High-dimensional CCA

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May 9, 2023

Introduction and outline

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Structure of talk

- Population CCA
- CCA as a tool for data analysis
- Our specific motivations and contributions

Population CCA

In words: Given random variables $X \in \mathbb{R}^p$, $Y \in \mathbb{R}^q$ find linear combinations $u^T X, v^T Y$ with maximal correlation, successively, subject to orthogonality.

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\underset{u \in \mathbb{R}^p, v \in \mathbb{R}^q}{\text{maximize}} \quad & \operatorname{Cov}\left(u^T X, v^T Y\right) \\
\text{subject to} \quad & \operatorname{Var}\left(u^T X\right) = \operatorname{Var}\left(v^T Y\right) = 1, \\
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Notation:

- ρ_k the optimal value called k^{th} *canonical correlation*
- $u_k^T X, v_k^T Y$ called *canonical variates*
- u_k, v_k called *weights*

Visualisation of CCA

$$\underset{u\in\mathbb{R}^p, v\in\mathbb{R}^q}{\text{maximize}} \ \text{Cov}\left(u^T X, v^T Y\right)$$
$$\text{subject to} \ \text{Var}\left(u^T X\right) = \text{Var}\left(v^T Y\right) = 1,$$
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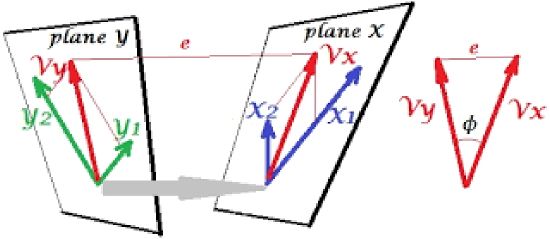

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Notation: Define *canonical loadings*

$$\Sigma_{xx} u_k = \text{Cov}(X, u_k^T X), \quad \Sigma_{yy} v_k = \text{Cov}(Y, v_k^T Y)$$

Reconstruction

Orthonormality constraints $u_k^T \Sigma_{xx} u_j = v_k^T \Sigma_{yy} v_j = \delta_{jk}$ for $1 \leq j \leq k - 1$.

So $(u_k), (\Sigma_{xx} u_k)$ and $(v_k), (\Sigma_{yy} v_k)$ are each pairs of *dual bases*.

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Hence

$$X = \sum_{k=1}^{p} \Sigma_{xx} u_k \langle u_k, X \rangle, \qquad Y = \sum_{k=1}^{q} \Sigma_{yy} v_k \langle v_k, Y \rangle$$

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Probabilistic CCA: Consider the model

$$\begin{aligned} Z &\sim \mathcal{N}(0, I_d), & \min(p,q) \geq d \geq 1 \\ X|Z &\sim \mathcal{N}(W_1 Z + \mu_1, \Psi_1), & W_1 \in \mathbb{R}^{p \times d}, \Psi_1 \succcurlyeq 0 \\ Y|Z &\sim \mathcal{N}(W_2 Z + \mu_2, \Psi_2), & W_2 \in \mathbb{R}^{p \times d}, \Psi_2 \succcurlyeq 0 \end{aligned}$$

Then MLEs for W_1, W_2 are essentially matrices of canonical loadings

Practical Uses

- **High-level:** two sets of data and want to understand interactions
- **Different perspectives:**
  - stats: estimation
  - bio-informatics: algorithm for data matrices, part of pipeline...
- **Uses:** Dimension reduction, visualisation / interpretation, multi-view / self-supervised learning
- **Motivating Example:** Multi-OMICS for human microbiome measuring $p = 200$ metabolites, and $q = 800$ enzymes for $n = 500$ individuals.

Classical Estimator / Sample CCA algorithm

Just stick in sample covariances

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Classical Theory: asymptotic distributions, significance tests...

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Problem: Arbitrary correlations of 1 in high dimensions ($q \geq n$).

Classical Estimator / Sample CCA algorithm

Add regularisation

$$\underset{u \in \mathbb{R}^p, v \in \mathbb{R}^q}{\text{maximize}} \widehat{\text{Cov}}(u^\top \mathbf{X}, v^\top \mathbf{Y}) - \tau_u \|u\|_1 - \tau_v \|v\|_1$$

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Setting the stage

- **Main perspective:** Exploratory Data Analysis (EDA) with an eye on physical interpretation. Loosely frequentist approach.
- **Regularised CCA algorithms:**
  - ridge CCA: l2 penalty
  - sparse CCA: l1 penalty
- **Practical considerations:**
  - model / tuning parameter selection
  - number of pairs to consider
  - interpretation
- **Unanswered question:** Are these regularised CCA methods appropriate for real data? Might other structural assumptions be more natural.

Our contributions

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- **Main conclusions:**
  - CCA is fundamentally a subspace problem
  - Variates and loadings are easier to estimate than weights
  - Powerful visualisation via biplots
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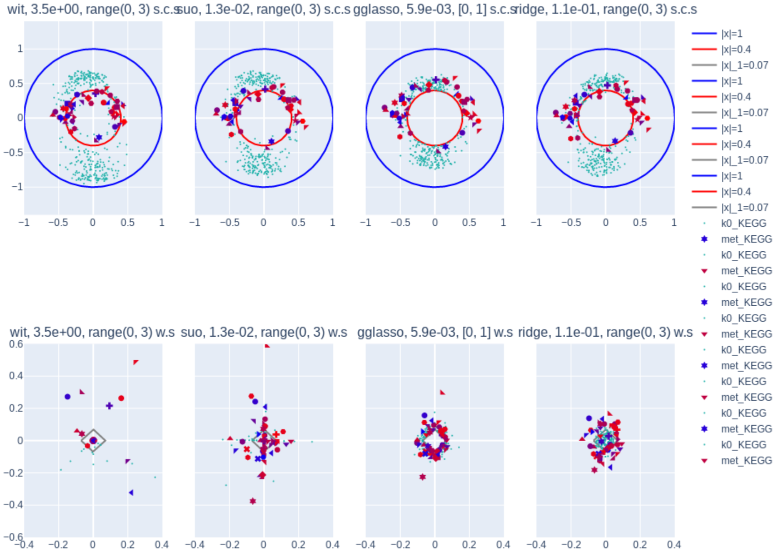
- **New algorithm:** using **graphical lasso**; motivated by graphical models and conditional independence.
- **Practical advice:** for model comparison and interpretation motivated by the fundamental geometry of population CCA.
- **Main conclusions:**
  - CCA is fundamentally a subspace problem
  - Variates and loadings are easier to estimate than weights
  - Powerful visualisation via biplots
  - Model selection is subtle
  - Graphical lasso approach works well!

These may seem natural, but are far from the accepted wisdom, and should be a welcome contribution to the field.

Questions?


wit, 3.5e+00, range(0, 3) s.c.s
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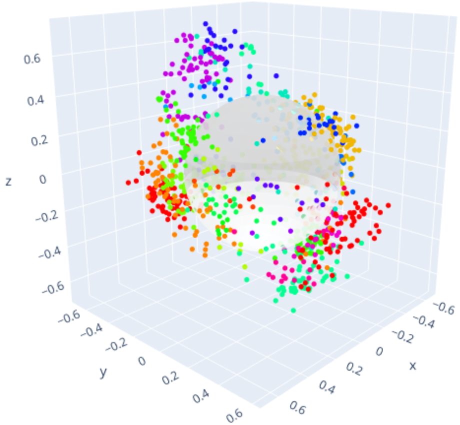
|x|=1
|x|=0.4
|x|_1=0.07
k0_KEGG
met_KEGG

Pretty picture



Links with matrix analysis

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- **Singular Value Decomposition**
  $(\rho_k, \Sigma_x^{1/2} u_k, \Sigma_y^{1/2} v_k)$ give SVD of $M := \Sigma_{xx}^{-1/2} \Sigma_{xy} \Sigma_{yy}^{-1/2}$

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$$A = \begin{pmatrix} 0 & \Sigma_{XY} \\ \Sigma_{YX} & 0 \end{pmatrix}, \quad B = \begin{pmatrix} \Sigma_{XX} & 0 \\ 0 & \Sigma_{YY} \end{pmatrix}, \quad w = \begin{pmatrix} u \\ v \end{pmatrix}, \quad d = p + q.$$

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- **Canonical Angles**
  $\mathcal{X} := \text{span}(\{X_j : j = 1, \dots, p\})$, $\mathcal{Y} := \text{span}(\{Y_j : j = 1, \dots, q\})$ then CCA is

$$\underset{W_k \in \mathcal{X}, Z_k \in \mathcal{Y}}{\text{maximize}} \; \langle W_k, Z_k \rangle$$

$$\text{subject to } \|W_k\|_2 \leq 1, \; \|Z_k\|_2 \leq 1,$$

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Probabilistic CCA

Consider the model:

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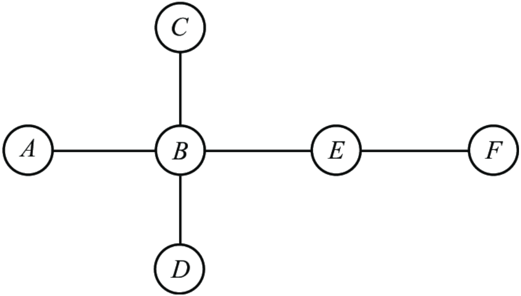
Then the MLEs of the parameters $W_1, W_2, \Psi_1, \Psi_2, \mu_1, \mu_2$ are

$$\begin{aligned} \hat{W}_1 &= \hat{\Sigma}_{xx} U_d M_1 \\ \hat{W}_2 &= \hat{\Sigma}_{yy} V_d M_2 \\ \hat{\Psi}_1 &= \hat{\Sigma}_{xx} - \hat{W}_1 \hat{W}_1^T \\ \hat{\Psi}_2 &= \hat{\Sigma}_{yy} - \hat{W}_2 \hat{W}_2^T \end{aligned}$$

and $\hat{\mu_1} = \bar{X}$, $\hat{\mu_2} = \bar{Y}$ where $M_1, M_2 \in \mathbb{R}^{d\times d}$ are arbitrary matrices with $M_1 M_2^T = R$, $\|M_1\| \leq 1, \|M_2\| \leq 1$

Graphical Models

- Setup: $X = (X^1, \dots, X^p)$ a random vector; $G = (V, E)$ graph with $V = \{1, \dots, p\}$
- Key idea: graph structure constrains distribution of X
- Gaussian graphical models: $X^i \perp X^j | (X^k)_{k \neq i,j}$ whenever $(i, j) \notin E$



Graphical Lasso

- Aim: Solve structure estimation problem
- Setup: samples $x_1, \dots, x_n$ from some zero-mean Gaussian with precision matrix $\in \mathbb{R}^{p \times p}$
- Write: $\mathbf{S} = \frac{1}{n} \sum_{i=1}^{n} x_i x_i^T \in \mathbb{R}^{p \times p}$
- Log-likelihood:

$$l(\Omega; \mathbf{X}) = \log\det \; - \mathrm{trace}(\mathbf{S})$$

- Penalised Objective:

$$\hat{} \in \mathrm{argmax}_{\succeq \mathbf{0}} \{\log\det \; - \mathrm{trace}(\mathbf{S}) - \alpha \rho_1()\}$$

where: $\alpha \in (0, \infty)$ is a penalty parameter, $\rho_1() = \sum_{i \neq j} |\Omega_{ij}|$

Our Approach

Observations:

- $\Sigma = \Omega^{-1}$ is differentiable function of Ω.
- M is a differentiable function of Σ
- So $M = f(\Omega)$ where f is differentiable

Algorithm: Estimate Ω with graphical lasso, plug-in $\hat{M} = f(\hat{\Omega})$, then apply SVD

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Theorem: can combine results in the literature to see convergence rate

$$\sin \Theta(\hat{B}, B) \lesssim s_0(p) \left(\frac{\log p}{n} \right)^{1/2}$$

Existing Methods: PMD [WTH09]

Penalised Matrix Decomposition

A natural but difficult objective:

$$\begin{aligned}
&\underset{u\in\mathbb{R}^p, v\in\mathbb{R}^q}{\text{maximize}} \ \frac{1}{n} u^T \mathbf{X}^T \mathbf{Y} v \\
&\text{subject to } \frac{1}{n}\|\mathbf{X}u\|_2^2 \leqslant 1, \ \ \frac{1}{n}\|\mathbf{Y}v\|_2^2 \leqslant 1, \ \ \|u\|_1 \leqslant c_1, \ \ \|v\|_1 \leqslant c_2
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Make constraints tractable:

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Later pairs: Apply with $\frac{1}{n}\mathbf{X}^T\mathbf{Y} - \sum_{j=1}^{k-1} d_j u_j v_j^T$

Existing Methods: AMA [SMN+17]

Alternating Minimisation Algorithm

Use Lagrange multiplier penalty rather than explicit constraints:

$$\underset{u,v}{\text{minimize}} \; -\frac{1}{n}u^T\mathbf{X}^T\mathbf{Y}v + \tau_1\|u\|_1 + \tau_2\|v\|_1 \\ + \mathbb{1}\left\{u : \frac{1}{n}\|\mathbf{X}u\|_2^2 \leq 1\right\} + \mathbb{1}\left\{v : \frac{1}{n}\|\mathbf{Y}v\|_2^2 \leq 1\right\}$$

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For v fixed get:

$$\underset{u\in\mathbb{R}^p, z\in\mathbb{R}^n}{\text{minimize}} \; \underbrace{-u^T\mathbf{X}^T\mathbf{Y}v + \tau_1\|u\|_1}_{f(u)} + \underbrace{\mathbb{1}\left\{\|z\|_2 \leq 1\right\}}_{g(z)}$$

$$\text{subject to } \mathbf{X}u = z$$

Tool: Linearized ADMM

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Alternating Minimisation Algorithm

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For v fixed get:

$$\underset{u\in\mathbb{R}^p, z\in\mathbb{R}^n}{\text{minimize}} \; \underbrace{-u^T\mathbf{X}^T\mathbf{Y}v + \tau_1\|u\|_1}_{f(u)} + \underbrace{\mathbb{1}\left\{\|z\|_2 \leq 1\right\}}_{g(z)}$$

$$\text{subject to } \mathbf{X}u = z$$

Tool: Linearized ADMM

Later pairs: Add constraint $U^T\mathbf{X}^T\mathbf{X}u = 0$; $V^T\mathbf{Y}^T\mathbf{Y}v = 0$

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