Compositional PCA based on projection onto simplicial subspace with application to microbiome data

Kipoong Kim, Jaesung Park, and Sungkyu Jung

Department of Statistics, Seoul National University

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Compositional data

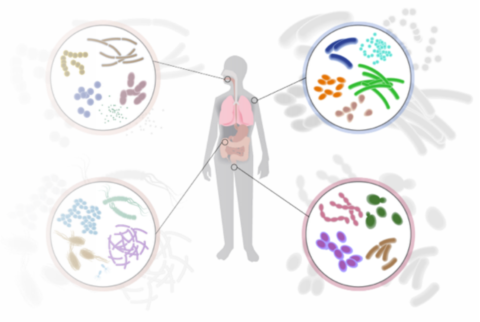
- Compositional data consists of vectors of proportions summing to one: e.g.
  - Geology, a rock composed of different minerals $[0.1, 0.3, 0.6]$;
  - Demography, a town or country
  - Epidemiology, 24-hour time-use data

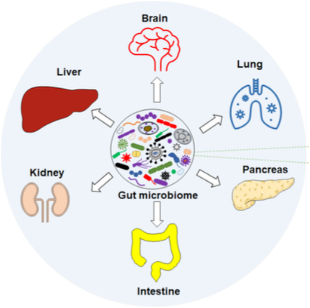
Table: Average monthly expenses per household

Type	ID	Housing	Foodstuff	Transport	Commun.	Sum
Absolute information	1	269	430	287	128	1114
	2	403	645	431	192	1671
	3	592	946	631	282	2450
Information expressed in %	1	24	39	26	11	100
	2	24	39	26	11	100
	3	24	39	26	11	100

Our motivating data

- 16s rRNA microbiome sequencing data
  - Formation of the Human Microbiome
    - Initial Colonization: Begins at birth, influenced by delivery method (vaginal vs. C-section) and breastfeeding.
    - Early Life ($\sim$ 1000 days): Shaped by diet transition and environmental exposure, including family and pets.
    - Adulthood: Continuously influenced by diet, lifestyle, and medication.
    - Other Factors: Genetics, geography, health status, and age also play roles.





Our motivating data

- 16s rRNA microbiome sequencing data
  - The data is collected by **counts of reads**, which can vary significantly between samples due to the DNA extraction process, the concentration of microbial cells, and technical problem.
  - For example,

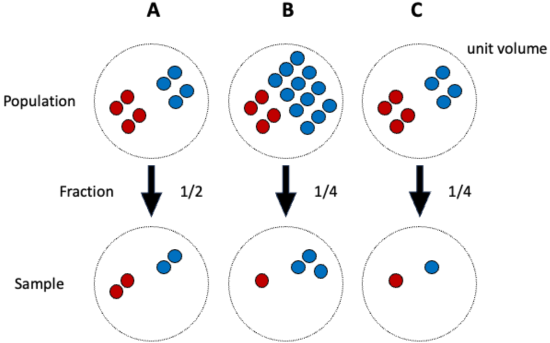


Figure: A vs B, C: different sampling fraction; A, B vs C: different library size

Compositional microbiome data

- Normalization to compositional data to create equal library sizes:

The number of counts

	x	y	z
A	1	4	6
B	5	15	30

⇒

The proportion of counts

	x	y	z
A	0.09	0.36	0.54
B	0.1	0.3	0.6

- Sample space of compositional data is a simplex defined as

$$\mathbb{S}^p = \{(x_1, \dots, x_p) : x_1 \geq 0, \dots, x_p \geq 0; x_1 + \cdots + x_p = 1\}.$$

- Closure operation $\mathcal{C} : \mathbb{R}^p_+ \to \mathbb{S}^p$ is defined as

$$\mathcal{C}(\boldsymbol{x}) = \left[\frac{x_1}{\sum_{j=1}^p x_j}, \dots, \frac{x_p}{\sum_{j=1}^p x_j} \right]$$

- In microbiome data,
  - Counts of reads: $\boldsymbol{x}^* \in \mathbb{R}^p_+$
  - Relative abundance: $\boldsymbol{x} = \mathcal{C}(\boldsymbol{x}^*) \in \mathbb{S}^p$

Compositional data

- Subcomposition and Amalgamation
  - Given a composition $\boldsymbol{x}$ and a selection of interest $\mathcal{A} = \{j_1, \ldots, j_a\}$, a `subcomposition` $\boldsymbol{x}_{\mathcal{A}}$, with a parts, can be written as

    $$\boldsymbol{x}_{\mathcal{A}} = \mathcal{C}[x_{j_1}, \ldots, x_{j_a}] = \left[\frac{x_{j_1}}{\sum x_{j_\ell}}, \ldots, \frac{x_{j_a}}{\sum x_{j_\ell}} \right],$$

    and the value $\sum_{j \in \mathcal{A}} x_j$ is called `amalgamated component`.
- Spurious correlation (bias towards negative correlation):

  $$\begin{aligned} 0 &= cov(x_1, x_1 + \cdots + x_p) \\ &= var(x_1) + cov(x_1, x_2) + \cdots + cov(x_1, x_p) \\ -var(x_1) &= cov(x_1, x_2) + \cdots + cov(x_1, x_p) \end{aligned}$$

  At least one of the covariances on the right must be negative.

Compositional data

- Simplex can be thought of as $p-1$ dimensional `convex hull` embedded in p-dimensional real space.

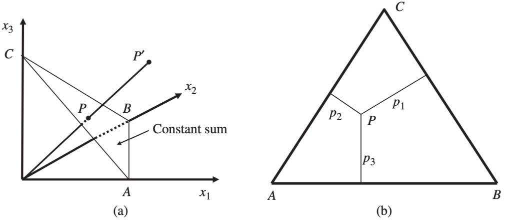


Figure: (a) Simplex embedded in the positive orthant of $\mathbb{R}^3$. (b) Ternary diagram.

- Compositional data that reside on a simplex does not admit the standard Euclidean geometry
    - e.g., not closed under addition and scalar multiplication

Aitchison geometry

- There have been developments on compositional data analysis based on the so-called *Aitchison geometry*[1], which is based on the log-ratio transformation.

- The most common log-ratio transformation is *centered log-ratio (clr) transformation*.
  - Additive log-ratio operator: $alr(\boldsymbol{x}) = \log x_j - \log x_J,\ J \in \{1, \dots, p\}$
  - Centered log-ratio operator: $clr(\boldsymbol{x}) = \log x_j - \frac{1}{p} \sum_{j=1}^{p} \log x_j$
  - Isometric log-ratio operator: $ilr(\boldsymbol{x}) = \log x_j - \frac{1}{p} \sum_{j=1}^{p} \log x_j$

- The inverse operator:

$$inv(\boldsymbol{z}) = \mathcal{C}(\exp \boldsymbol{z}) = \left[\frac{\exp z_1}{\sum_{j=1}^{p} \exp z_j}, \dots, \frac{\exp z_p}{\sum_{j=1}^{p} \exp z_j} \right].$$

[1] J. Aitchison, *Journal of the Royal Statistical Society: Series B* **44**, 139–160 (1982).

Existing PCA methods for compositional data

- Log-ratio PCA[2]: copes with both linear and curved data patterns.

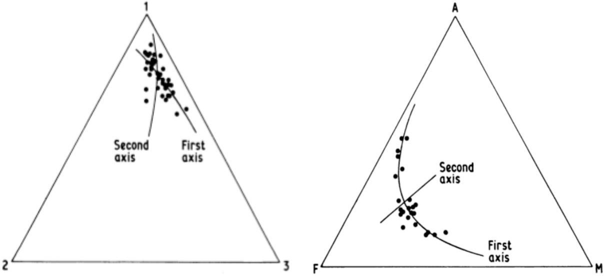


Figure: Ternary diagram with log-ratio principal axes

- Limitation
  - the log-ratio transformation could be inadequate to accommodate the *distinctive features of microbiome data* such as zero inflation, over dispersion and the presence of taxonomic tree structure among microbes.

[2] J. Aitchison, *Biometrika* **70**, 57–65 (1983).

Dealing with zeros in log-ratio transformation

- Zero replacement strategies
  - Simple replacement

$$r_j = \begin{cases} \frac{1}{1+\sum_{k:x_k=0} \delta_k}\delta_j, & \text{if } x_j = 0, \\ \frac{1}{1+\sum_{k:x_k=0} \delta_k}x_j, & \text{if } x_j > 0, \end{cases}$$

  - Additive replacement

$$r_j = \begin{cases} \frac{\delta_j(Z+1)N}{(N+Z)^2}, & \text{if } x_j = 0, \\ x_j - \frac{\delta_j(Z+1)Z}{(N+Z)^2}, & \text{if } x_j > 0, \end{cases}$$

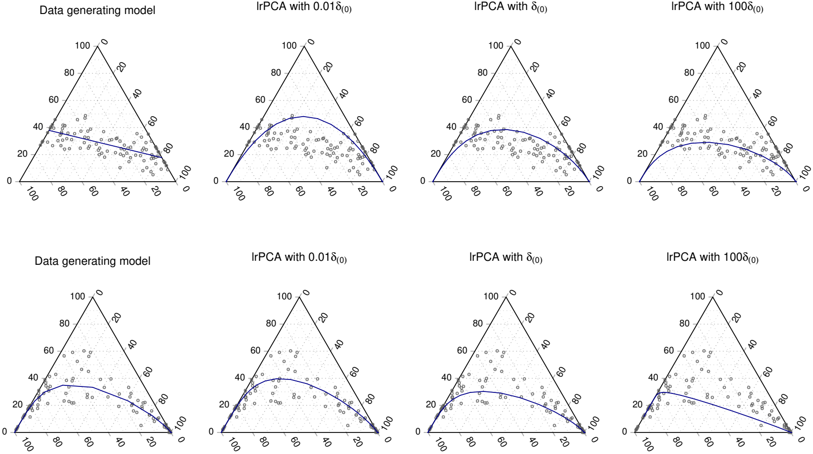
  - Multiplicative replacement

$$r_j = \begin{cases} \delta_j, & \text{if } x_j = 0, \\ (1 - \frac{\sum_{k:x_k=0} \delta_k}{1})x_j, & \text{if } x_j > 0, \end{cases}$$

where δ_j is a small value (e.g. $\min\{x_j : x_j > 0\}$), Z is the number of zeros, and N is the number of nonzeros $(i.e., N + Z = p)$.

Sensitivity analysis for the zero replacement

- Based on $\delta_{(0)} = \min\{x_j : x_j > 0\}$ (minimum of nonzero compositions),



Data generating model

lrPCA with $0.01\delta_{(0)}$

lrPCA with $\delta_{(0)}$

lrPCA with $100\delta_{(0)}$

Data generating model

lrPCA with $0.01\delta_{(0)}$

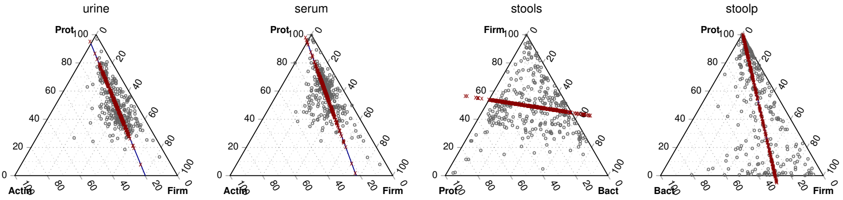
lrPCA with $\delta_{(0)}$

lrPCA with $100\delta_{(0)}$

- The log-ratio PCA result highly depends on the zero-replacement value.

Subcompositional plot: linearity pattern

- Subcomposition plot for the three most abundant microbes with naive PCA axes



*Prot: Proteobacteria; Firm: Firmicutes; Actin: Actinobacteria; Bact: Bacteroidetes

- Low-rank approximation of compositional data do not belong to a simplex.
    - New statistical method (Compositional PCA).

Main goal

- We denote the transpose of the i-th row vector by $\boldsymbol{a}_i$ and the k-th column vector by $\mathbf{A}_k$ for a matrix $\mathbf{A}$.
- We want to solve the following problem:

$$\underset{\mathbf{U}\in\mathbb{R}^{n\times r},\ \mathbf{V}\in\mathbb{R}^{p\times r}}{\arg\min} \|\mathbf{X} - \mathbf{1}\boldsymbol{\mu}^T - \mathbf{U}\mathbf{V}^T\|_F^2,$$

  subject to

  - $\mathbf{U}$ and $\mathbf{V}$ have `orthogonal` and `orthonormal` columns
  - $\boldsymbol{\mu} + \mathbf{V}\boldsymbol{u}_i^T \in \mathbb{S}^p \ \forall i$ for $\boldsymbol{\mu} \in \mathbb{S}^p$

- Simplicial subspace

$$\mathbb{S}^p_{\mathbf{V}_1,\ldots,\mathbf{V}_k} := \mathbb{S}^p \cap span(\{\mathbf{V}_1, \ldots, \mathbf{V}_k\})$$

  (intersection of affine subspace spanned by $\mathbf{V}_1, \ldots, \mathbf{V}_k$ and $\mathbb{S}^p$)

- There is no relationship between $(\mathbf{U}_{k-1}, \mathbf{V}_{k-1})$ and $(\mathbf{U}_k, \mathbf{V}_k)$: e.g. $\mathbb{S}^p_{\mathbf{V}_1,\ldots,\mathbf{V}_{k-1}} \not\subseteq \mathbb{S}^p_{\mathbf{V}_1,\ldots,\mathbf{V}_{k-1},\mathbf{V}_k}$.

Main ideas

- (Direction) Construction of a nested sequence of principal simplicial subspaces:

$$\mathbb{S}^p_{\mathbf{V}_1} \subset \mathbb{S}^p_{\mathbf{V}_1,\mathbf{V}_2} \subset \cdots \subset \mathbb{S}^p_{\mathbf{V}_1,\ldots,\mathbf{V}_k} \subset \cdots .$$

- (Score) Projection onto principal simplicial subspace:

$$\boldsymbol{u}_i = \Pi_{\mathbf{V}_1,\ldots,\mathbf{V}_k}(\boldsymbol{x}_i;\boldsymbol{\mu})$$
$$\text{such that } \boldsymbol{\mu} + u_{i1}\mathbf{V}_1 + \cdots + u_{ik}\mathbf{V}_k \in \mathbb{S}^p_{\mathbf{V}_1,\ldots,\mathbf{V}_k}$$

  for $\boldsymbol{x}_i \in \mathbb{S}^p$ and $\mathbf{V}_1,\ldots,\mathbf{V}_k \perp \mathbf{1}_p$.

Two types of projection approaches

- One-dimensional projection

$$\Pi_{\boldsymbol{v}}^{one}(\boldsymbol{x}_i;\boldsymbol{\mu}) = \mathop{\arg\min}_{u_i \in \mathbb{R}} \|\boldsymbol{x}_i - \boldsymbol{\mu} - u_i\boldsymbol{v}\|_2^2 \quad \text{s.t. } \boldsymbol{\mu} + u_i\boldsymbol{v} \in \mathbb{S}_{\boldsymbol{v}}^p$$

- Multi-dimensional projection

$$\Pi_{\mathbf{V}_1,\ldots,\mathbf{V}_k}^{mult}(\boldsymbol{x}_i;\boldsymbol{\mu}) = \mathop{\arg\min}_{u_{i1},\ldots,u_{ik} \in \mathbb{R}} \|\boldsymbol{x}_i - \boldsymbol{\mu} - u_{i1}\mathbf{V}_1 - \cdots - u_{ik}\mathbf{V}_k\|_2^2$$

$$\text{subject to } \boldsymbol{\mu} + u_{i1}\mathbf{V}_1 + \cdots + u_{ik}\mathbf{V}_k \in \mathbb{S}_{\mathbf{V}_1,\ldots,\mathbf{V}_k}^p$$

- Example with 2-dimensional simplicial subspace embedded in $\mathbb{S}^4$, where the blue cross is out of the subspace and the red cross is the projected point.

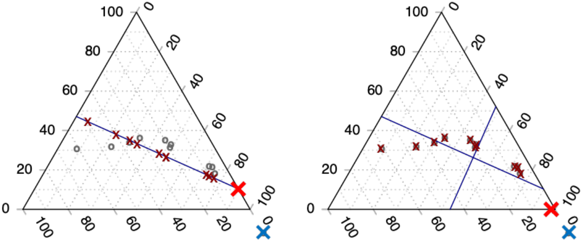


Figure: Left: one-dimensional projection; Right: multi-dimensional projection

Three types of compositional PCA

- Compositional PCA (CPCA): Given $\hat{\mathbf{V}}_1, \ldots, \hat{\mathbf{V}}_{k-1}$,

$$\underset{\mathbf{U}_1,\ldots,\mathbf{U}_k,\mathbf{V}_k}{\arg\min} \; \|\mathbf{X} - \mathbf{1}\boldsymbol{\mu}^T - \mathbf{U}_1\hat{\mathbf{V}}_1^T - \cdots - \mathbf{U}_{k-1}\hat{\mathbf{V}}_{k-1}^T - \mathbf{U}_k\mathbf{V}_k^T\|_F^2$$

- Approximated CPCA (aCPCA): Given $(\hat{\mathbf{U}}_1, \hat{\mathbf{V}}_1), \ldots, (\hat{\mathbf{U}}_{k-1}, \hat{\mathbf{V}}_{k-1})$,

$$\underset{\mathbf{U}_k,\mathbf{V}_k}{\arg\min} \; \|\mathbf{X} - \mathbf{1}\boldsymbol{\mu}^T - \hat{\mathbf{U}}_1\hat{\mathbf{V}}_1^T - \cdots - \hat{\mathbf{U}}_{k-1}\hat{\mathbf{V}}_{k-1}^T - \mathbf{U}_k\mathbf{V}_k^T\|_F^2$$

- Compositional Reconstructed PCA (crPCA): Given $\hat{\mathbf{V}}_1^{PC}, \ldots, \hat{\mathbf{V}}_r^{PC}$,

$$\underset{\mathbf{U}_1,\ldots,\mathbf{U}_r}{\arg\min} \; \|\mathbf{X} - \mathbf{1}\boldsymbol{\mu}^T - \mathbf{U}_1{\hat{\mathbf{V}}_1^{PC}}^T - \cdots - \mathbf{U}_r{\hat{\mathbf{V}}_r^{PC}}^T\|_F^2$$

  under the appropriate compositional constraints.

- Sequential alternating minimization:
  - update $\mathbf{U}_k$ and $\mathbf{V}_k$

    (a) sequentially for $k = 2, \ldots, r$ and (b) alternately by fixing another.

Alternating algorithm: Rank-1 estimation

- Repeat the followings for $t = 0, 1, \ldots$:
    - U-update: Given $\mathbf{V}_1^{(t)}$,

$$u_{i1}^{(t+1)} = \Pi^{one}_{\mathbf{V}_1^{(t)}}(\boldsymbol{x}_i; \boldsymbol{\mu}) = \Pi^{mult}_{\mathbf{V}_1^{(t)}}(\boldsymbol{x}_i; \boldsymbol{\mu}) \quad \forall i$$

    - U-shrinkage: $\mathbf{U}_1^{(t+1)} \leftarrow (1 - \frac{\gamma}{t+1})\mathbf{U}_1^{(t+1)}$.
    - V-update: Given $\mathbf{U}_1^{(t+1)}$,

$$\mathbf{V}_1^{(t+1)} = \underset{\mathbf{V}_1 : \mathbf{V}_1 \perp \mathbf{1}_p}{\arg\min} \left\| \mathbf{X} - \mathbf{1}\boldsymbol{\mu}^T - \mathbf{U}_1^{(t+1)} \mathbf{V}_1^T \right\|_F^2 \quad \text{s.t. } \boldsymbol{\mu} + u_{i1}^{(t+1)} \mathbf{V}_1 \in \mathbb{S}^p \ \forall i.$$

    - V-scaling: $\mathbf{V}_1^{(t+1)} \leftarrow \mathbf{V}_1^{(t+1)} / \|\mathbf{V}_1^{(t+1)}\|_2$

  until convergence, $\|\mathbf{V}_1^{(t+1)} - \mathbf{V}_1^{(t)}\|_F^2 < \epsilon = 10^{-10}$.

- Re-estimation of $\mathbf{U}_1$:

$$u_{i1}^{(t+1)} \leftarrow \Pi^{one}_{\mathbf{V}_1^{(t+1)}}(\boldsymbol{x}_i; \boldsymbol{\mu}) = \Pi^{mult}_{\mathbf{V}_1^{(t+1)}}(\boldsymbol{x}_i; \boldsymbol{\mu}) \quad \forall i \quad \text{for a given } \mathbf{V}_1^{(t+1)}.$$

Alternating algorithm: Rank-k estimation in aCPCA

- For $(\hat{\mathbf{U}}_1, \hat{\mathbf{V}}_1, \dots, \hat{\mathbf{U}}_{k-1}, \hat{\mathbf{V}}_{k-1})$ fixed, repeat the followings for $t = 0, 1, \dots$:
  - Let $\hat{\mathbf{C}}_{k-1} = \mathbf{1}\boldsymbol{\mu}^T + \sum_{h=1}^{k-1} \hat{\mathbf{U}}_h \hat{\mathbf{V}}_h^T$.
  - U-update: Given $\mathbf{V}_k^{(t)}$,

$$u_{ik}^{(t+1)} = \Pi^{one}_{\mathbf{V}_k^{(t)}}(\boldsymbol{x}_i; \hat{\boldsymbol{c}}_{i,k-1}) \ \ \forall i.$$

  - U-shrinkage: $\mathbf{U}_k^{(t+1)} \leftarrow (1 - \frac{\gamma}{t+1})\mathbf{U}_k^{(t+1)}$.
  - V-update: Given $\mathbf{U}_k^{(t+1)}$,

$$\mathbf{V}_k^{(t+1)} = \underset{\mathbf{V}_k : \mathbf{V}_k \perp \mathbf{1}_p}{\arg\min} \left\| \mathbf{X} - \mathbf{1}\boldsymbol{\mu}^T - \sum_{h=1}^{k-1} \hat{\mathbf{U}}_h \hat{\mathbf{V}}_h^T - \mathbf{U}_k^{(t+1)} \mathbf{V}_k^T \right\|_F^2$$

$$\text{s.t. } \boldsymbol{\mu} + \sum_{h=1}^{k-1} \hat{u}_{ih} \hat{\mathbf{V}}_h + u_{ik}^{(t+1)} \mathbf{V}_k \in \mathbb{S}^p \ \forall i.$$

  - V-scaling: $\mathbf{V}_k^{(t+1)} \leftarrow \mathbf{V}_k^{(t+1)} / \|\mathbf{V}_k^{(t+1)}\|_2$

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- For $(\hat{\mathbf{V}}_1, \ldots, \hat{\mathbf{V}}_{k-1})$ fixed, repeat the followings for $t = 0, 1, \ldots$:
  - U-update: Given $\mathbf{V}_k^{(t)}$,

$$\boldsymbol{u}_i^{(t+1)} = \Pi^{mult}_{\hat{\mathbf{V}}_1,\ldots,\hat{\mathbf{V}}_{k-1},\mathbf{V}_k}(\boldsymbol{x}_i; \boldsymbol{\mu}) \ \ \forall i$$

  - U-shrinkage: $[\mathbf{U}_1^{(t+1)}, \ldots, \mathbf{U}_k^{(t+1)}] \leftarrow (1 - \frac{\gamma}{t+1})[\mathbf{U}_1^{(t+1)}, \ldots, \mathbf{U}_k^{(t+1)}]$.
  - V-update: Given $\mathbf{U}_1^{(t+1)}, \ldots, \mathbf{U}_k^{(t+1)}$,

$$\mathbf{V}_k^{(t+1)} = \underset{\mathbf{V}_k : \mathbf{V}_k \perp \mathbf{1}_p}{\arg\min} \left\| \mathbf{X} - \mathbf{1}\boldsymbol{\mu}^T - \sum_{h=1}^{k-1} \mathbf{U}_h^{(t+1)} \hat{\mathbf{V}}_h^T - \mathbf{U}_k^{(t+1)} \mathbf{V}_k^T \right\|_F^2$$

$$\text{s.t. } \boldsymbol{\mu} + \sum_{h=1}^{k-1} u_{ih}^{(t+1)} \hat{\mathbf{V}}_h + u_{ik}^{(t+1)} \mathbf{V}_k \in \mathbb{S}^p \ \forall i.$$

  - V-scaling: $\mathbf{V}_k^{(t+1)} \leftarrow \mathbf{V}_k^{(t+1)} / \|\mathbf{V}_k^{(t+1)}\|_2$

  until convergence, $\|\mathbf{V}_k^{(t+1)} - \mathbf{V}_k^{(t)}\|_F^2 < \epsilon = 10^{-10}$.

- Re-estimation of $\mathbf{U}_1, \ldots, \mathbf{U}_k$:

$$\boldsymbol{u}_i^{(t+1)} \leftarrow \Pi^{mult}_{\hat{\mathbf{V}}_1,\ldots,\hat{\mathbf{V}}_{k-1},\mathbf{V}_k^{(t+1)}}(\boldsymbol{x}_i; \boldsymbol{\mu}) \ \ \forall i \ \ \text{for a given } \mathbf{V}_k^{(t+1)}.$$

Optimization problems

- One-dimensional projection problem

$$\arg\min_{u_i \in \mathbb{R}} \|\boldsymbol{x}_i - \boldsymbol{\mu} - u_i \boldsymbol{v}\|_2^2$$

: Closed form solution

- Multi-dimensional projection problem

$$\arg\min_{u_{i1},\ldots,u_{ik} \in \mathbb{R}^p} \|\boldsymbol{x}_i - \boldsymbol{\mu} - u_{i1}\mathbf{V}_1 - \cdots - u_{ik}\mathbf{V}_k\|_2^2$$

$$\text{subject to } \boldsymbol{\mu} + u_i 1\mathbf{V}_1 + \cdots + u_{ik}\mathbf{V}_k \in \mathbb{S}^p_{\mathbf{V}_1,\ldots,\mathbf{V}_k}$$

: Quadratic Programming (QP)

- Update of $\mathbf{V}_k$

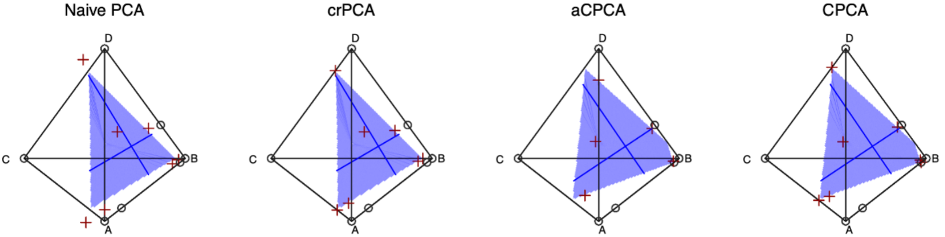
$$\mathbf{V}_k = \arg\min_{\mathbf{V}_k} \left\| \mathbf{X} - \mathbf{1}\boldsymbol{\mu}^T - \sum_{h=1}^{k-1} \mathbf{U}_h \hat{\mathbf{V}}_h^T - \mathbf{U}_k \mathbf{V}_k^T \right\|_F^2$$

$$\text{subject to } \boldsymbol{\mu} + u_{i1}\hat{\mathbf{V}}_1 + \cdots + u_{i,k-1}\hat{\mathbf{V}}_{k-1} + u_{ik}\hat{\mathbf{V}}_k \in \mathbb{S}^p \quad \forall i;$$

$$\mathbf{V}_k \perp \hat{\mathbf{V}}_1, \ldots, \hat{\mathbf{V}}_{k-1}; \ \|\mathbf{V}_k\|_2 = 1$$

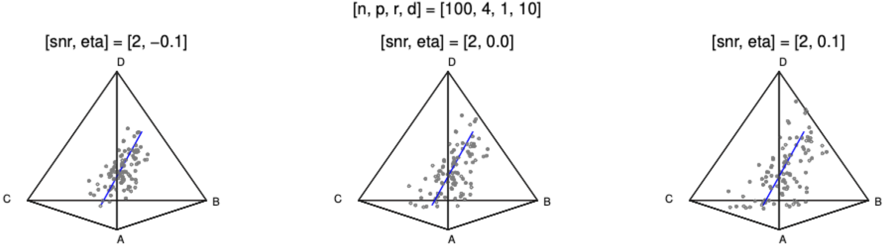
: Quadratic Programming (QP)

Comparative illustration



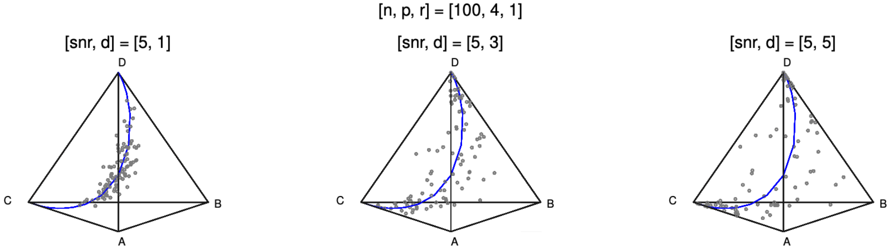
Simulation design: Linear pattern

- Centroid: $\boldsymbol{\mu} \sim Dir(10, \ldots, 10)$
- Loadings: $\mathbf{V} = Orth(\mathbf{V}^*)$ where $v^*_{jk} \sim N(0, 1)$, $\mathbf{V}^T\mathbf{V} = \mathbf{I}_r$, and $\mathbf{V}_1, \ldots, \mathbf{V}_r \perp \mathbf{1}_p \;\; (r = 5)$.
- Scores: $\mathbf{U} = \{u_{ik}\}$ with $u_{ik} \sim TN(0, (d/k)^2; a_k - \frac{\eta}{\log(p)}, b_k + \frac{\eta}{\log(p)})$, where $[a_k, b_k]$ is the confined support which ensures any vectors within $[\boldsymbol{\mu} + a_k\mathbf{V}_k, \boldsymbol{\mu} + b_k\mathbf{V}_k]$ to be inside $\mathbb{S}^p$ $(d = 10 \;\&\; \eta = 0.1)$.
- Simulated data: $\boldsymbol{x}_i = Proj_{\,\mathbb{S}^p}\left[\boldsymbol{\mu}^T + \mathbf{V}\boldsymbol{u}_i + (\mathbf{I}_p - \frac{1}{p}\mathbf{1}_p\mathbf{1}_p^T)\boldsymbol{e}_i\right]$, where $e_{ij} \sim U(-\delta, \delta)$, $Proj_{\,\mathbb{S}^p}$ is a projection operator onto a simplex, and δ was set to achive a specified SNR.



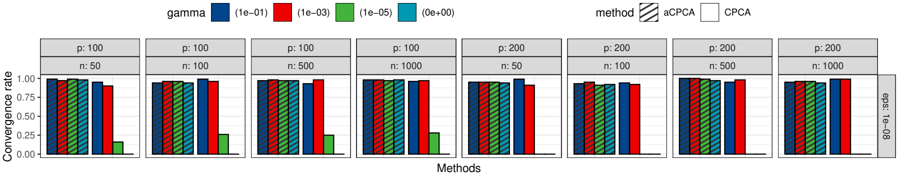
Simulation design: Curved pattern

- Centroid: $\boldsymbol{\mu} = (0, \ldots, 0)$
- Loadings: $\mathbf{V} = Orth(\mathbf{V}^*)$ where $v^*_{jk} \sim N(0,1)$, $\mathbf{V}^T\mathbf{V} = \mathbf{I}_r$, and $\mathbf{V}_1, \ldots, \mathbf{V}_r \perp \mathbf{1}_p \;\; (r = 5)$.
- Scores: $\mathbf{U} = \{u_{ik}\}$ with $u_{ik} \sim N(0, (d/k)^2)$ $(d = 3)$
- Simulated data: $\boldsymbol{x}_i = \mathcal{C}\left[\exp(\boldsymbol{\mu} + \mathbf{V}\boldsymbol{u}_i + \boldsymbol{e}_i)\right]$, where $\boldsymbol{e}_i = (e_{i1}, \ldots, e_{ip})$ with $e_{ij} \sim N(0, \sigma_e^2)$.

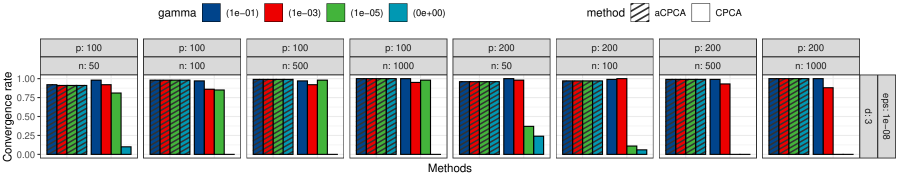


Simulation result: Convergence rate

- The proportion of cases that converged over 100 simulation replicates



Linear

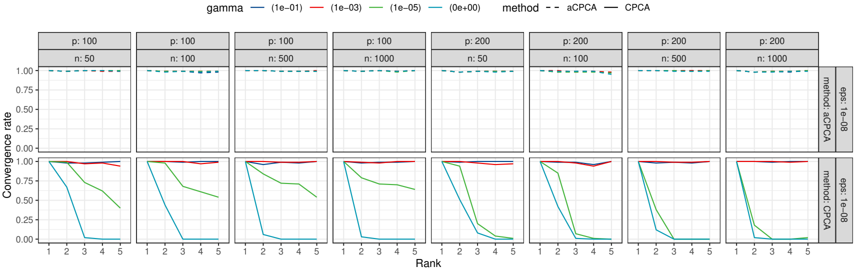


Curved

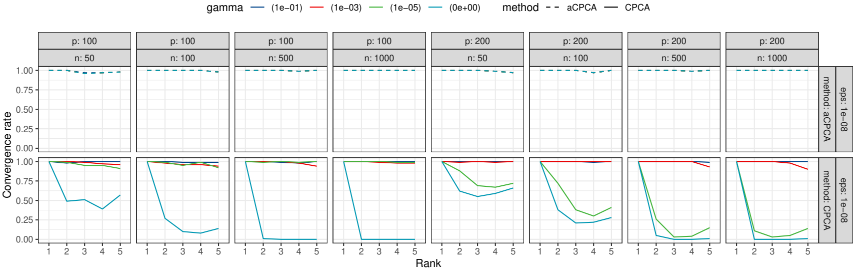
- We choose the shrinkage parameter $\gamma = 0.1$ as an optimal.

Simulation result: Convergence rate for each rank

Linear



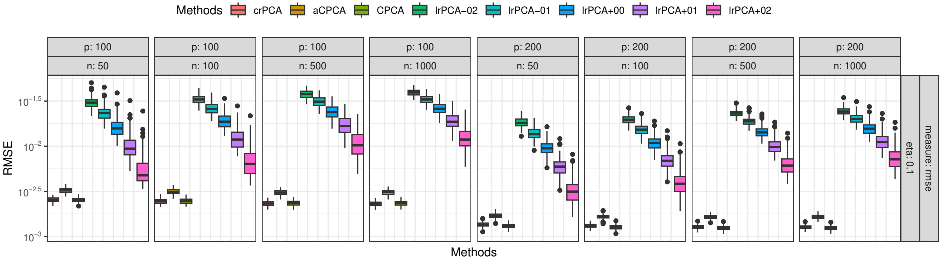
Curved



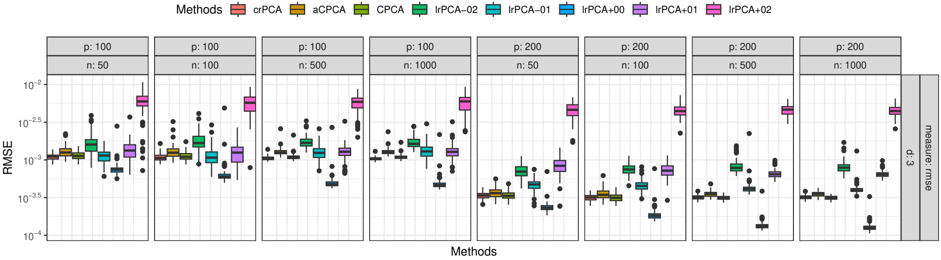
Simulation result: Estimation performance

- RMSE: $\|(\mathbf{1}\boldsymbol{\mu}^T + \mathbf{U}\mathbf{V}^T) - (\mathbf{1}\hat{\boldsymbol{\mu}}^T + \hat{\mathbf{U}}\hat{\mathbf{V}}^T)\|_F / \sqrt{np}$

Linear

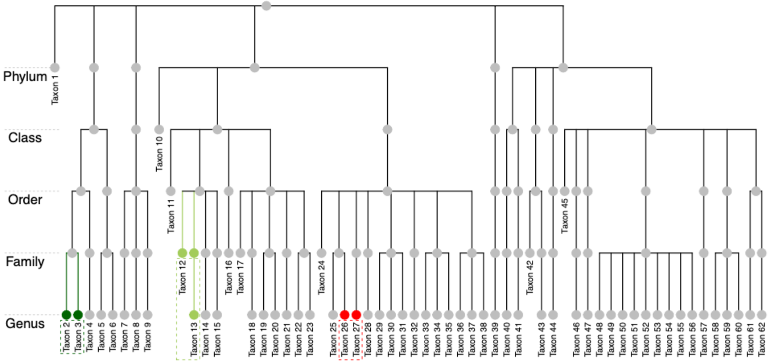


Curved



Real data analysis: microbiome data

- Microbiome counts of reads were measured at four different body sites (urine, serum, stool-s, stool-p) for $n = 293$ individuals. The counts of reads were amalgamated to the phylum level, resulting in data dimensions of $p = 40, 44, 46,$ and 32, respectively.
- Microbiome data is highly sparse so that 70-76% of elements are zero.
- Data dimension (p) can vary according to the taxonomic level.



Cross-validated reconstruction error

- Reconstruction error on test: $\sqrt{\frac{1}{n_{\text{test}}p}\sum_i \|\boldsymbol{x}_i^{\text{test}} - u_{i1}^{\text{test}}\hat{\mathbf{V}}_1 - \cdots - u_{ir}^{\text{test}}\hat{\mathbf{V}}_r\|_2^2}$ where $\boldsymbol{u}_i^{\text{test}} = \Pi_{\hat{\mathbf{V}}_1,\ldots,\hat{\mathbf{V}}_r}(\boldsymbol{x}_i^{\text{test}};\hat{\boldsymbol{\mu}})$.
- 10-fold CV reconstruction error with rank=1 and rank=5.

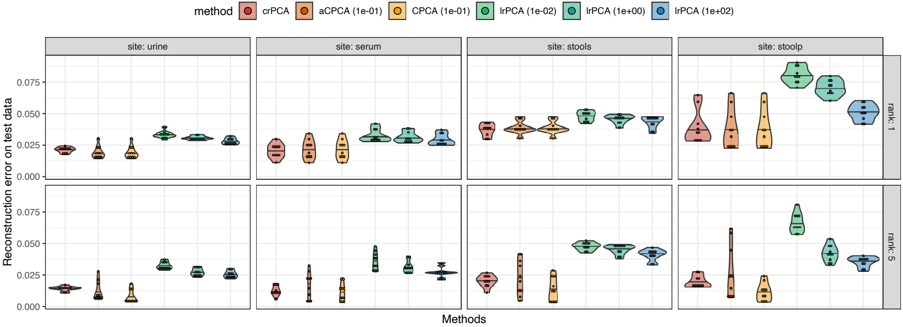
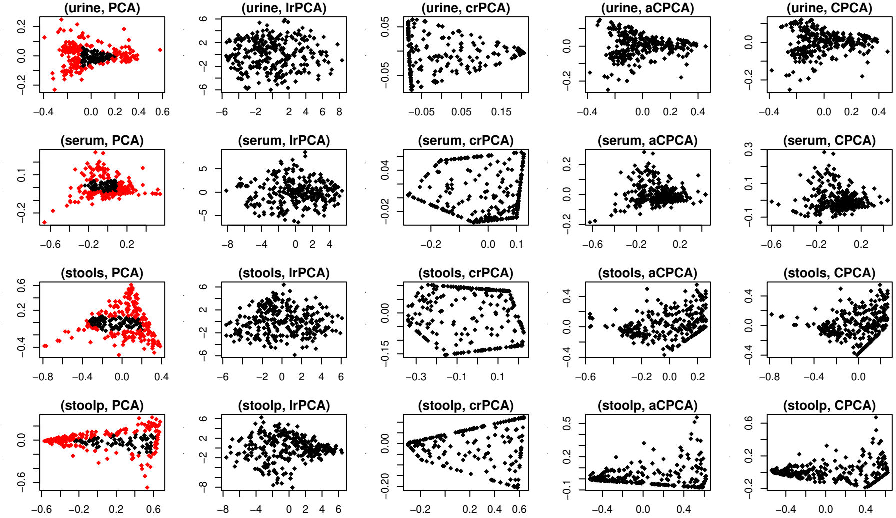


Figure: Top: rank-1; Bottom: rank-5. The lrPCA methods with zero-replacement value $\frac{1}{100}\delta_{(0)}, \delta_{(0)}, 100\delta_{(0)}$ are denoted by lrPCA (1e-02), lrPCA (1e+00), lrPCA (1e+02), respectively.

Real data analysis: The first two PC scores



- The red points represents the samples out of a simplex.

Real data analysis: Compositional plot

- Compositional plot for the rank-1 reconstructed data.

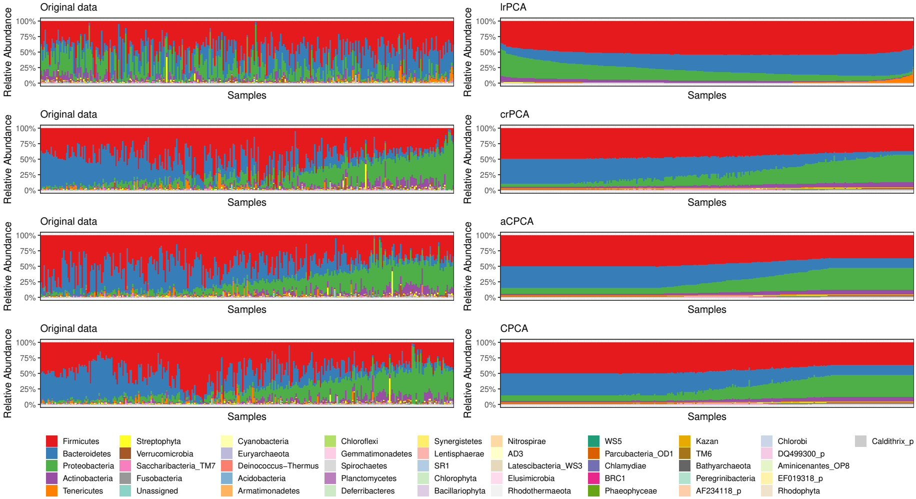


Figure: Right: reconstructed data by PCA; Left: original data. The samples of both the right and left panels are sorted in the same order based on the first PC score.

Conclusion

- In this work, we proposed three types of compositional PCA based on the projection onto the simplicial subspace.
- They performed better than the existing log-ratio PCA in the presence of linear pattern in zero-inflated data.
- Although the proposed optimization problem is clearly non-convex, the convergence is empirically guaranteed by a proper shrinkage parameter.
- We will show the existence and consistency of the simplicial subspace. Furthermore, we are also interested in the robust compositional PCA for future research.

Thank you for your attention ! ☺