Compositional Data Analysis in a Nutshell

report errors to: Raimon Tolosana-Delgado, raimon.tolosana@geo.uni-goettingen.de

version: November 10, 2008

Geometry

Characteristics

- Compositional data are vectors of non-negative components showing the *relative* weight or importance of a set of *parts in a total*.
- The total sum of a compositional vector is *considered* irrelevant, or an artifact of the sampling procedure.
- No individual component can be interpreted isolated from the other. A composition carries no absolute information on increment/decrement of mass.
- The sample space (or set of possible values) is called the *simplex*: this is the set of vectors of positive (or zero) components and constant sum:

$$S^D = \{\mathbf{x} = [x_1;\ldots;x_D] | x_i \geq 0 \,\text{and}\, \sum_{j=1}^{D} x_j = \kappa\}$$

with $\kappa = 1, 100, 10^6, 10^9$ (proportions, %, ppm, ppb), etc.

Compositional operations

Take $\mathbf{x} = [x_1, \ldots x_D]$, $\mathbf{y} = [y_1, \ldots y_D]$, $\mathbf{z} = [z_1, \ldots z_D]$ compositions of D parts, and λ a real value. The compositional operations are

- closure:
$$\mathbf{x} = \mathcal{C}[\mathbf{x}'] = \frac{\kappa}{\sum_{i=1}^{D} x'_i}\mathbf{x}'$$
- perturbation (replacing sum and subtraction):
$$\begin{aligned} \mathbf{z} &= \mathbf{x} \oplus \mathbf{y} = \mathcal{C}[x_1 \cdot y_1; \ldots; x_D \cdot y_D] \\ \mathbf{z} &= \mathbf{x} \ominus \mathbf{y} = \mathcal{C}[x_1/y_1; \ldots; x_D/y_D] \end{aligned}$$
- power transformation (replacing scaling):
$$\mathbf{z} = \lambda \odot \mathbf{x} = \mathcal{C}[x_1^\lambda; \ldots; x_D^\lambda]$$
- Aitchison scalar product (repl. dot product):
$$\langle \mathbf{x} | \mathbf{y} \rangle_a = \frac{1}{2D} \sum_{i=1}^{D} \sum_{j=1}^{D} \ln \frac{x_i}{x_j} \ln \frac{y_i}{y_j}$$
- Aitchison distance (repl. Euclidean distance):
$$d^2(\mathbf{x}, \mathbf{y})_a = \frac{1}{2D} \sum_{i=1}^{D} \sum_{j=1}^{D} \left(\ln \frac{x_i}{x_j} - \ln \frac{y_i}{y_j} \right)^2$$

Log-ratio transformations

- additive log-ratio transform (and inverse)
$$\begin{aligned} \mathrm{alr}(\mathbf{x}) &= \mathbf{y} = \left[\ln \frac{x_1}{x_D}; \ldots; \ln \frac{x_{D-1}}{x_D} \right] = \\ &= \ln(\mathbf{x}) \cdot \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \\ -1 & -1 & \cdots & -1 \end{pmatrix} \\ \mathrm{alr}^{-1}(\mathbf{y}) &= \mathcal{C}[\exp(\,[\mathbf{y}; 0]\,)] \end{aligned}$$
- centered log-ratio transform ($g(\mathbf{x}) = \sqrt[D]{x_1 \cdots x_D}$)
$$\begin{aligned} \mathrm{clr}(\mathbf{x}) &= \mathbf{z} = \left[\ln \frac{x_1}{g(\mathbf{x})}; \ldots; \ln \frac{x_D}{g(\mathbf{x})} \right] \\ &= \frac{\ln(\mathbf{x})}{D} \cdot \begin{pmatrix} D-1 & -1 & \cdots & -1 \\ -1 & D-1 & \cdots & -1 \\ \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & \cdots & D-1 \end{pmatrix} \\ \mathrm{clr}^{-1}(\mathbf{z}) &= \mathcal{C}[\exp(\mathbf{z})] \end{aligned}$$
- isometric log-ratio transform
$$\mathrm{ilr}_V(\mathbf{x}) = \mathrm{clr}(\mathbf{x}) \cdot \mathbf{V} = \ln(\mathbf{x}) \cdot \mathbf{V},$$
for a given matrix $\mathbf{V}$ of D rows and $(D-1)$ columns such that $\mathbf{V} \cdot \mathbf{V}^t = \mathbf{I}_{D-1}$ (identity matrix of D-1 elements) and $\mathbf{V} \cdot \mathbf{V}^t = \mathbf{I}_D + a\mathbf{1}$, where a may be any value, and $\mathbf{1}$ is a matrix full of ones. The inverse is
$$\mathrm{ilr}_V^{-1}(\mathbf{x}) = \mathcal{C}[\exp(\mathbf{x} \cdot \mathbf{V}^t)].$$
- examples for $D = 3$:

$$\begin{aligned} \mathrm{alr}(\mathbf{x}) &= [y_1; y_2] = \left[\ln \frac{x_1}{x_3}; \ln \frac{x_2}{x_3} \right] \\ \mathbf{x} &= \frac{[\exp(y_1); \exp(y_2); 1]}{\exp(y_1) + \exp(y_2) + 1} \\ \mathrm{clr}_i(\mathbf{x}) &= z_i = \ln \frac{x_i}{\sqrt[3]{x_1 x_2 x_3}} \\ x_i &= \frac{\exp(z_i)}{\exp(z_1) + \exp(z_2) + \exp(z_3)} \\ \mathrm{ilr}_V(\mathbf{x}) &= \left[\frac{1}{\sqrt{2}} \ln \frac{x_2}{x_3}; \frac{1}{\sqrt{6}} \ln \frac{x_1^2}{x_2 x_3} \right] \\ \mathbf{V} &= \begin{pmatrix} 0 & \frac{2}{\sqrt{6}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{6}} \\ \frac{-1}{\sqrt{2}} & \frac{-1}{\sqrt{6}} \end{pmatrix} \end{aligned}$$

Statistics

Descriptive statistics

Take $\mathbf{X}$ as a compositional data set, with N rows (individuals) and D columns (compositional variables). Notation $*$lr means one of the log-ratio transforms.

center (repl. average)

$$\mathrm{Mean}_A[\mathbf{X}] = \mathrm{clr}^{-1}(\mathrm{Mean}[\ln \mathbf{X}]) = *\mathrm{lr}^{-1}(\mathrm{Mean}[*\mathrm{lr}(\mathbf{X})])$$

- *centering*: $\mathbf{X}' = \mathbf{X} \ominus \mathrm{Mean}_A[\mathbf{X}]$

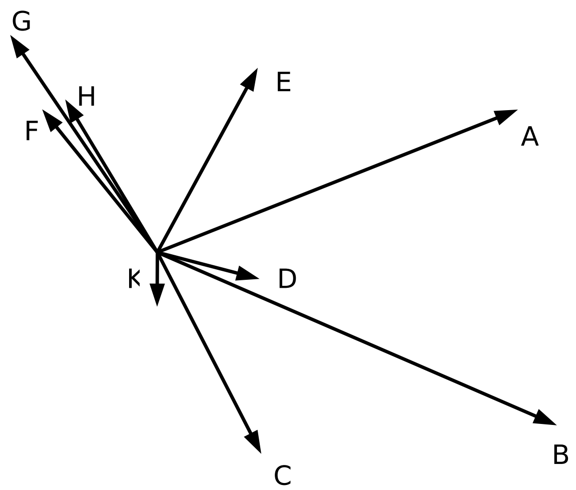
variation matrix (repl. correlation) $\mathbf{T} = [\tau_{ij}]$ with

$$\tau_{ij} = \mathrm{Var}\left[\ln \frac{x_i}{x_j}\right]$$

- if $\tau_{ij} \to 0$, then $\ln(x_i/x_j) \approx$ constant, then x_i and x_j proportional
- larger τ_{ij}, less proportional x_i and x_j

***lr-variance matrix** (repl. covariance) $\mathrm{Var}[*\mathrm{lr}(\mathbf{X})]$ (no back-transformation, difficult to interpet)

Compositional biplot



Best 2D simultaneous representation of data variability and relationships between variables; linked to principal components of the covariance matrix of a centered clr-transformed data set:

- **warning**: do not interpret rays; focus on links
- short link: small t_{ij}, x_i and x_j proportional (FH)
- 3 separate, very long rays: subcomposition defining a high-variance ternary diagram (ABG)
- collinear links: subcomposition showing a one-dimensional pattern (AFH, AEG or CDE)
- orthogonal links: the two subcompositions are uncorrelated (AFH vs. CDE)

Normal inference on the simplex

Normal on the simplex: normal distribution of a *lr-transformed composition, with parameters: a central composition $\mathbf{x}$ and a dispersion (positive-semidefinite symmetric) matrix $\mathbf{\Sigma}$ of eigen-decomposition $\mathbf{\Sigma} = \mathbf{V} \cdot \mathbf{\Lambda} \cdot \mathbf{V}^t$:

$$\mathbf{x} \sim \mathcal{N}_S^D(\mathbf{m}, \mathbf{\Sigma}) \quad \Leftrightarrow \quad -2\ln f(\mathbf{x}|\mathbf{m}, \mathbf{\Sigma}) = (D-1)\ln(2\pi) + \sum_{i=1}^{D-1} \ln \lambda_i \quad + \quad \mathrm{ilr}_V(\mathbf{x} \ominus \mathbf{m}) \cdot \mathbf{\Lambda}^{-1} \cdot \mathrm{ilr}_V^t(\mathbf{x} \ominus \mathbf{m}),$$

where $\mathrm{ilr}_V(\cdot)$ is the ilr with matrix $\mathbf{V}$ giving the eigenvectors in columns, and λ_i are the diagonal elements of $\mathbf{\Lambda}$, the non-zero eigenvalues of $\mathbf{\Sigma}$.

Given $\mathbf{m}$ and $\mathbf{\Sigma}$ mean composition and dispersion matrix (theoretical or estimated)

- Regions on a ternary diagram ($D = 3$): ellipses, centered on $\mathbf{m}$, with principal axes along the eigenvectors of the columns of $\mathbf{V}$, semiaxes $\sqrt{\lambda_i}$ and radius r:
  - $(1-\alpha)$-probability regions for observations, $r = \sqrt{\chi^2_\alpha(2)}$
  - $(1-\alpha)$-confidence regions on the mean, $r = \sqrt{\mathcal{F}_\alpha(2, N-2) \cdot 2/(N-2)}$.
- Test statistic on equivalence of population of two groups, with $\mathbf{m}_i$ and $\mathbf{\Sigma}_i$ center and dispersion in group i:

  $$Q(\mathbf{X}) = N \ln|\mathbf{\Sigma}_0| - N_1 \ln|\mathbf{\Sigma}_1| - N_2 \ln|\mathbf{\Sigma}_2| \sim \chi^2(\nu)$$

  1. = center, = dispersion: $\nu = D(D-1)/2$, and $\mathbf{\Sigma}_0$ the joint covariance matrix (computed as if no groups existed)
  2. $\neq$ center, = dispersion: $\nu = (D-1)(D-2)/2$ and $\mathbf{\Sigma}_0 = \frac{N_1}{N}\mathbf{\Sigma}_1 + \frac{N_2}{N}\mathbf{\Sigma}_2$ the pooled covariance matrix
  3. = center, $\neq$ dispersion: $\nu = (D-1)$; see lecture notes or book for $\mathbf{\Sigma}_0$ expression;

  $\ln|\mathbf{\Sigma}|$= log-determinant, computed as the sum of logs of the non-zero eigenvalues of $\mathbf{\Sigma}$.

Most basic references

Grounding book: Aitchison, J. (1986) *The statistical analysis of compositional data*. Reprinted in 2003 by The Blackburn Press.

General paper: Pawlowsky-Glahn, V. (2003) Statistical modelling in coordinates. In: Proceedings of the 1st CoDaWork.

Lecture notes: Pawlowsky-Glahn, V., Egozcue, J.J. and Tolosana-Delgado, R. (2007) *Lecture notes on compostional data analysis*
http://hdl.handle.net/10256/297

Ongoing research several CoDaWork proceedings, available online at:
http://dugi-doc.udg.edu/handle/10256/150