Outlier Detection with Application to Geochemistry

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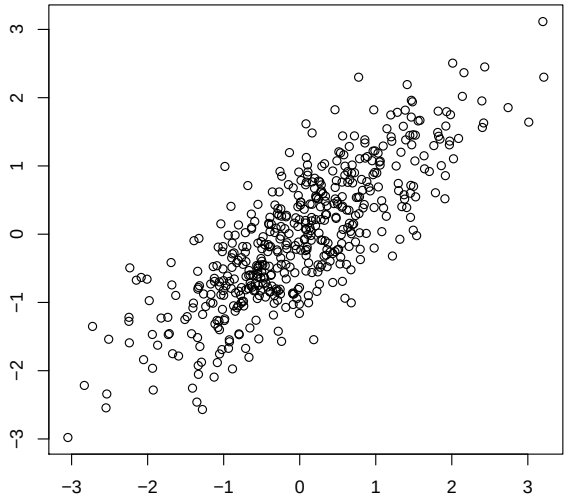
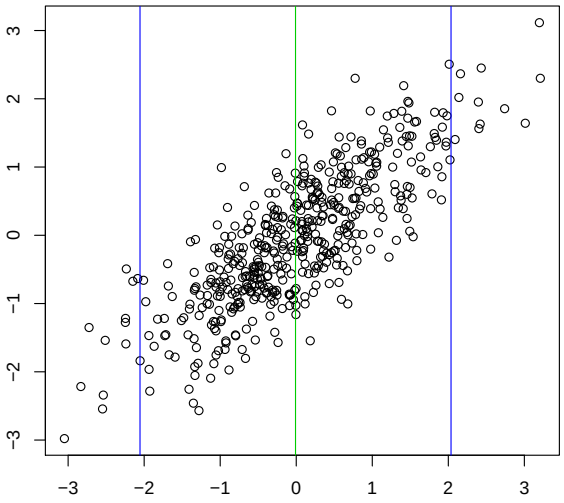
Univariate versus Multivariate Outliers



Univariate versus Multivariate Outliers



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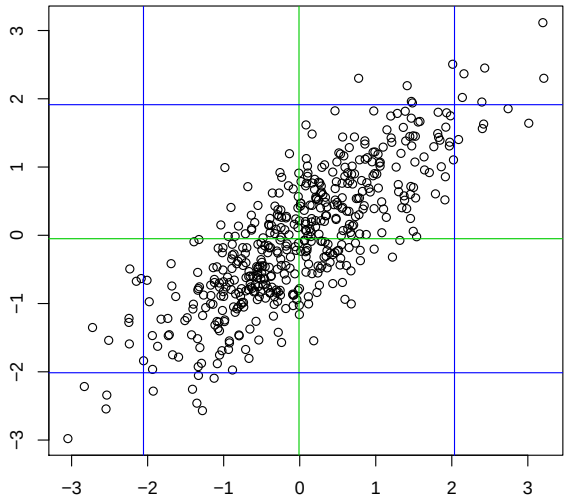

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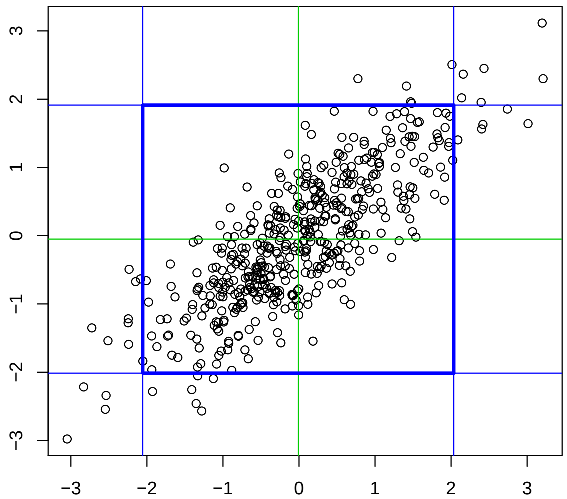

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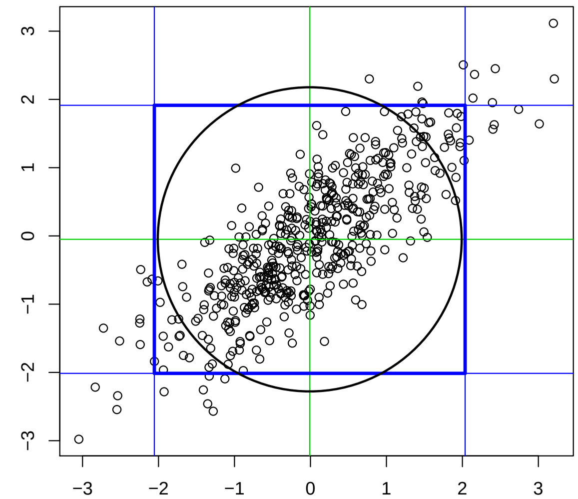

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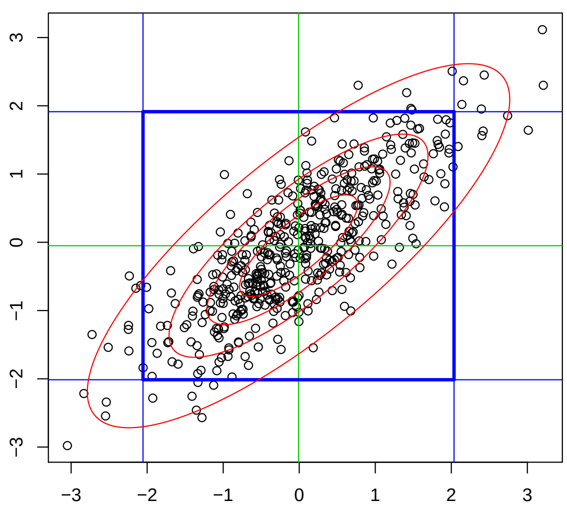

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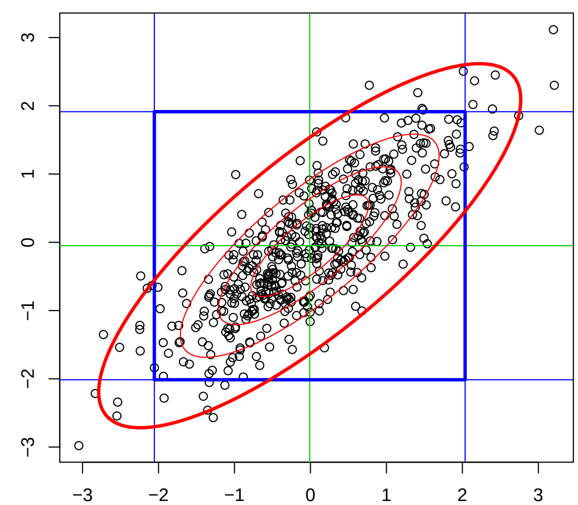


Multivariate Outlier Detection Methods

Standard methods are based on the **Mahalanobis distances** (MD):

$$\text{MD}_i := d(\boldsymbol{x}_i, \boldsymbol{t}, \boldsymbol{C}) = \{(\boldsymbol{x}_i - \boldsymbol{t})^\top \boldsymbol{C}^{-1} (\boldsymbol{x}_i - \boldsymbol{t})\}^{1/2}$$

for a sample $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n \in I\!R^p$ and estimators of location $\boldsymbol{t}$ and covariance $\boldsymbol{C}$.

$\Longrightarrow$ **Robust estimates of location and covariance are needed!**

Outlier detection:
Outliers will typically have large distance. If multivariate normal distribution is assumed, MD_i^2 is approx. χ^2_p distributed.

$\Longrightarrow$ suspect observations: $\text{MD}_i^2 > \chi^2_{p,0.975}$

- does not account for different sample size
- χ^2_p-approximation is poor

Garrett (1989)

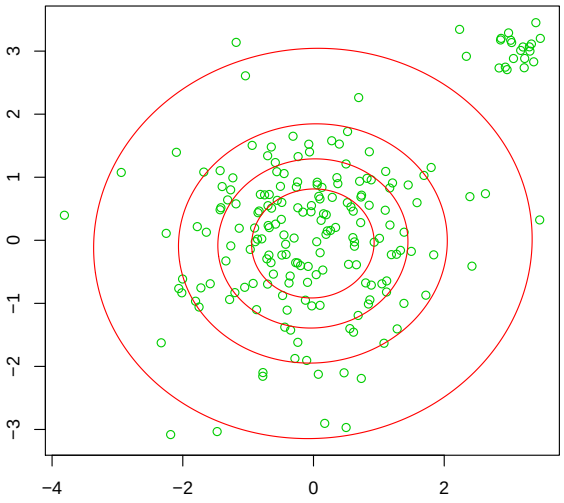
Chi-square plot:

Plot robust MD_i^2 against quantiles of χ^2_p.

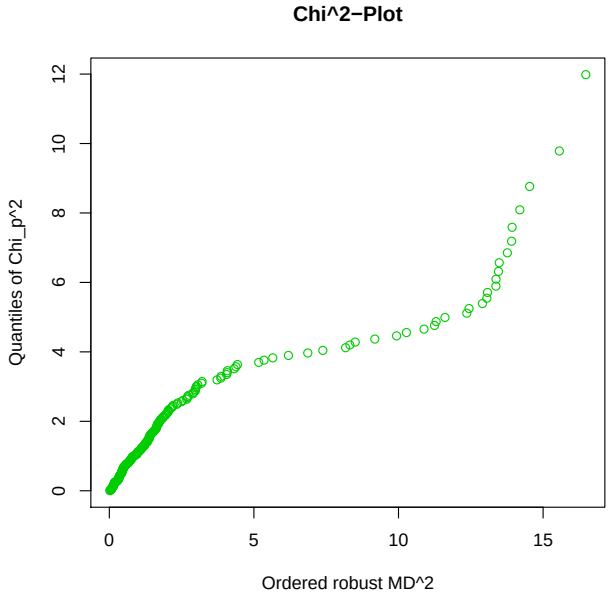
$\Longrightarrow$ iterative deletion of points with large distance until a straight line appears.

Drawback: no automatic procedure, needs user interaction.

Example: Simulated data with outliers



Iterative deletion of outliers:



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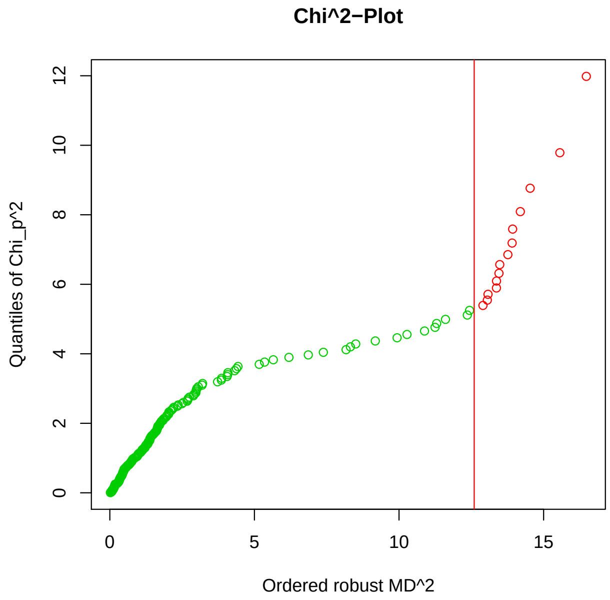

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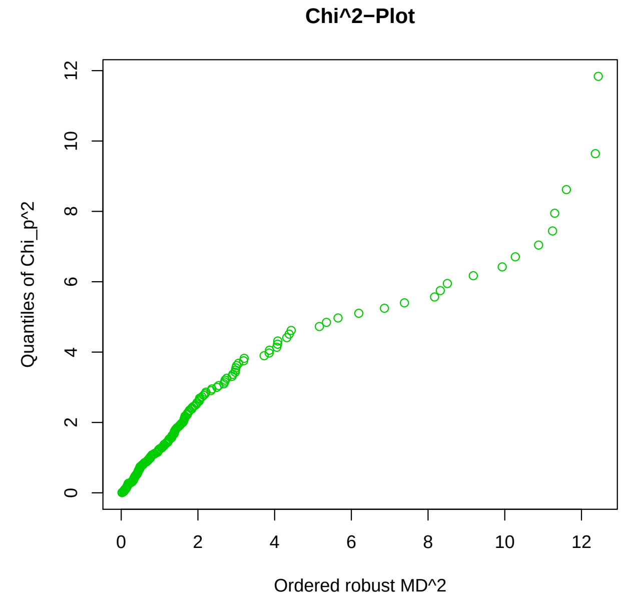

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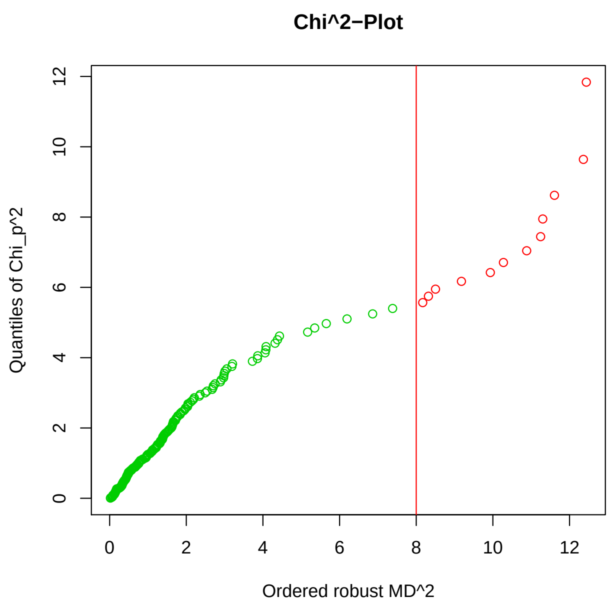
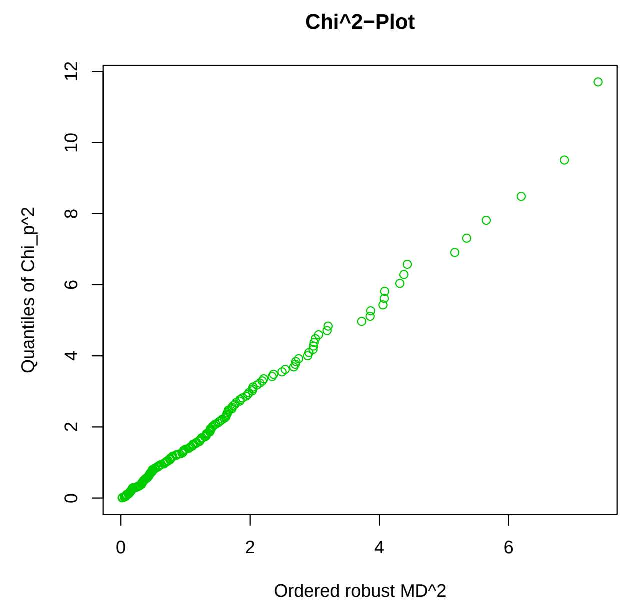


Iterative deletion of outliers:



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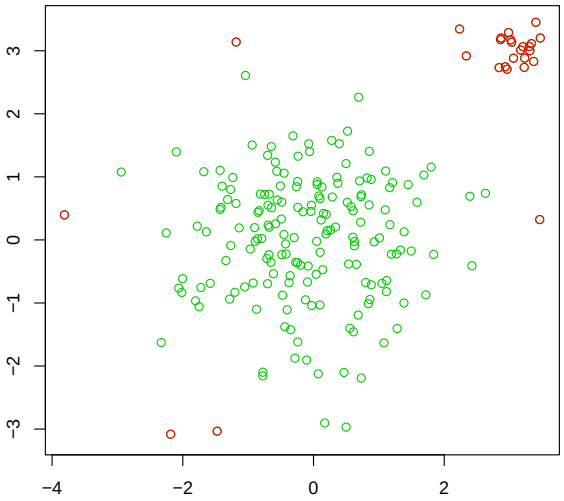


New Proposal

$G(u)$ ... theoretical distribution function of χ^2_p,
$G_n(u)$ ... empirical distribution function of MD_i^2.

For $\eta = \chi^2_{p,1-\alpha}$ define

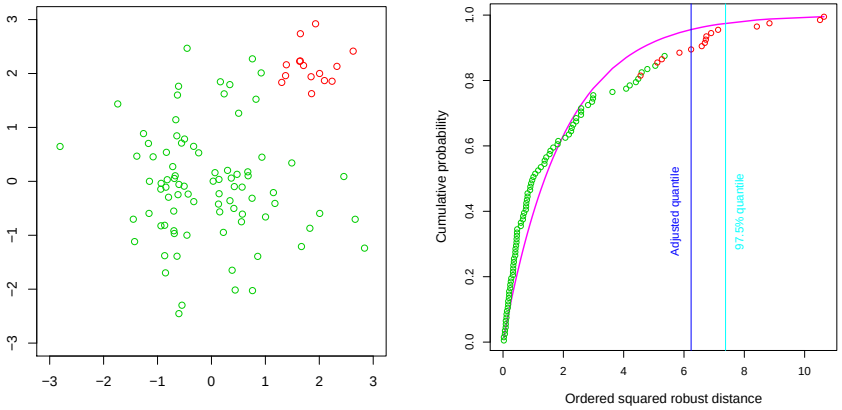
$$p_n(\eta) = \sup_{u \geq \eta} \{G(u) - G_n(u)\}^+.$$

Then a measure of *outliers* in the sample is

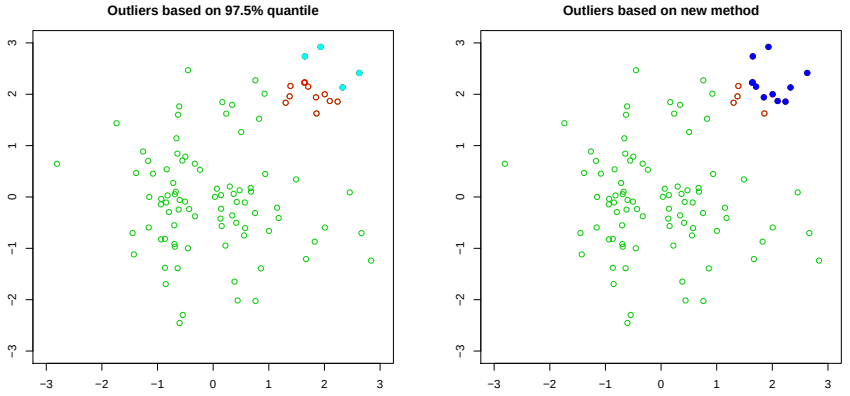
$$\alpha_n(\eta) = \begin{cases} 0 & \text{if } \; p_n(\eta) \leq p_{crit}(\eta, n, p) \\ p_n(\eta) & \text{if } \; p_n(\eta) > p_{crit}(\eta, n, p). \end{cases}$$

$p_{crit}(\eta, n, p)$ can be obtained by simulations.

Simulated Data Example



Example: Simulated Data



Example: Kola Data

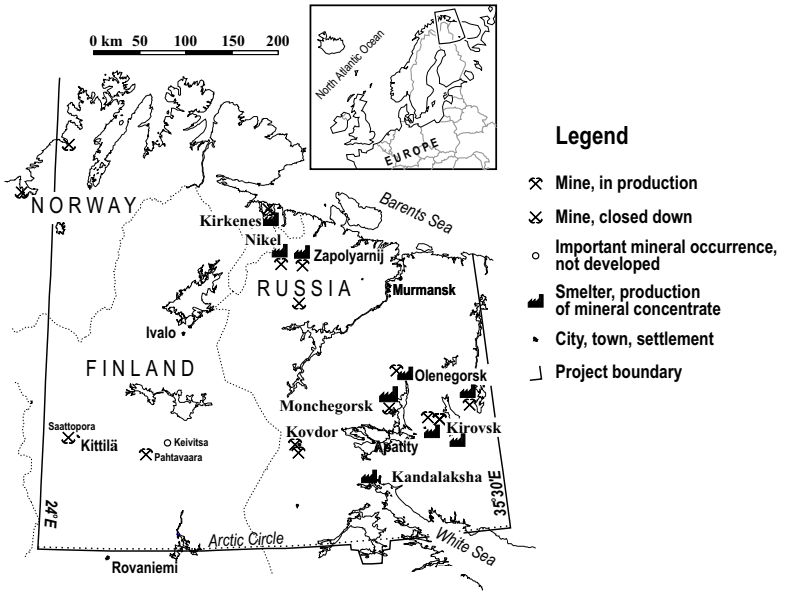
Consider the O-horizon (organic surface soil) of the Kola data set.

Take (more or less) typical elements for "pollution":

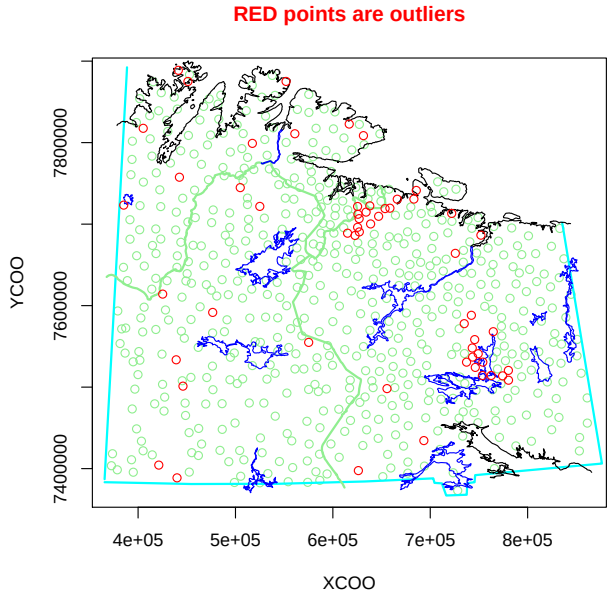
As, Cd, Co, Cu, Mg, Pb, Zn

Question: *Where are the multivariate outliers?*

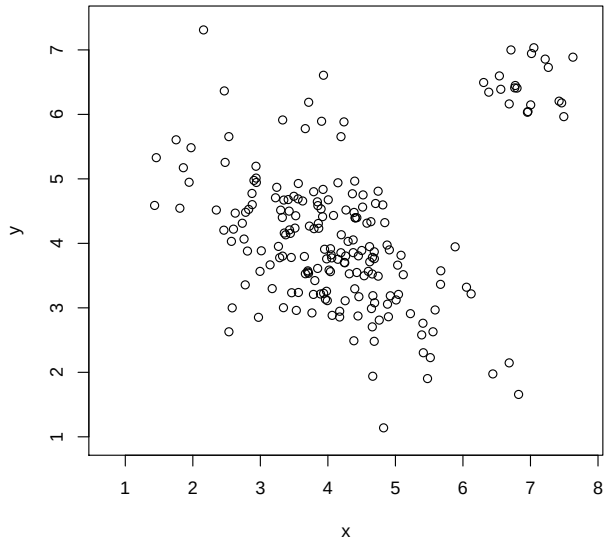
KOLA-Project



Example: Map showing outliers



Choice of Symbols



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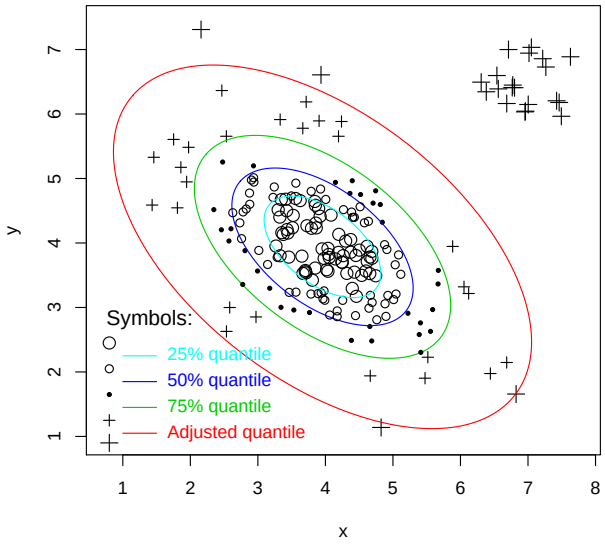

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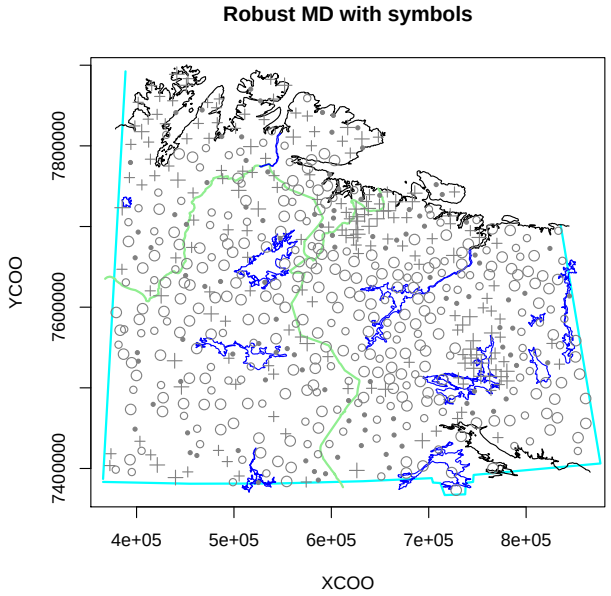
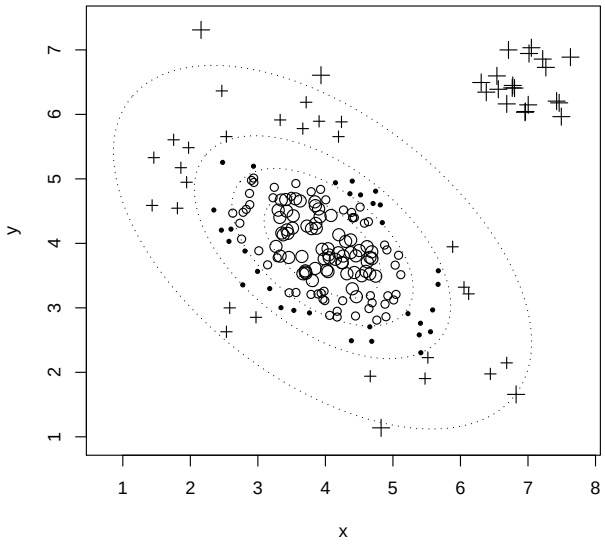


Which Outliers?



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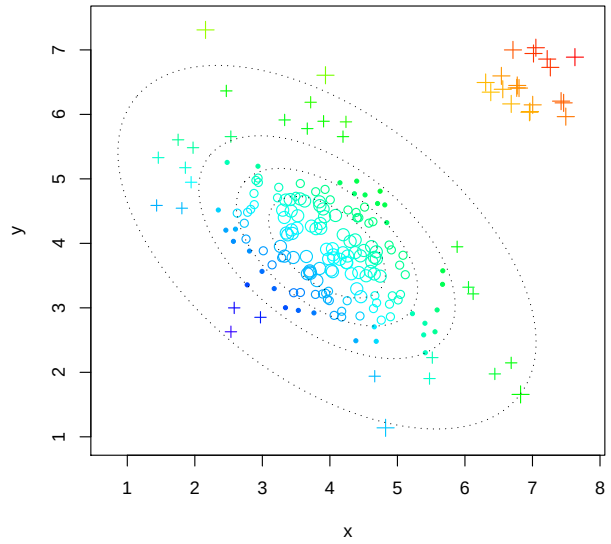

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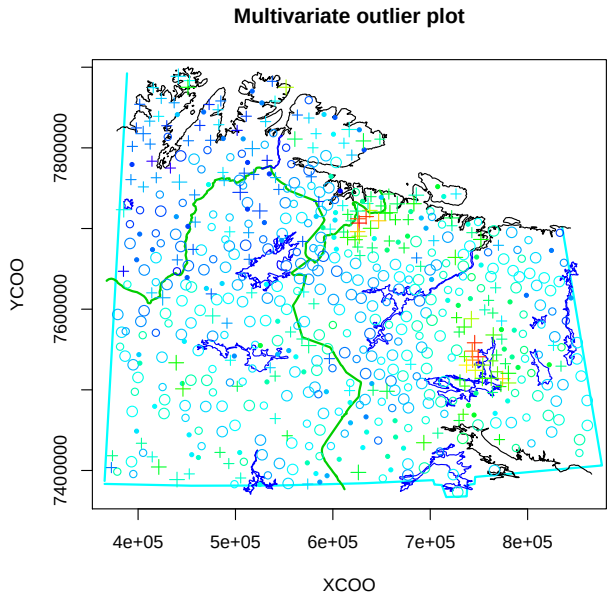
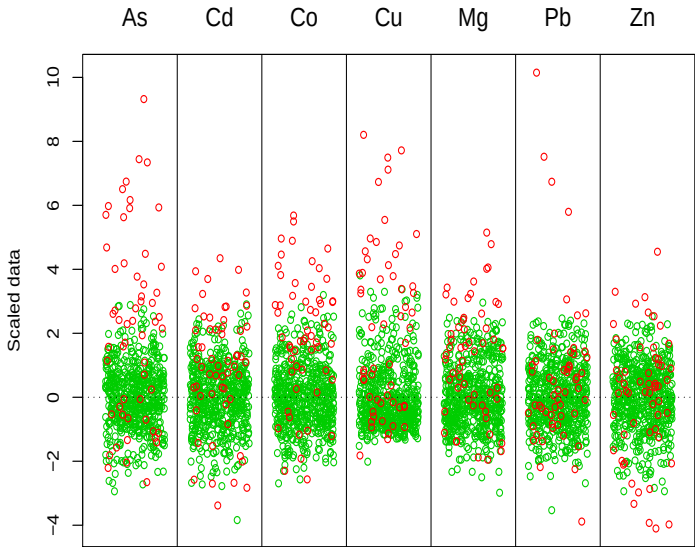
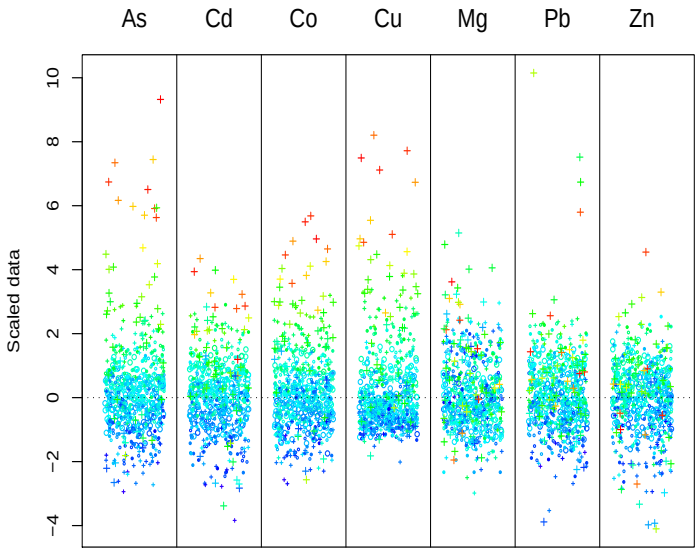


Example: From Multivariate to Univariate



Example: Symbols from multivariate plot



Summary

`library(mvoutlier)`

includes

- all routines to generate the presented plots
- Kola data and other interesting geochemical data sets