Geochemical Data Evaluation and Interpretation

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Geological Survey of Canada

Workshop 2: Exploration Geochemistry -
Basic Principles & Concepts
Exploration 07
8-Sep-2007
Outline

- What is geochemical data?
- The Basics of how geochemical data is evaluated.
- Case Studies:
  - Levelling geochemical survey data
  - Lithology/Alteration/Mineralization signatures in metavolcanics
  - Multivariate geochemical signatures & topography in the tropics.
- Concluding Remarks
Goals of Geochemical Data Analysis

• Detect inter-element relationships of geochemical data reflect that mineralogy or chemical species interactions and describe or infer geological processes.

• Isolate atypical observations or groups of observations that are potentially identified with processes of interest (mineral deposit, hazardous environment).

• Pattern recognition is a key concept in data analysis.
Evaluation of Geochemical Data

• Variable Space
  - Statistics and Data visualization. Numerous graphical and statistical methods characterize the variables.

• Geographic Space
  - Geographic representation of data using Geographic Information Systems (GIS) or Image Analysis Systems
  - Geostatistical Analysis - spatial processes.
Geochemical Sample Media

- Choice of sample media reflects different processes.
- Method of sample preparation affects analytical results.
- Method of instrumentation affects analytical results.
- Spatial density (support) affects the ability to detect various processes.
Measures of Geochemical Data

- Common practice to express major elements as weight % oxides (e.g. SiO2).
- Trace elements commonly expressed as parts per million (ppm).
- Mixing major element oxides with elements reported without oxides is not a good idea (scale differences).
- Convert to moles and then evaluate.
Ideal Distribution of Elements
The True Nature of Distributions

- Censoring
- Non-normal
- Quantization
- Au-As
Univariate Exploratory Approach

• Histograms
• Ranked data
• Q-Q plots
• Density plot
• Summary tables

A “near perfect” distribution.
Typical Distribution

- Non-normal
- Censoring
- Bimodal
## Summary Table

**Summary Statistics for Lake Sediments, Batchawan Area, Ontario**

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Comparative Boxplots
Multivariate Exploratory Approach

Multivariate

- Principal components
- Independent Components
- Multi-dimensional scaling
- Cluster analysis
- $\chi^2$ plots
- Empirical Indices
  (NUMCHI, CHI*-6X, PEG-4, Weighted Sums, SCORESUM)
Modelled Approach based on Target and Background Populations

Groups chosen from exploratory analysis & orientation studies

- Canonical Variate Analysis
- Posterior Probability/Typicality
- Neural Networks / Self Organizing Maps / Random Forests / Support Vector Machines
Special Problems

- Censoring - samples < detection limit - replacement,
- Non-normal distributions that hamper statistical testing - transformations,
- Missing values and zeros - replacements,
- Different limits of detection and instrumentation - levelling,
- Constant sum (closure) problem - Logratio analysis.
Transformations

Transformations are useful to:

• Scale the data in order to view subtle features and minimize the effects of outliers,

• Apply statistical tests (i.e. log-ratios)
Transformations

- Outliers
- "Breaks"
- Censored

Sulphur

Log10 Sulphur

Outliers

"Breaks"

Values < L.L.D.

Censored
Exploratory Data Analysis & Transformations

Histogram

Box Plot

As [ppm]

Frequency

Histogram

Box Plot

As Log10

Frequency

Density Plot

Q-Q Plot

As

Density

Q-Q Plot

Density

As

Theoretical Quantiles

Theoretical Quantiles

Exploration07
Lake Sediments - Logcentred
Robust Statistics

- Presence of extreme or atypical values in a sample population can have a dramatic effect on the estimation of the mean and variance.

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![Histogram of Zn ppm with Mode, Median, and Mean labeled]
Multivariate Visualization
Quantile-Quantile Plots

Batchawana Lake Sediments - Log-centred

- Normal Q-Q Plot
  - As
  - Au
  - Ba
- Normal Q-Q Plot
  - Cd
  - Cu
  - Mg
- Normal Q-Q Plot
  - Ni
  - W
  - Zn
Multi-element Relationships
Pairs Plots
Spatial Evaluation
Bubble Plots
Adequate Support - Spatial Analysis

- Spatial Structure - Fe - Lake Sediments
- Adequate sampling density (support)

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Distance | Distance
Spatial Presentation

Bubble Plot

Interpolated Image
Spatial Analysis and Anomaly Recognition Using Fractals
## Compositional Data

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Compositional Relationships
Aitchison (1982) described the use of logratios as a way of overcoming the problem of compositional data for statistical analysis.

Logratio
\[ y_i = \log \left( \frac{x_i}{x_D} \right) \quad (i = 1, \ldots, D-1) \]
where \( x_D \) is a compositional component of choice

Centred Logratio
\[ z_i = \log \left( \frac{x_i}{g(x_D)} \right) \quad (i = 1, \ldots, D), \]
where \( g(x_D) \) is the geometric mean of the composition
Assessing the Entire Composition with Multivariate Methods
Pearce Element Ratios

• PER’s are based on the “preservation” of a constituent within a magmatic system.
• It is the relative change of a constituent w.r.t another constituent that describes compositional variation.
• $y_i = x_i / x_j$ (where $x_j$ is the preserved constituent and $i = 1, \ldots, D-1$)
• The analysis of $y_i (i = 1, \ldots, D-1)$ is more likely to define compositional variation related to stoichiometric processes.
Levelling Geochemical Survey Data
Levelling Geochemical Survey Data

> 35 elements  Batchawana Greenstone Belt

3047 Sites
Parametric Levelling Scenarios
Cr - Lake Sediment Surveys

Quantile Interval = 0.05
Comparative Boxplots for Levelling
Zn in Lake Sediments
Batchawana Area
Zn [C] = 2.7 + 0.57 \times Zn [H]
Zn in Lake Sediments after levelling
Multivariate Methods

• In many surveys a number of elements may be important.
  - Commodity elements
  - Pathfinder elements
  - Background characterization

• There are many methods to evaluate multi-element geochemical data.
Empirical Methods

- Weighted Sums - a choice of specific elements that define a process of interest. Weights are assigned in terms of importance.
- SCORESUM - a score is given for each element that exceeds a predetermined threshold (i.e. if 6 elements exceed their respective thresholds, the SCORESUM value is 6).
- Specific Indices
  - $\text{CHI-6}*X = \text{As} + 3.56x\text{Sb} + 10x\text{Bi} + 3x\text{Mo} + 30x\text{Ag} + 30x\text{Sn} + 10xW + 3.5xSe$
- Mahalanobis Distance Plots ($X^2$ plots) - multivariate equivalent of a quantile-quantile plot.
The Mahalanobis distance is defined as:

\[ D^2 = (\mathbf{x} - \bar{\mathbf{x}})' \mathbf{C}^{-1} (\mathbf{x} - \bar{\mathbf{x}}) \]

Where:

- \( \mathbf{x} \) is a vector of variables for the observations,
- \( \bar{\mathbf{x}} \) is a vector of the group mean,
- \( \mathbf{C}^{-1} \) is the inverse of the covariance matrix.
Chi-square Plot
Thresholds for the elements:

- As = 1.25
- Au = 1.1
- Ba = 2.7
- Cd = 0.6
- Cu = 2.2
- Mo = 1.2
- Ni = 1.7
- W = 1.0
- Zn = 2.4
Principal Components Analysis

- A multivariate method based on the correlation/covariance of groups of elements.
- Based on correlations linear combinations of elements can be extracted that are orthogonal (independent of each other).
- Each successive component accounts for less of the overall data variation.
Metavolcanics & Mafic Intrusions
Metavolcanics & Mafic Intrusions

Principal Components Analysis

\[ \lambda_1 = 1.8 \text{ (93\% of data variation)} \]
\[ \lambda_2 = 0.1 \text{ (7\% of data variation)} \]
Principal Components Analysis
Metavolcanics & Mafic Intrusions

Overall

Depletion  Enrichment

Relative Cr enrichment

Relative Ni enrichment

PC1

PC2

Cr

Ni
Mapping Volcanic Stratigraphy, zones of alteration and mineralization

Sample Location Map – 825 sites
Ben Nevis Metavolcanics
Principal Components Analysis
Ben Nevis Metavolcanics
Principal Components Analysis
Ben Nevis Metavolcanics
Principal Component 1
Log-centred Data
Ben Nevis Metavolcanics
Principal Component 3
Log-centred Data
Ben Nevis Metavolcanics
Principal Component 4
Log-centred Data
Soil Sediment Geochemistry in a Tropical Environment
Geology of the Area

- Crystal Tuff
- Andesite
- Granodiorite
- Hydrothermal Breccia

Sample Spacing
25m along lines
100 m between lines

Up to 7.5 g/t Au.

Clay altered

Altered Felsic Tuff

Soil Survey Grid

0 0.5 1
Kilometers
Soil Geochemistry

Principal Components Analysis

PC1

PC2

PC1

PC2

Cu Enrichment

K

Ca

Mg

Cr

Ti

Fe

V

Co

Ni
PC2 - Cu Mineralization

- Breccia Zone
- Granodiorite
- Andesite
Soil Geochemistry
PC1 over Topography
Soil Geochemistry
PC1 over Topography

Recent Volcanic Ash
Soil Geochemistry
PC2 - Cu Signature

Cu Enrichment
Software for Geochemical Data Analysis

- Desktop statistical and mapping packages are common today.
- Many public domain and commercial packages available for geochemical data analysis.
- See Exploration 2007 proceedings.
Software for Evaluating Geochemical Data

- Evaluation of data in the spatial and variable domains are currently separate.
- GIS and Geostatistics packages are best for the spatial evaluation.
- Statistical packages best for the variable domain.
The R Project for Statistical Computing (www.r-project.org) provides a comprehensive environment for evaluating data.

- Specific packages include:
  - rgr (The GSC Applied Geochemistry EDA Package)
  - gstat (geostatistical modelling, prediction and simulation)
- Other packages (cluster, fastICA, MASS, e1071, kohonen, nnet, randomForest)
Some Comments

• To Assess/Interpret multi-element geochemistry:
  - Data analysis methods (exploratory),
  - Statistical methods (modelling),
  - Visualization in the variable and geospatial domains,
  - Geographic rendering in 2, 2.5 and 3 dimensions.
In Conclusion....

From Mess to Message ....
Get to know your data ....
There are a wealth of tools available to investigate and evaluate.
Use them all!