

## Motivation

Develop tool which allows to:

- Identify important log-ratios for the detection of subcropping mineralizations.
- Identify features related to specific type of mineralization.
- Indicate sampling target - mineralization.

## Generalized Additive Models (GAMs)

Generalized Additive Models allow one to model the mean and variance of a random variable  $y|x$  dependent on the predictor  $x$  in a very flexible way:

$$h(\mathbb{E}(y|x)) = \eta(x) \quad \mathbb{V}(y|x) = V(\mathbb{E}(y|x)) \frac{\psi}{\omega}$$

for a fixed function  $V$  depending on the distribution of  $y|x$ .

Assumptions and fitting:

- The response belongs to the exponential family and the linear predictor  $\eta$  is a sufficiently smooth function.
- We solve the following optimization problem

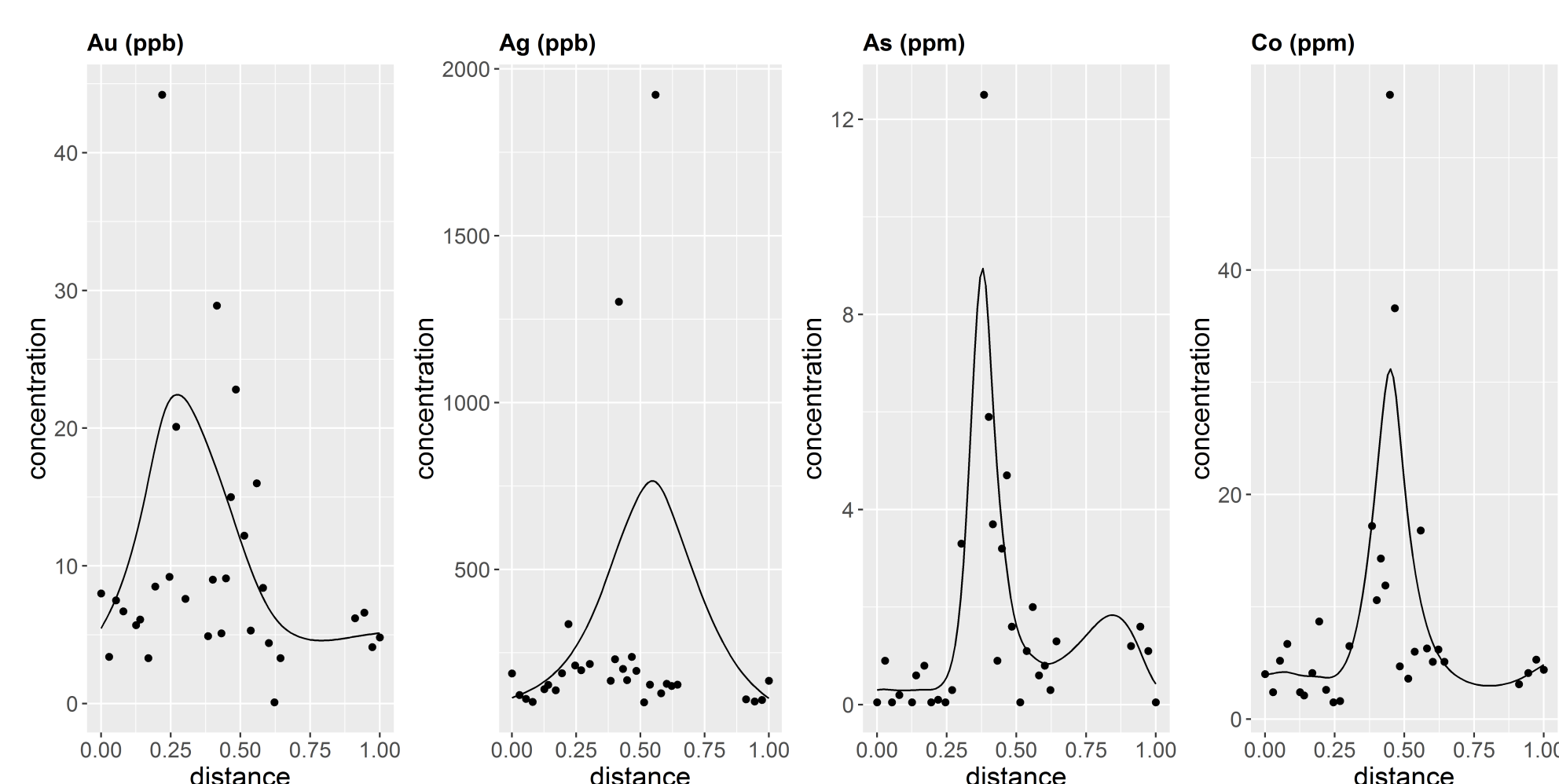
$$\max_{\eta} \sum_{i=1}^n \omega_i l(y_i | x_i; \eta) - \lambda \int (\eta''(x))^2 dx,$$

where  $\lambda$  controls the smoothness of  $\eta$ .

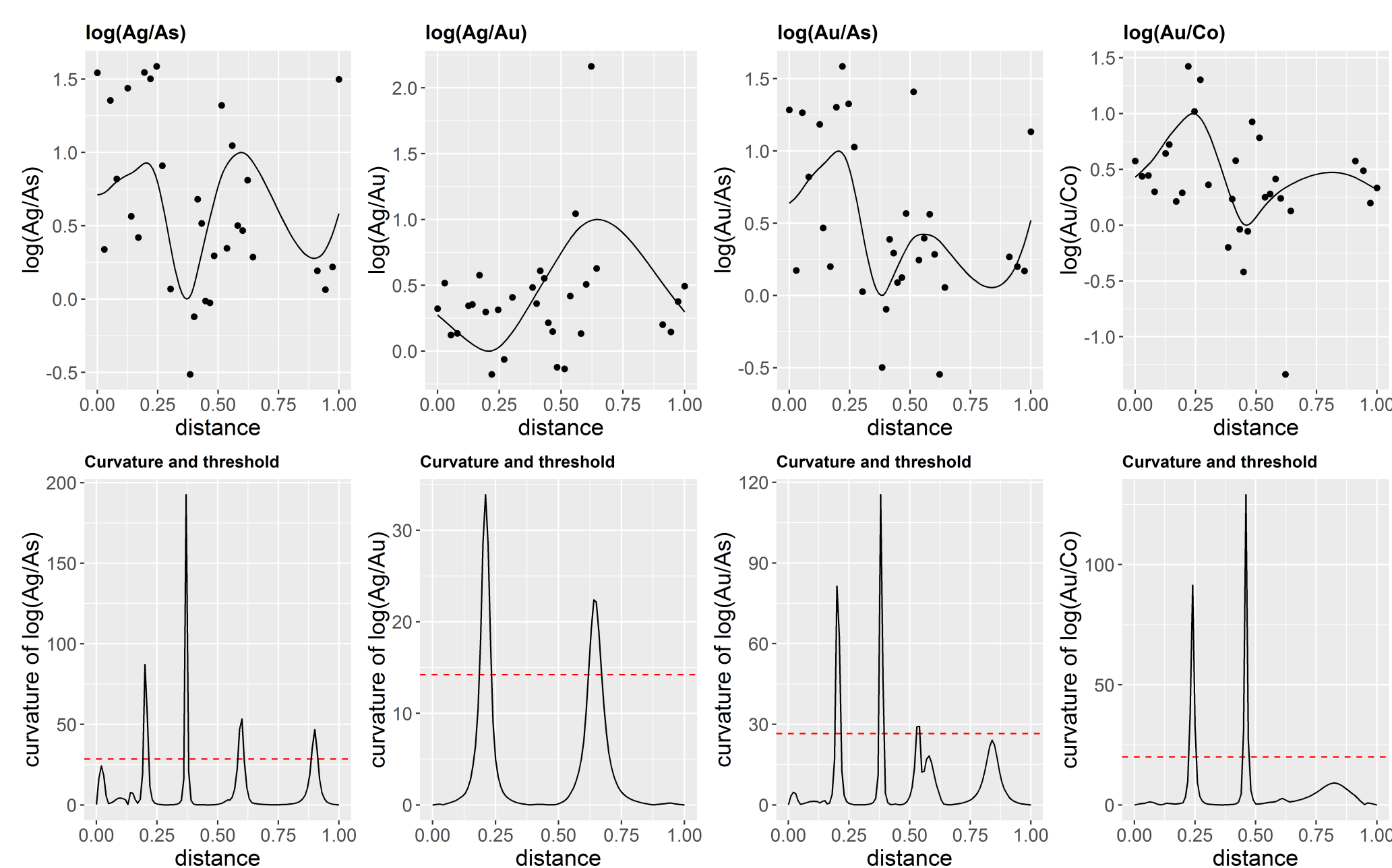
- The weights  $\omega_i$  can be used up or downweight outliers; we upweighted outliers.

## Juomasuo - Selected GAM fits and log-ratios

- The Juomasuo dataset consists of 64 different elements measured at 30 locations each. Each measurement is comprised of 6 different species respectively organs, e.g. Strawberry, Bilberry, etc respectively leaf, twig, etc.
- We fit Generalized Additive Models to the concentration of elements at certain positions:

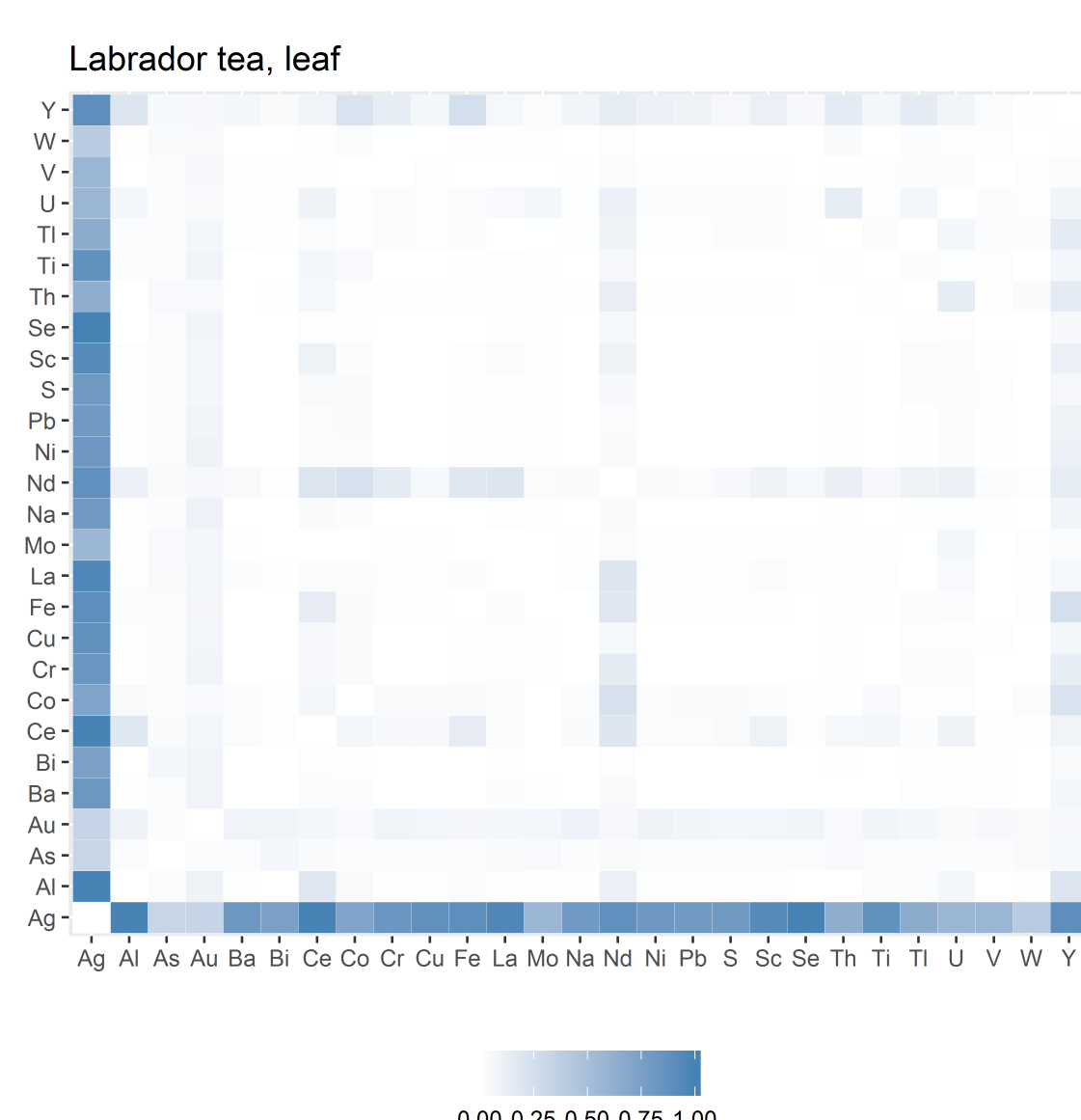


- The curvature can be used to measure a quick behavioural change of log-ratio:



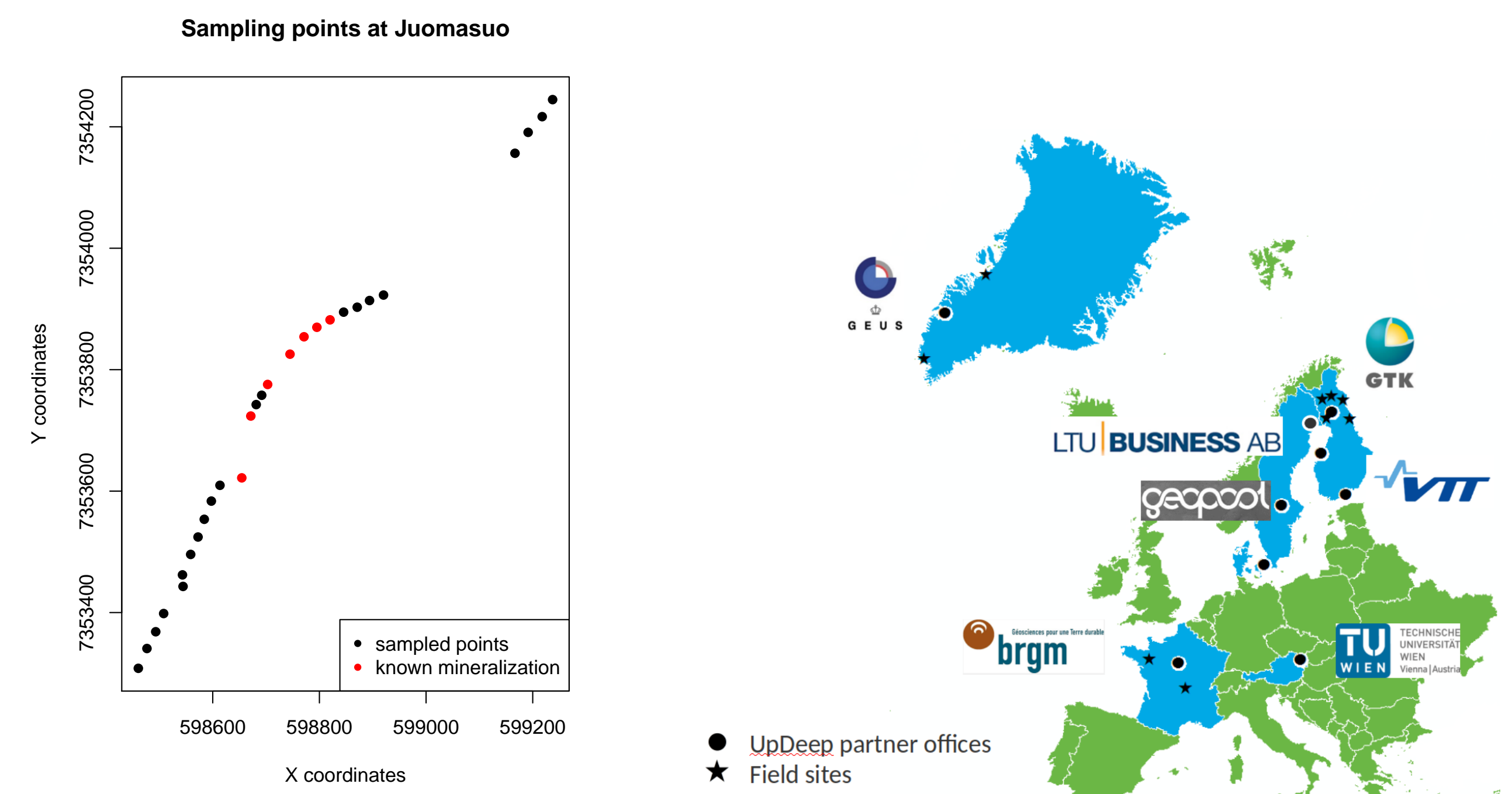
## Juomasuo - Heatmaps of the measures

- The ranked log-ratios can be displayed in a heatmap, e.g. for Labrador tea, Silver seems to be a meaningful pathfinder for mineralization:



## UpDeep project

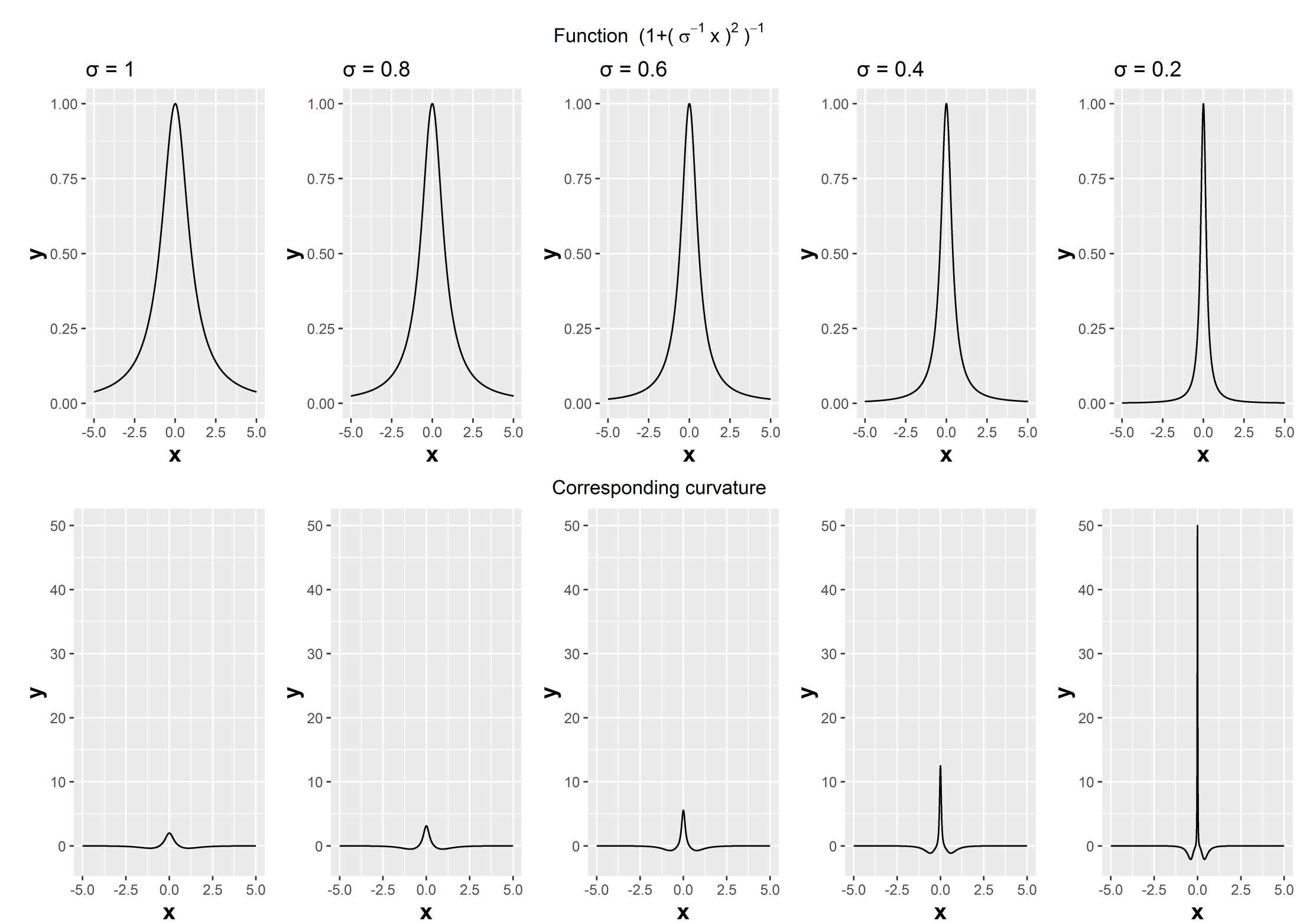
Upscaling deep buried geochemical exploration techniques into European business. TU Wien is responsible for statistical data analysis.



## Detection of interesting log-ratios

With the use of GAMs we construct the log-ratios of all the combinations, which are then ranked from the most interesting to the least interesting by the use of a measure, between zero and one, based on the curvature.

- Geochemically interesting log-ratios have presumably sharp peaks.
- The curvature of a  $[0, 1]$  scaled function can be used to measure a sudden change, e.g.:



- Once GAMs are fitted to the concentration of each element the curvature  $\kappa$  of each log-ratio  $g$  is calculated:

$$\kappa(x) := \frac{|g''(x)|}{(1 + (g'(x))^2)^{\frac{3}{2}}}$$

- For multiple peaks we use for each pair of elements,

$$\frac{1}{J} \sum_{j=1}^J \max_{x \in I_j} (\kappa(x) - \mathcal{T})_+^2$$

to measure the average deviation of the peaks from a threshold  $\mathcal{T}$ .

- $\mathcal{T}$  is  $\mu + \sigma$ , where  $\mu$  is the mean of  $\kappa$  over the whole range and  $\sigma$  is respectively its variance.
- The intervals  $I_j$  mark the intervals for which  $\kappa$  lies above  $\mathcal{T}$ .

## Summary and future work

Summary:

- A statistical tool which can identify meaningful features related to mineralization.
- Based on curvature of log-ratios of chemical elements.
- Developed for the case where sampling was done on (linear) transects.

Future work:

- Extension to the two dimensional predictor case.
- Individual modelling of mean and variance through VGAMs.

## References

- UltraLIM-project, Ultra low-impact exploration methods in the subarctic (2013–2015). Funded from Tekes Green Mining Programme.
- KAVA Reference: 16329, UpDeep, Upscaling deep buried geochemical exploration techniques into European business (2017–2020).
- Wood, S. N. (2017). *Generalized Additive Models: An Introduction With R*. Chapman and Gall/CRC, Boca Raton, USA.