Identification of mineralization in geochemistry based on the spatial curvature of log-ratios

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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:

$$h(E(y|x)) = \eta(x)$$
$$V(y|x) = V(E(y|x)) \frac{\omega_0}{\omega(x)}$$

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

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

where $\lambda$ controls the smoothness of $\eta$.
- The weights $\omega_i$ can be used up or downweigh outliers; we upweighted outliers.

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.:

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

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

$$1 \sum_{k < l} \max_{x} (\kappa(x) - T)^2$$

to measure the average deviation of the peaks from a threshold $T$.
- $T$ 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 $T$.

UpDeep project

Upscaling deep buried geochemical exploration techniques into European business.

TU Wien is responsible for statistical data analysis.

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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