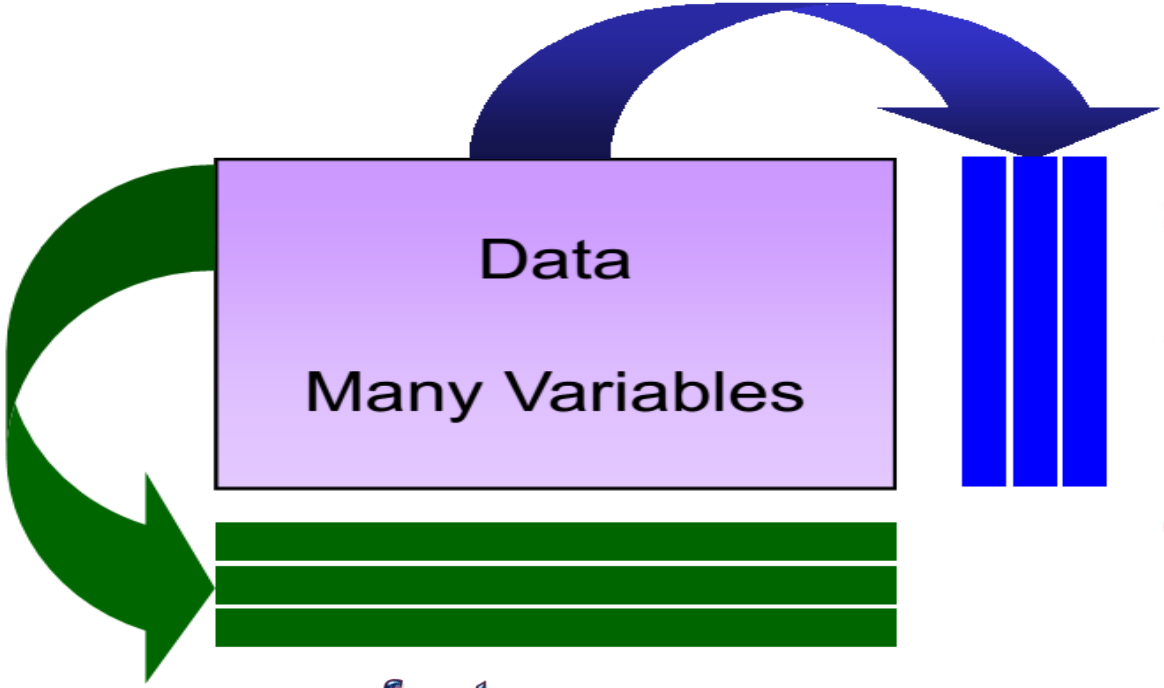
Pre-treatment procedure for Hasse diagram technique is searching for!!!

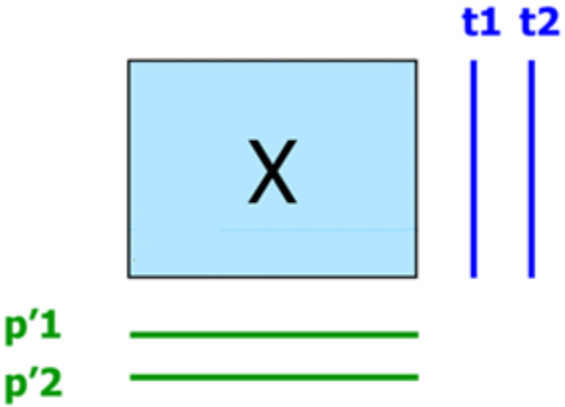
MULTIVARIATE ANALYSIS



- Using all variables (K) and experiments (N);
- No loss of substantial information;
- Revealing of “latent” factors explaining data variation;
- Detection and/or recognition of similarity groups.

Principal Component Analysis





Principal Component Analysis (source apportioning)

$$x_{ik} = \sum_{j=1}^{p} f_{ip} g_{pk} + e_{ik}$$

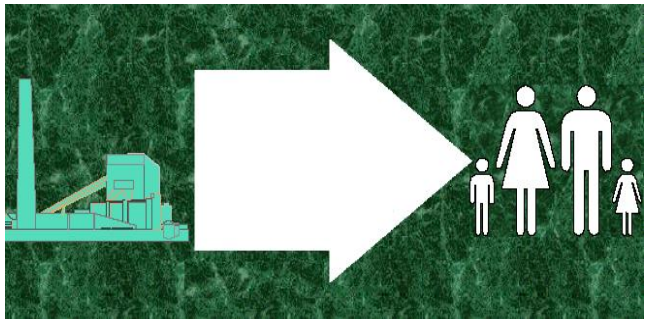
x_{ik} – measured variable i for day k

p – number of sources

f_{ip} – fraction concentration of variable i for source p

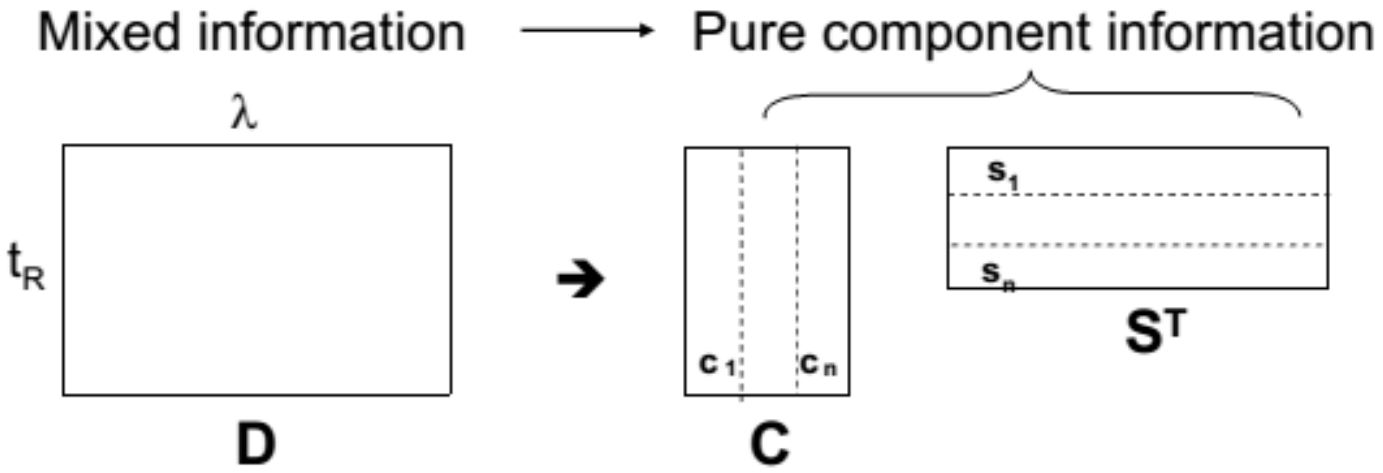
g_{pk} – contribution mass of factor p for day k

e_{ik} – error



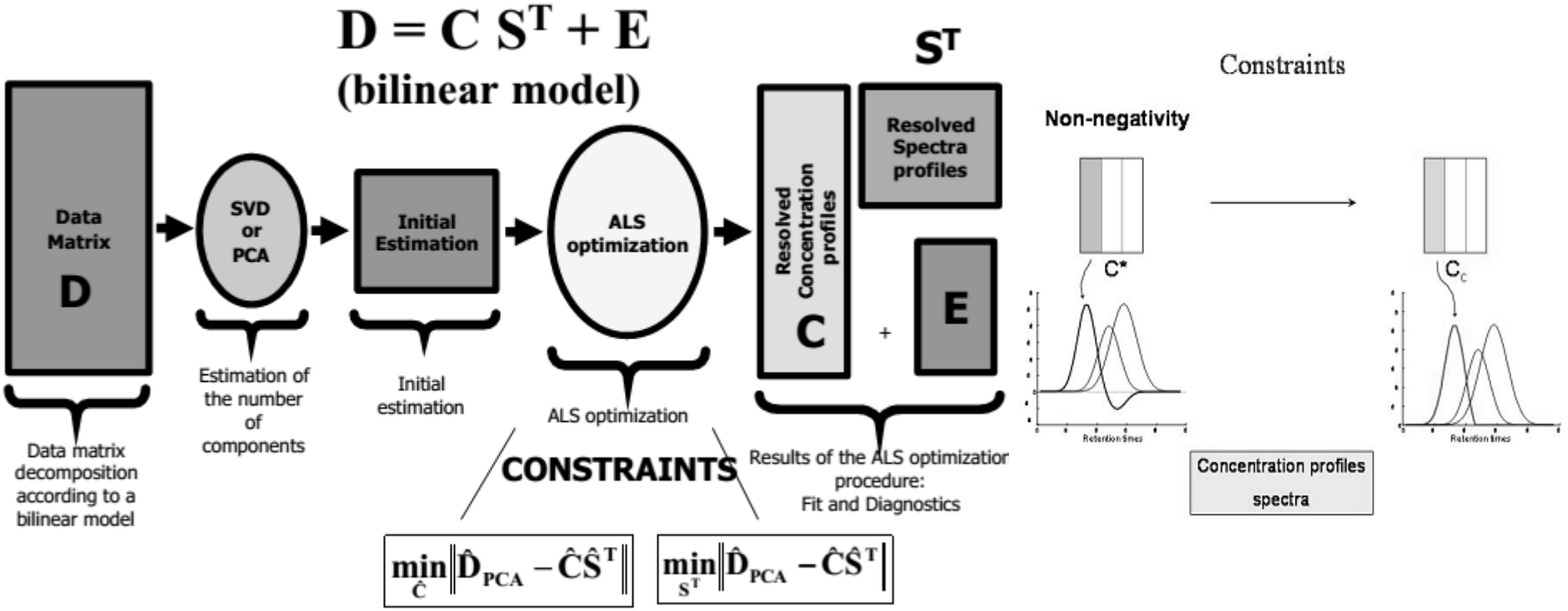
Thurston, G.D., Spengler, J.D., 1985. A quantitative assessment of source contributions to inhalable particulate matter pollution in metropolitan Boston. ***Atmospheric Environment*** 19 (1), 9–25

Multivariate curve resolution (1)

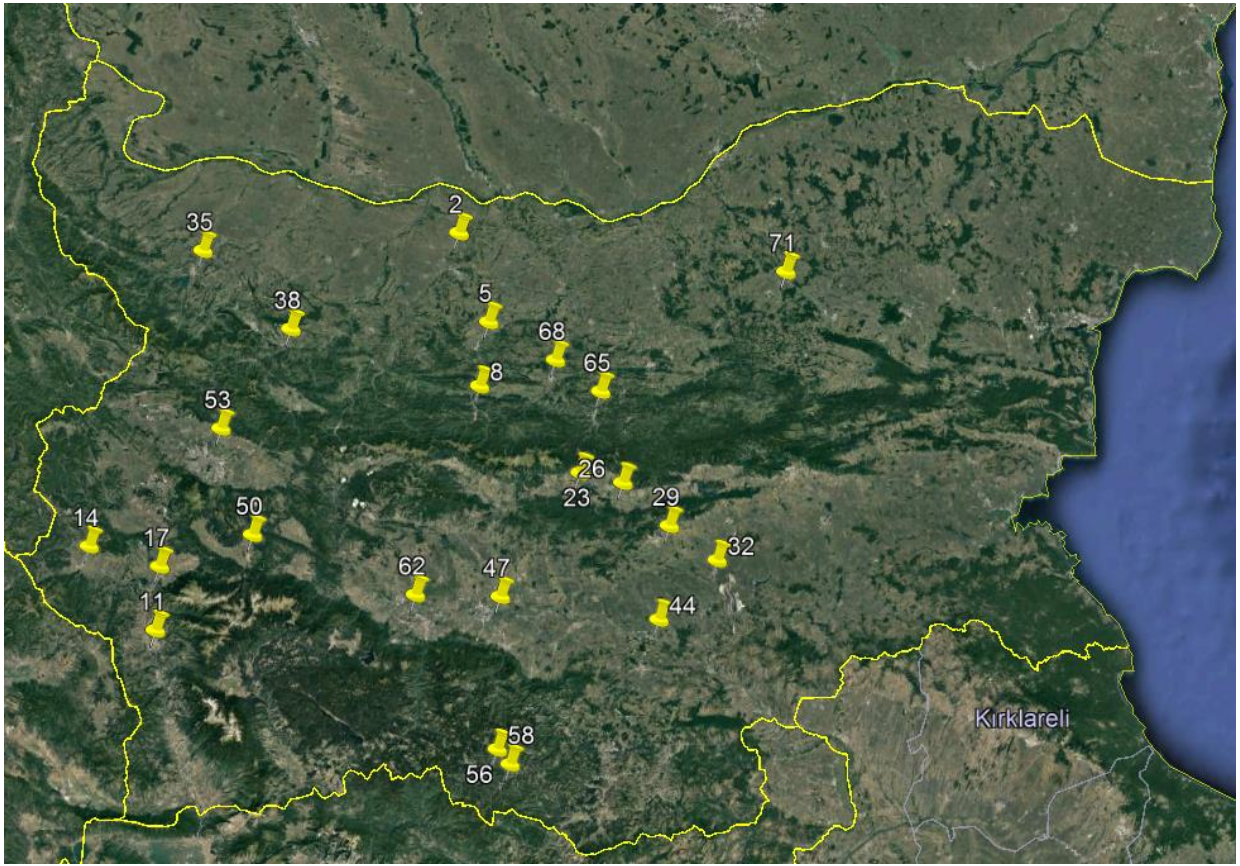


Multivariate Curve resolution applied to Spectral Data from Multiple Runs of an Industrial Process. R.Tauler, B.R.Kowalski and S.Fleming. **Analytical Chemistry**, 1993, 65, 2040-2047

Multivariate curve resolution (2)

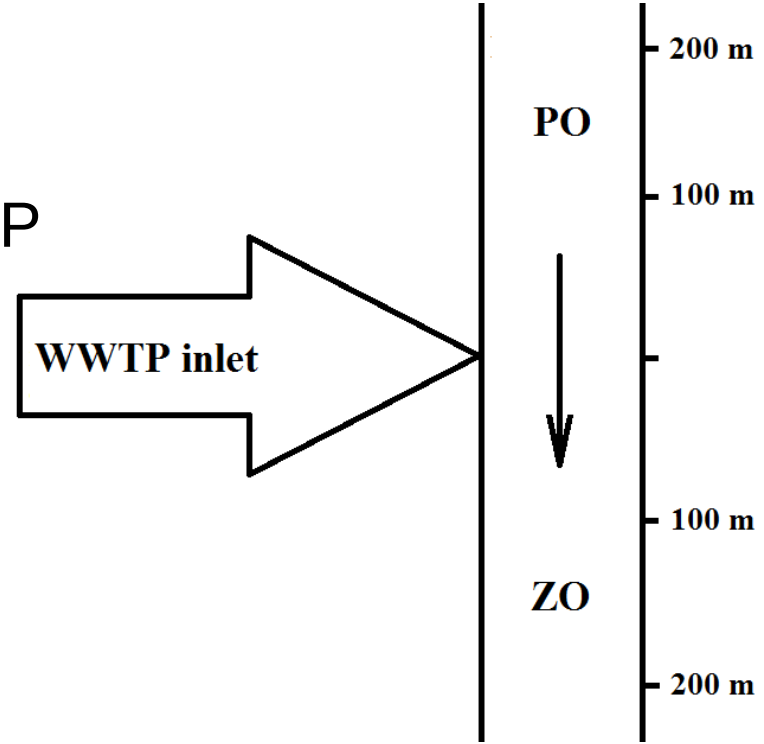


WWTP data - sampling map



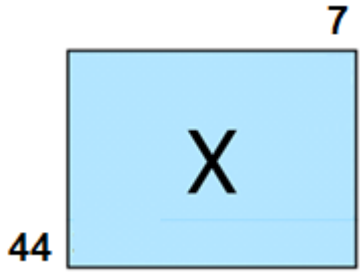
Sampling…

Sampling period: august 2018
Monitored WWTPs: 22
Samples: three samples per WWTP
PO – prior to inflow (n)
ZO – after release (n+1)

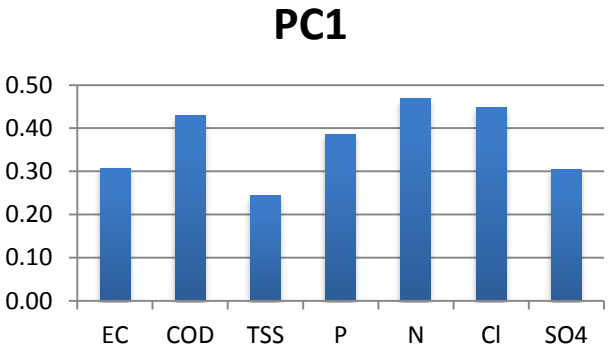


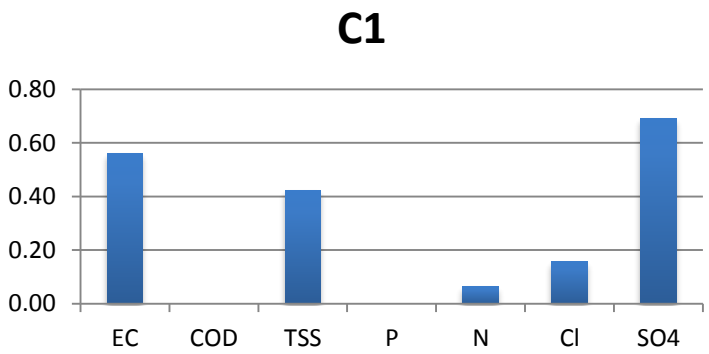
Water quality indicators

- EC – conductivity^{-};
- COD – chemical oxygen demand;
- TSS – total suspended solids;
- P – total phosphorous;
- N – total total nitrogen;
- Cl^{-} – chloride;
- SO_4^{2-} - sulphates.

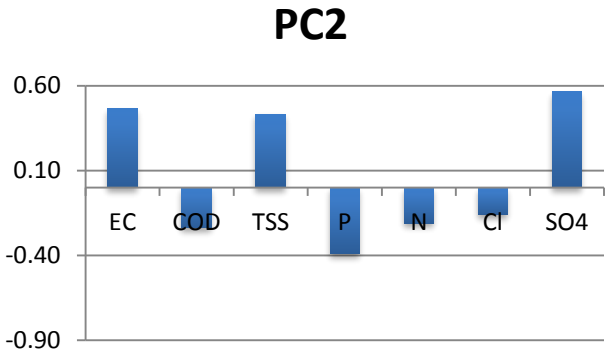


Sources…

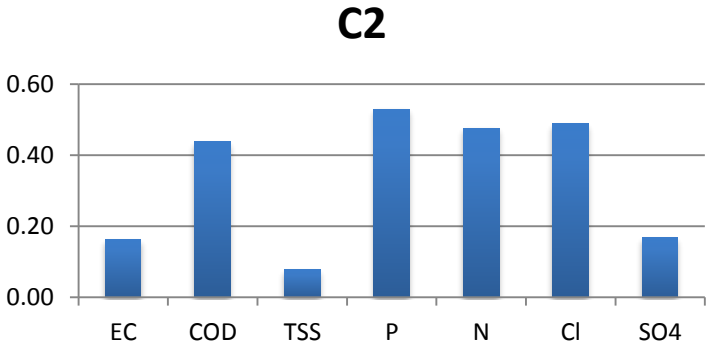




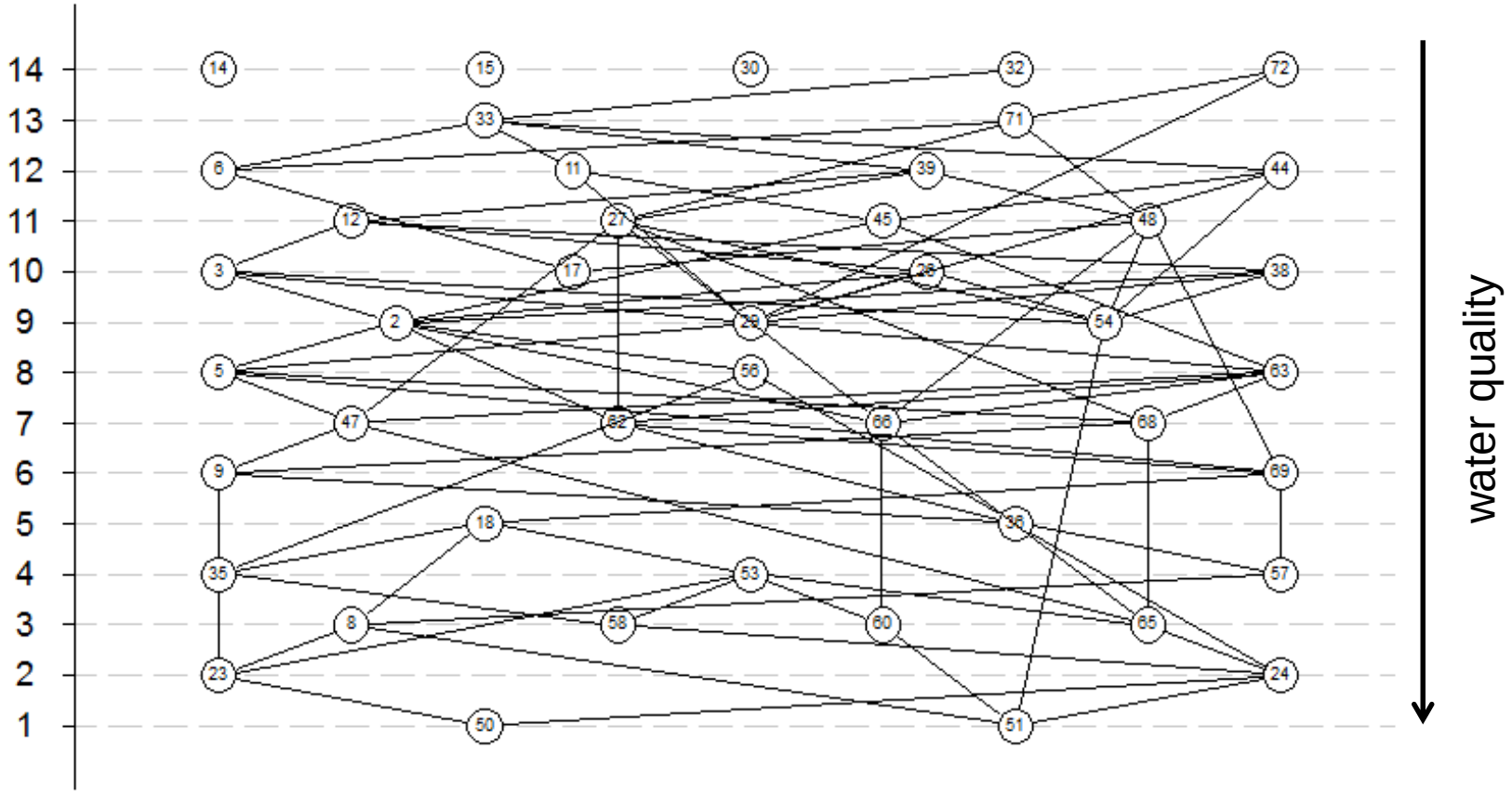
„conductivity“



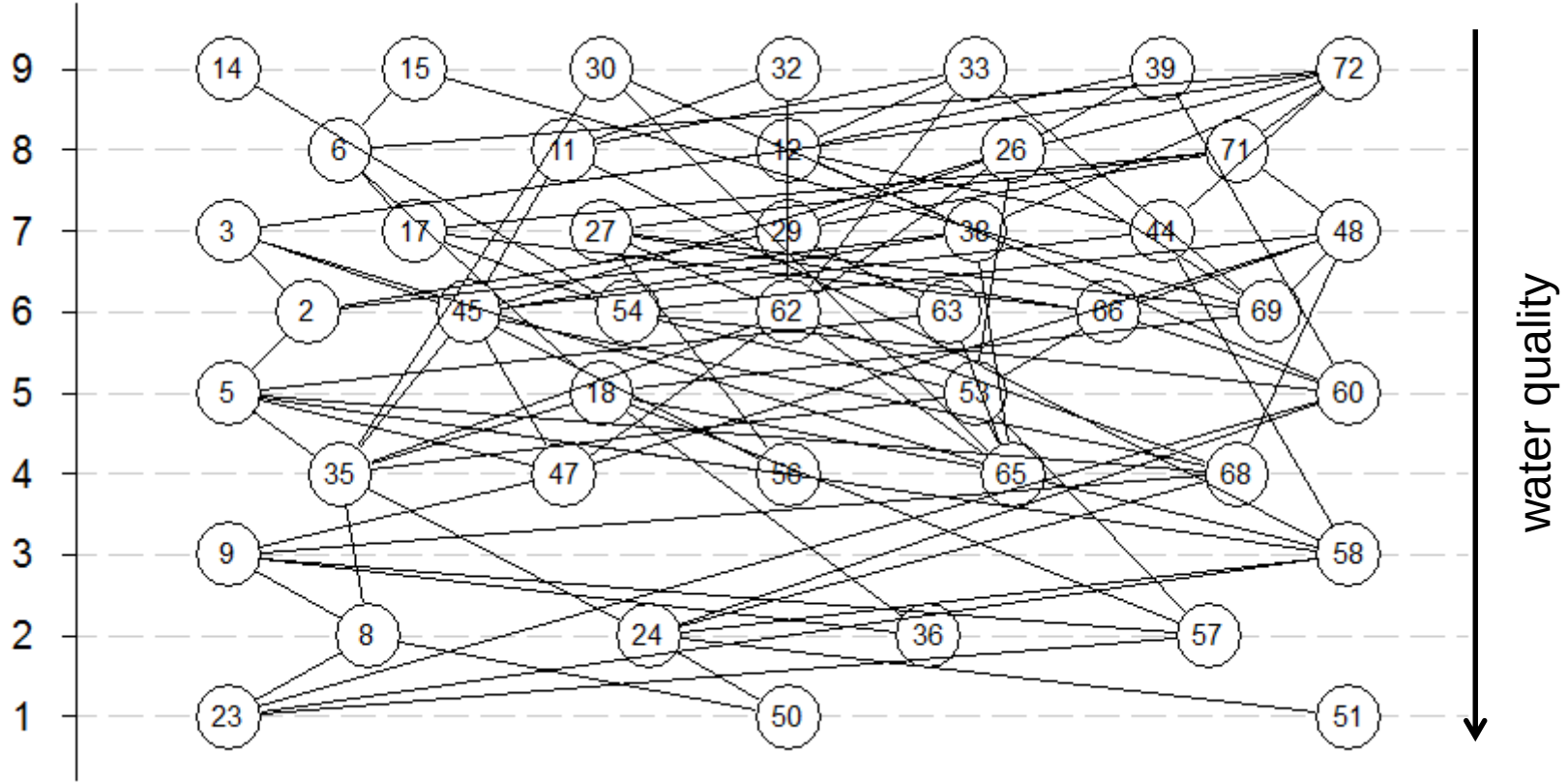
„oxygen demand“



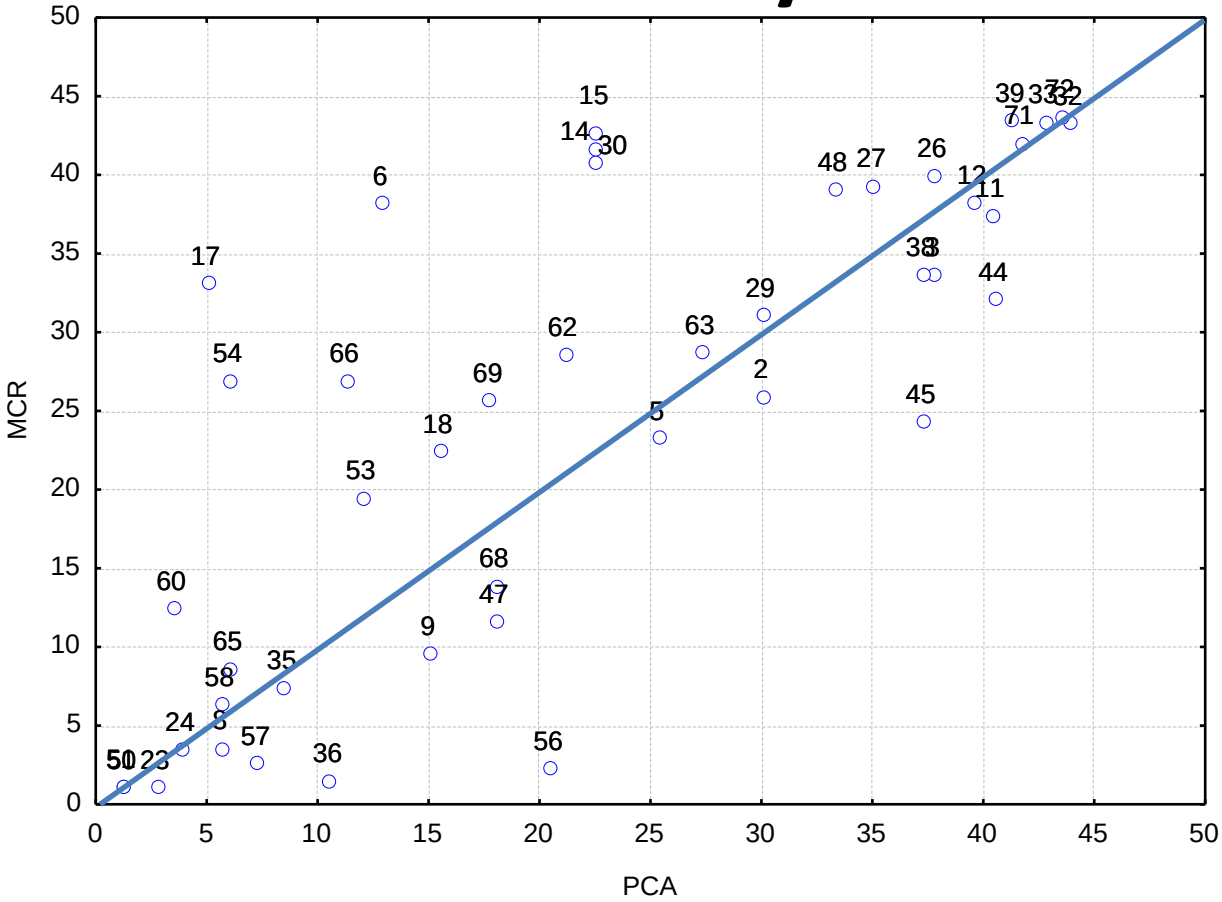
Hasse diagram based on PCA factor scores



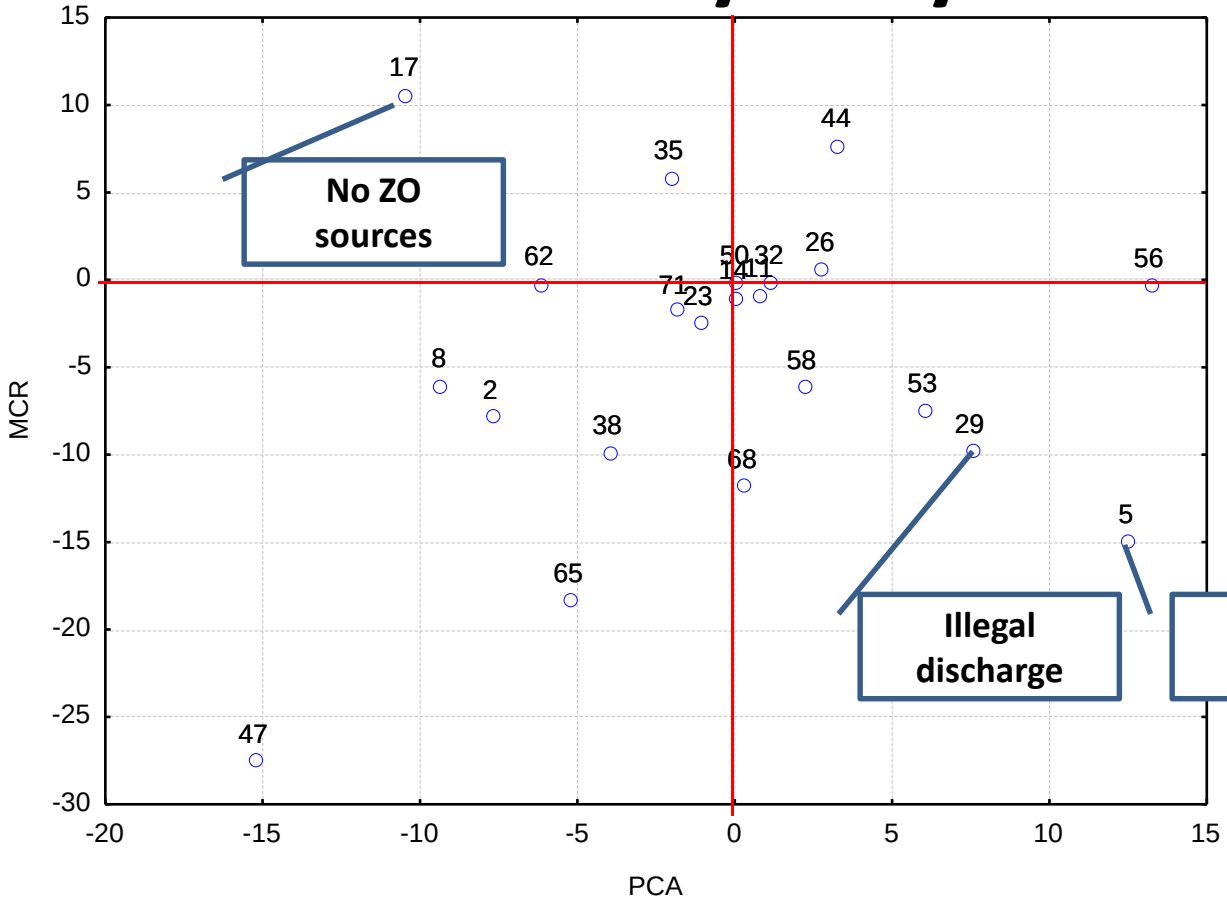
Hasse diagram based on MCR spectra



LPOM analysis



LPOM analysis by WWTP



$$PO - ZO$$

(-) quality decrease

(+) quality increase

Conclusions

- PCA and MCR extract similar sources controlling surface water quality as MCR “concentration profiles” seem more appropriate concerning processes in natural waters;
- HDT based on MCR spectra gives more reliable results concerning a prior knowledge for “conflict” WWTPs ;
- MCR-HDT could be appropriate approach for estimating of WWTPs’ impact on receiving water bodies.

Future work…

- To complete data set;
- To work by loads then concentrations;
- To estimate WWTPs' impact based on gray water footprint;
- To have look inside HDT…

Acknowledgments

- H2020-TWINN-2015 - project “Materials Networking”, Project ID: 692146
- NSF DN 19/15 (20.12.2017) – “Environmental impact assessment of WWTP on receiving water bodies”

Thank you for your attention