SCF Iteration for Orthogonal Canonical Correlation Analysis

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joint work with
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Outline

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Single-Vector CCA

Canonical Correlation Analysis (CCA) is a two-view multivariate statistical method (H. Hotelling, 1936), where the variables of observations is partitioned into two sets, i.e., two views of the data.

Data matrices $S_1 \in \mathbb{R}^{n\times q}$ (view 1, n features), $S_2 \in \mathbb{R}^{m\times q}$ (view 2, m features), q is the number of samples.
Both centralized: $S_i \mathbf{1}_q = 0$; otherwise, $S_i \leftarrow S_i - \frac{1}{q}(S_i\mathbf{1}_q)\mathbf{1}_q^{\mathrm{T}}$.

Canonical Variates $\boldsymbol{z}_1 = S_1^{\mathrm{T}}\boldsymbol{x}_1$, $\boldsymbol{z}_2 = S_2^{\mathrm{T}}\boldsymbol{x}_2$ defined in terms of Canonical Weight Vectors: $\boldsymbol{x}_1 \in \mathbb{R}^n$, $\boldsymbol{x}_2 \in \mathbb{R}^m$.

Canonical Correlation: $\rho(\boldsymbol{x}_1, \boldsymbol{x}_2) := \dfrac{\boldsymbol{z}_1^{\mathrm{T}}\boldsymbol{z}_2}{||\boldsymbol{z}_1||_2||\boldsymbol{z}_2||_2} = \dfrac{\boldsymbol{x}_1^{\mathrm{T}}C_{1,2}\boldsymbol{x}_2}{\sqrt{\boldsymbol{x}_1^{\mathrm{T}}C_{1,1}\boldsymbol{x}_1}\sqrt{\boldsymbol{x}_2^{\mathrm{T}}C_{2,2}\boldsymbol{x}_2}}$,

where $C_{i,j} = S_i S_j^{\mathrm{T}}$, (Cross-)Covariance.

CCA aims to find the pair of canonical weight vectors to maximize canonical correlation:

$$\max_{\boldsymbol{x}_1,\boldsymbol{x}_2} \rho(\boldsymbol{x}_1, \boldsymbol{x}_2). \tag{1}$$

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CCA in General

Single-vector CCA (1) has been extended to Canonical Weight Matrices.

Canonical Weight Matrices: $X_1 \in \mathbb{R}^{n\times k}$, $X_2 \in \mathbb{R}^{m\times k}$.

Canonical Correlation: $f(X_1, X_2) = \dfrac{\operatorname{tr}(X_1^{\mathrm{T}} C_{1,2} X_2)}{\sqrt{\operatorname{tr}(X_1^{\mathrm{T}} C_{1,1} X_1)}\sqrt{\operatorname{tr}(X_2^{\mathrm{T}} C_{2,2} X_2)}}$,

CCA in general seeks to maximize canonical correlation:

$$\max_{X_1, X_2} f(X_1, X_2), \text{ s.t. } X_i^{\mathrm{T}} C_{i,i} X_i = I_k,\ i = 1, 2, \tag{2}$$

Closed form solution in terms of SVD for $C_{1,1}^{-1/2} C_{1,2} C_{2,2}^{-1/2}$. Collectively, traditional CCA or, simply, CCA is referred to either (1) or (2).

CCA is not suitable for: orthogonal projections are required such as for data visualization in an orthogonal coordinate system, because optimal X_1 and X_2 in (2) usually do not have orthonormal columns.

One can orthogonalize the columns of X_1 and X_2 as a post-processing step, but outcome is often suboptimal – less discriminatory.

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1. Introduction to CCA
2. Orthogonal CCA (OCCA)
3. Submaximization Problem
4. Orthogonal Multiset CCA (OMCCA)
5. Applications
6. Summary

Orthogonal CCA (OCCA)

Orthogonal CCA (OCCA) seeks to maximize the correlation:

$$\max_{X_1 \in \mathbb{O}^{n\times k}, X_2 \in \mathbb{O}^{m\times k}} f(X_1, X_2) \tag{3}$$

directly over orthonormal matrices in $\mathbb{O}^{n\times k} = \{X \in \mathbb{R}^{n\times k} : X^{\mathrm{T}}X = I_k\}$.

Different from CCA, OCCA preserves the covariance of the original data S_1 and S_2 while correlation is maximized.

Can use generic optimization methods over the product of the Stiefel manifolds, and indeed applied.

Essentially, they are classical steepest ascent, trust-region, nonlinear CG methods over the Euclidean space extended to Riemannian manifolds. These methods don't recognize any special structure in f: less efficient, low accuracy, ...

P. Cunningham and Z. Ghahramani, Linear dimensionality reduction: Survey, insights, and generalizations, *J. Mach. Learning Res.*, 16(2015), 2859–2900.

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OCCA model (abstraction)

Data of both views centralized in advance: $S_1\mathbf{1}_q = 0$ and $S_2\mathbf{1}_q$. Define

$$A = S_1S_1^{\mathrm{T}} \in \mathbb{R}^{n\times n},\ B = S_2S_2^{\mathrm{T}} \in \mathbb{R}^{m\times m},\ C = S_1S_2^{\mathrm{T}} \in \mathbb{R}^{n\times m}.$$

OCCA: given an integer $1 \le k < \min\{m,n\}$ (usually $k \ll \min\{m,n\}$), solve

$$\max_{X\in\mathbb{O}^{n\times k}, Y\in\mathbb{O}^{m\times k}} f(X,Y) := \frac{\mathrm{tr}(X^{\mathrm{T}}CY)}{\sqrt{\mathrm{tr}(X^{\mathrm{T}}AX)}\sqrt{\mathrm{tr}(Y^{\mathrm{T}}BY)}}. \tag{4}$$

Propose to maximize $f(X,Y)$ alternatingly with respective to X and Y.

Although the framework of the proposed numerical scheme is rather natural, novelty lies in the way how its core sub-maximization problems are solved.

Algorithm framework for 2-view OCCA

Algorithm 1. Alternating optimization scheme for (4)

Input: $\{X^{(0)}, Y^{(0)}\}$ with $X^{(0)} \in \mathbb{O}^{n\times k}, Y^{(0)} \in \mathbb{O}^{m\times k}$.

Output: a solution $\{X^{(\nu)}, Y^{(\nu)}\}$ to (4).

1: **for** $\nu = 1, 2, \ldots$ until convergence **do**

2: solve $X^{(\nu)} \in \arg\max_{X\in\mathbb{O}^{n\times k}} f(X, Y^{(\nu-1)})$;

3: solve $Y^{(\nu)} \in \arg\max_{Y\in\mathbb{O}^{m\times k}} f(X^{(\nu)}, Y)$;

4: compute SVD: $(X^{(\nu)})^{\mathrm{T}} C Y^{(\nu)} = \widetilde{U}\widetilde{\Sigma}\widetilde{V}^{\mathrm{T}}$, and set $X^{(\nu)} \leftarrow X^{(\nu)}\widetilde{U}$ and $Y^{(\nu)} \leftarrow Y^{(\nu)}\widetilde{V}$;

5: **end for**

6: **return** $\{X^{(\nu)}, Y^{(\nu)}\}$ as a numerical solution to (4).

The role of line 4 in Algorithm 1 is to make sure $X^{(\nu)}$ and $Y^{(\nu)}$ are best-aligned. In particular, $\mathrm{tr}({X^{(\nu)}}^{\mathrm{T}} C Y^{(\nu)}) > 0$ and maximized within the column spaces of $X^{(\nu)}$ and $Y^{(\nu)}$ at lines 2 & 3.

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Convergence

Convergence Theorem

Let $\{X_{\rm opt}, Y_{\rm opt}\}$ be the optimal solution to (4) and $\{X^{(\nu)}, Y^{(\nu)}\}$ be the νth approximation of Algorithm 1. Then

(i) $X_{\rm opt}^{\rm T} C Y_{\rm opt}$ is symmetric and positive semidefinite.

(ii) $(X^{(\nu)})^{\rm T} C Y^{(\nu)}$ is symmetric and positive semidefinite for $\nu \geq 1$, and thus for any limit pair $\{X_*, Y_*\}$ of $\{X^{(\nu)}, Y^{(\nu)}\}_{\nu=1}^{\infty}$, $X_*^{\rm T} C Y_*$ is symmetric and positive semidefinite.

(iii) The sequence $\{f(X^{(\nu)}, Y^{(\nu)})\}_{\nu=1}^{\infty}$ is monotonically increasing and converges.

Efficiency of Algorithm 1 relies heavily on solving the sub-maximization problems at Lines 2 and 3.

Abstractly, they are of the following type

$$\max_{X \in \mathbb{O}^{n \times k}} \eta(X) \quad \text{with } \eta(X) := \frac{\operatorname{tr}(X^{\rm T} D)}{\sqrt{\operatorname{tr}(X^{\rm T} A X)}}, \tag{5}$$

where $0 \neq D \in \mathbb{R}^{n \times k}$ and $A \succ 0$.

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Local but non-global maximizers

Problem (5) may admit local but non-global maximizers.

Example. Consider the case with $n = 5,\ k = 2$,

$$A = \begin{bmatrix} 4 & 0 & -5 & -5 & 1 \\ 0 & 2 & 1 & -1 & 1 \\ -5 & 1 & 9 & 5 & 1 \\ -5 & -1 & 5 & 18 & 4 \\ -1 & 1 & 1 & 4 & 2 \end{bmatrix} \quad \text{and} \quad D = \begin{bmatrix} -1 & 1 \\ 0 & 0 \\ 0 & 2 \\ 0 & 0 \\ 1 & 0 \end{bmatrix}.$$

By calling MATLAB's `fmincon`, we find two (numerical) local maximizers:

$$X_+ = \begin{bmatrix} -0.358041496119094 & 0.770164268103322 \\ -0.453284095949462 & -0.326431512218038 \\ -0.091335437376569 & 0.497561512998402 \\ -0.269574025133855 & 0.008593213179154 \\ 0.765066989399257 & 0.229451880441015 \end{bmatrix},$$

Local but non-global maximizers (cont'd)

$$X_* = \begin{bmatrix} -0.506648923972689 & 0.664385053189626 \\ 0.619602876311725 & 0.312889763321350 \\ -0.337893503149209 & 0.384494340924914 \\ 0.103073503143856 & 0.210902556071053 \\ -0.484358314662567 & -0.518050876600301 \end{bmatrix}.$$

$$\eta(X_+) \approx 1.517 < \eta(X_*) \approx 3.187.$$

We argue that they are (numerical) local maximizers:

- $\|\operatorname{grad} \eta(X)\|_F \le 10^{-6}$ (on $\mathbb{O}^{n\times k}$) for $X = X_+$ or X_*;
- Second order sufficient condition: verified at 10^7 random tangent "vectors" in $\mathcal{T}_X\mathbb{O}^{n\times k}$ for both X_+ and X_*.

This example numerically shows (5) in general admits local but non-global maximizers.

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SCF Iteration

$$\max_{X \in \mathbb{O}^{n\times k}} \eta(X) \quad \text{with } \eta(X) := \frac{\operatorname{tr}(X^{\mathrm{T}}D)}{\sqrt{\operatorname{tr}(X^{\mathrm{T}}AX)}}. \tag{5}$$

Gradient:

$$\operatorname{grad}\eta(X) = \Pi_X\left(\frac{\partial \eta(X)}{\partial X}\right) \in \mathcal{T}_X\mathbb{O}^{n\times k}, \tag{6}$$

where $\Pi_X(Z) = Z - X\,\operatorname{sym}(X^{\mathrm{T}}Z)$ for $Z \in \mathbb{R}^{n\times k}$. By calculations,

$$\frac{\partial \eta(X)}{\partial X} = \frac{1}{\sqrt{\operatorname{tr}(X^{\mathrm{T}}AX)}}\,D - \frac{\operatorname{tr}(X^{\mathrm{T}}D}{[\operatorname{tr}(X^{\mathrm{T}}AX)]^{3/2}}\,AX,$$

$$\frac{[\operatorname{tr}(X^{\mathrm{T}}AX)]^{3/2}}{\operatorname{tr}(X^{\mathrm{T}}D)}\operatorname{grad}\eta(X) = [\xi(X)D - AX] - X\Lambda(X) \in \mathbb{R}^{n\times k},$$

where $\xi(X) = \frac{\operatorname{tr}(X^{\mathrm{T}}AX)}{\operatorname{tr}(X^{\mathrm{T}}D)}$,

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First Order KKT Condition

Lemma 1. First Order KKT Condition

If X is a maximizer of (5), then $X^{\mathrm{T}}D = D^{\mathrm{T}}X$ and

$$\xi(X)D - AX = X\Lambda(X). \tag{8}$$

Condition (8) is a type of nonlinear Sylvester equation but with the orthogonality constraint $X^{\mathrm{T}}X = I_k$. Not clear how to solve.

Turn it into nonlinear eigenvalue problem (NEPv):

$$E(X)X = X\widehat{\Lambda}(X), \tag{9}$$

where $\widehat{\Lambda}(X)^{\mathrm{T}} = \widehat{\Lambda}(X)$ and

$$E(X) := \xi(X)(DX^{\mathrm{T}} + XD^{\mathrm{T}}) - A.$$

Evidently, $E(X)$ is always symmetric. It is implied $\widehat{\Lambda}(X) = X^{\mathrm{T}}E(X)X \in \mathbb{R}^{k\times k}$.

Lemma 2. Equivalent KKT Condition

Suppose $X \in \mathbb{O}^{n\times k}$. Then X satisfies (8) if and only if X is an eigenbasis matrix of $E(X)$, i.e., X satisfies (9).

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Suppose $X \in \mathbb{O}^{n\times k}$. Then X satisfies (8) if and only if X is an eigenbasis matrix of $E(X)$, i.e., X satisfies (9).

First Order KKT Condition

Lemma 1. First Order KKT Condition

If X is a maximizer of (5), then $X^{\mathrm{T}}D = D^{\mathrm{T}}X$ and

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Condition (8) is a type of nonlinear Sylvester equation but with the orthogonality constraint $X^{\mathrm{T}}X = I_k$. Not clear how to solve.

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A self-consistent-field (SCF) iteration

Necessary condition of a global maximizer for (5)

If $X_{\rm opt}$ is a global maximizer to (5), then $X_{\rm opt}$ is an orthonormal eigenbasis matrix associated with the k largest eigenvalues of $E(X_{\rm opt})$.

Algorithm 2. An SCF iteration for solving (5)

Input: $X_{(0)} \in \mathbb{O}^{n\times k}$;
Output: approximate maximizer X to (5).

for $\nu = 1, 2, \ldots$ until convergence **do**
    construct $E_{(\nu)} = E(X_{(\nu-1)})$ as in (9);
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Comments on Algorithm 2 (SCF)

Use full eigen-decomposition of E for small n (e.g., ≤ 200); use an iterative method for large n such as LOBPCG, Inverse-free (Golub+Ye), LOBPECG, ...

The SCF iteration stops if

$$\frac{\operatorname{tr}(X^{\mathrm{T}}D)}{[\operatorname{tr}(X^{\mathrm{T}}AX)]^{3/2}}\frac{\|\operatorname{grad}\eta(G_{(\nu)})\|_1}{\|A\|_1+\|D\|_1}\leq\epsilon_{\mathrm{scf}}$$

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Convergence

Weak Convergence Theorem

Let $\{X_{(\nu)}\}$ be generated by the SCF iteration (Algorithm 2).

(i) For each $\nu \geq 1$, $D^{\mathrm{T}} X_{(\nu)} \succeq 0$ and $\mathrm{tr}(X_{(\nu)}^{\mathrm{T}} D) = \sum_{j=1}^{k} \sigma_j(X_{(\nu)}^{\mathrm{T}} D)$;

(ii) $\{\eta(X_{(\nu)})\}$ is monotonically increasing and convergent;

(iii) If
$$\mathrm{tr}(X_{(\nu)}^{\mathrm{T}} E(X_{(\nu-1)}) X_{(\nu)}) \geq \mathrm{tr}(X_{(\nu-1)}^{\mathrm{T}} E(X_{(\nu-1)}) X_{(\nu-1)}), \tag{10}$$
then $\eta(X_{(\nu-1)}) \leq \eta(X_{(\nu)})$; If (10) is strict, then also $\eta(X_{(\nu-1)}) < \eta(X_{(\nu)})$;

(iv) $\{X_{(\nu)}\}$ has a convergent subsequence $\{X_{(\nu)}\}_{\nu \in \mathcal{I}}$;

(v) Let $\{X_{(\nu)}\}_{\nu \in \mathcal{I}}$ be any convergent subsequence of $\{X_{(\nu)}\}$ with the accumulation point X_* satisfying
$$\zeta = \lambda_k(E(X_*)) - \lambda_{k+1}(E(X_*)) > 0. \tag{11}$$
Then X_* satisfies the first order optimality condition and also the necessary condition for a global minimizer.

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Convergence (cont'd)

Strong Convergence Theorem

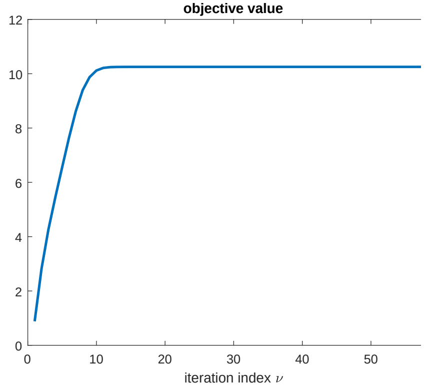
Let $\{X_{(\nu)}\}$ be generated by the SCF iteration (Algorithm 2), and let X_* be an accumulation point of $\{X_{(\nu)}\}$. Suppose that $\mathcal{R}(X_*)$ is an isolated accumulation point of $\{\mathcal{R}(X_{(\nu)})\}_{\nu=0}^{\infty}$.

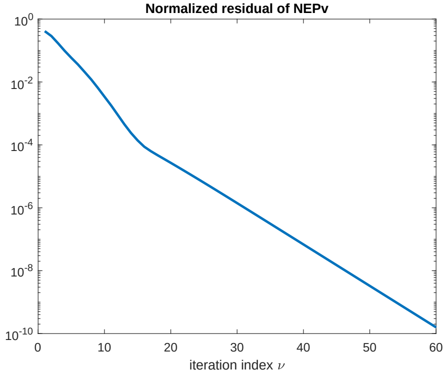
(i) $\{\mathcal{R}(X_{(\nu)})\}_{\nu=0}^{\infty}$ converges to $\mathcal{R}(X_*)$.

(ii) If also $\operatorname{rank}(X_*^{\mathrm{T}}D) = k$, then $\{X_{(\nu)}\}_{\nu=0}^{\infty}$ converges to X_*.

A random example for Algorithm 2

$$\eta(X) = \frac{\operatorname{tr}(X^{\mathrm{T}}D)}{\sqrt{\operatorname{tr}(X^{\mathrm{T}}AX)}}, \qquad \frac{\|E_{(\nu)}X_{(\nu)} - X_{(\nu)}\widehat{\Lambda}_{(\nu)}\|_2}{\|E_{(\nu)}\|_2}.$$





Earlier example with local minimizers

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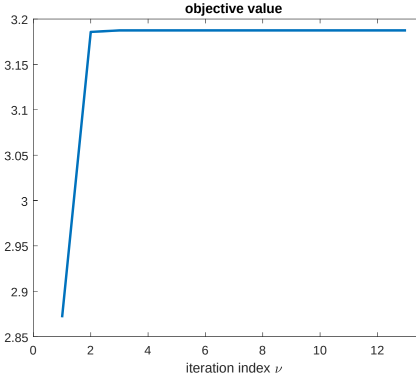

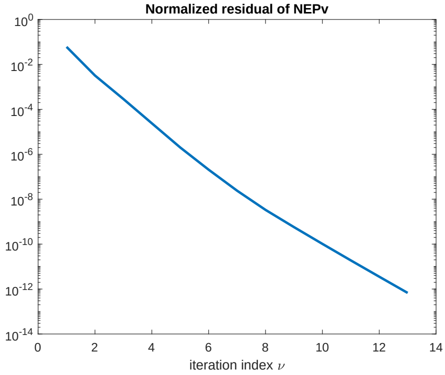

Digression: Compared to LDA

Fisher's linear discriminant analysis (LDA): given symmetric $B, A \in \mathbb{R}^{n\times n}$ and $A \succ 0$, solve

$$\max_{X\in\mathbb{O}^{n\times k}} \frac{\operatorname{tr}(X^{\mathrm{T}}BX)}{\operatorname{tr}(X^{\mathrm{T}}AX)}. \tag{12}$$

Equivalent to

$$H(X)X := \left(B - \frac{\operatorname{tr}(X^{\mathrm{T}}BX)}{\operatorname{tr}(X^{\mathrm{T}}AX)}A\right) = X(X^{\mathrm{T}}H(X)X) =: X\Lambda(X). \tag{13}$$

SCF:

$$H(X_{\nu-1})X_\nu = X_\nu\Lambda(X_\nu) \quad \text{for } \nu = 1, 2, \ldots \tag{14}$$

- (12) has global maximizers, but no local maximizer;
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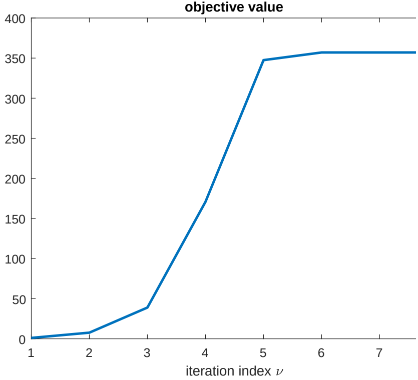

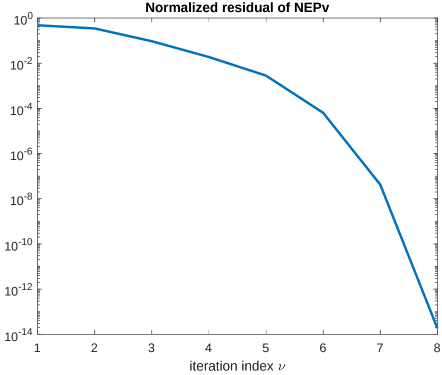

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Outline

Single-Vector Multiset CCA (MCCA)

Multiset CCA (MCCA) is to analyze linear relationships among more than two canonical variates, as a generalization of traditional two-view CCA.

Widely used model: Given ℓ datasets in the form of matrices

$$S_i \in \mathbb{R}^{n_i \times q} \quad \text{for } i = 1, 2, \ldots, \ell, \tag{15}$$

where n_i is the number of features in the ith view, and q is the number of sample data points.

Assume all S_i are centered, i.e., $S_i \mathbf{1}_q = 0$ for all i.

(Cross-)Covariance: $C_{i,j} = S_i S_j^{\mathrm{T}}$ for $i,\, j = 1, \ldots, \ell$. MCCA seeks to solve

$$\max_{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_\ell} \sum_{i,\, j=1}^{\ell} \boldsymbol{x}_i^{\mathrm{T}} C_{i,j} \boldsymbol{x}_j \quad \text{subject to} \begin{cases} \text{either} & \sum_{i=1}^{\ell} \boldsymbol{x}_i^{\mathrm{T}} C_{i,i} \boldsymbol{x}_i = 1, \\ \text{or} & \boldsymbol{x}_i^{\mathrm{T}} C_{i,i} \boldsymbol{x}_i = 1,\, i = 1, \ldots, \ell. \end{cases}$$

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Orthogonal Multiset CCA (OMCCA)

We seek Canonical Weight Matrices $X_i \in \mathbb{R}^{n_i \times k}$ that solve

$$\max_{\{X_i\}} f(\{X_i\}), \quad \text{s.t. } X_i^{\mathrm{T}} X_i = I_k,\ i = 1, \ldots, \ell, \tag{16}$$

where $1 \le k \le \min\{n_1, \ldots, n_\ell, q\}$, and

$$f(\{X_i\}) = \sum_{\substack{i,\, j=1 \\ i \ne j}}^{\ell} \rho_{ij} \frac{\mathrm{tr}(X_i^{\mathrm{T}} C_{i,j} X_j)}{\sqrt{\mathrm{tr}(X_i^{\mathrm{T}} C_{i,i} X_i)} \sqrt{\mathrm{tr}(X_j^{\mathrm{T}} C_{j,j} X_j)}}, \tag{17}$$

with some weighting factors $\rho_{ij} \ge 0$ that turn out to be extremely important.

- $\{\rho_{ij}\}$ dictate the contribution of the correlation between S_i and S_j to the total $f(\{X_i\})$;
- sparse $\{\rho_{ij}\}$ dramatically reduce the number terms in $f(\{X_i\})$ and thus speed up computations;
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It is known $0 \le \widehat{\rho}_{ij} \le 1$.

Envision a graph of ℓ nodes corresponding to dataset matrices X_i, respectively, with every two nodes connected with an edge whose weight ρ_{ij} to be determined.

Three heuristic strategies to select the weights $\rho_{ij} = \rho_{ji}$:

1. uniform weighting: use $\rho_{ij} = 1 \, \forall i,j$;
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2. tree weighting: find the minimal spanning tree of the graph with the same nodes but the edge (i, j) having weight $1 - \widehat{\rho}_{ij}$, and then let $\rho_{ij} = \widehat{\rho}_{ij}$ if the the edge (i, j) is on the tree and 0 otherwise.
3. top-p weighting: let $\widetilde{\rho}_{ij} = \widehat{\rho}_{ij}$ for the p largest $\widehat{\rho}_{ij}$ for $i > j$ and all other $\widetilde{\rho}_{ij} = 0$, and then apply the soft-max function to $\widetilde{\rho}_{ij}$ to yield ρ_{ij}.

SCF algorithm for OMCCA (1)

$$\max_{\{X_i\}} f(\{X_i\}), \quad \text{s.t. } X_i^{\mathrm{T}} C_{i,i} X_i = I_k,\ i = 1, \ldots, \ell,$$

where

$$f(\{X_i\}) = \sum_{\substack{i,\, j=1 \\ i \neq j}}^{\ell} \rho_{ij} \frac{\operatorname{tr}(X_i^{\mathrm{T}} C_{i,j} X_j)}{\sqrt{\operatorname{tr}(X_i^{\mathrm{T}} C_{i,i} X_i)} \sqrt{\operatorname{tr}(X_j^{\mathrm{T}} C_{j,j} X_j)}}.$$

Plan to optimize $f(\{X_i\})$ cyclically over each matrix variable X_i in the styles similar to either Jacobi or Gauss-Seidel updating for linear systems.

Specifically, an inner-outer iterative method:

- outer iteration – each step called a cycle – generates from the current approximation $\{X_i^{(\nu)}\}_{i=1}^{\ell}$ to the next $\{X_i^{(\nu+1)}\}_{i=1}^{\ell}$ of the maximizer of $f(\{X_i\})$;
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SCF algorithm for OMCCA (2)

Let the SVDs of S_i be ($r_i = \mathrm{rank}(S_i)$)

$$S_i = U_i \Sigma_i V_i^{\mathrm{T}},\ U_i \in \mathbb{R}^{n_i \times r_i},\ V_i \in \mathbb{R}^{q \times r_i},\ \Sigma_i \in \mathbb{R}^{r_i \times r_i}. \tag{19}$$

$$X_i^{\mathrm{T}} S_i S_j^{\mathrm{T}} X_j = X_i^{\mathrm{T}} U_i \Sigma_i V_i^{\mathrm{T}} V_j \Sigma_j U_j^{\mathrm{T}} X_j =: \widehat{X}_i^{\mathrm{T}} \Sigma_i V_i^{\mathrm{T}} V_j \Sigma_j \widehat{X}_j,$$

where $\widehat{X}_i = U_i^{\mathrm{T}} X_i \in \mathbb{R}^{r_i \times k}$. $X_i = U_i \widehat{X}_i$ by $\mathcal{R}(X_i) \subset \mathcal{R}(S_i)$.
The function $f(\{X_i\})$ is then transformed into

$$\sum_{i \neq j} \rho_{ij} \frac{\mathrm{tr}(\widehat{X}_i^{\mathrm{T}} \Sigma_i V_i^{\mathrm{T}} V_j \Sigma_j \widehat{X}_j)}{\sqrt{\mathrm{tr}(\widehat{X}_i^{\mathrm{T}} \Sigma_i^2 \widehat{X}_i)} \sqrt{\mathrm{tr}(\widehat{X}_j^{\mathrm{T}} \Sigma_j^2 \widehat{X}_j)}} =: g(\{\widehat{X}_i\}),$$

and, thus

$$\max_{X_i \in \mathbb{O}^{n_i \times k},\, \mathcal{R}(X_i) \subset \mathcal{R}(S_i),\ \forall i} f(\{X_i\}) = \max_{\widehat{X}_i \in \mathbb{O}^{r_i \times k},\, \forall i} g(\{\widehat{X}_i\}).$$

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SCF algorithm for OMCCA (3)

The key step to maximize $g(\{\widehat{X}_i\})$ by either the Jacobi- or Gauss-Seidel-style updating scheme is to maximize it, for any $s \in \{1, \cdots, \ell\}$, over $\widehat{X}_s$ while keeping all other $\widehat{X}_j$ for $j \neq s$ constant.

That is equivalent to

$$\max_{\widehat{X}_s \in \mathbb{O}^{n_s \times k}} \frac{\operatorname{tr}(\widehat{X}_s^{\mathrm{T}} D_s)}{\sqrt{\operatorname{tr}(\widehat{X}_s^{\mathrm{T}} \Sigma_s^2 \widehat{X}_s)}}, \tag{20}$$

where $D_s(\{\widehat{X}_i\}_{i\neq s}) = \Sigma_s V_s^{\mathrm{T}} \sum_{j\neq s} \rho_{sj} \frac{V_j \Sigma_j \widehat{X}_j}{\sqrt{\operatorname{tr}(\widehat{X}_j^{\mathrm{T}} \Sigma_j^2 \widehat{X}_j)}}$.

Problem (20) is equivalent to solving:

$$\max_{\widehat{X}_s \in \mathbb{O}^{n_s \times k}} \frac{\operatorname{tr}^2(\widehat{X}_s^{\mathrm{T}} D_s)}{\operatorname{tr}(\widehat{X}_s^{\mathrm{T}} \Sigma_s^2 \widehat{X}_s)}. \tag{21}$$

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Algorithm 3. RCOMCCA: Range Constrained OMCCA

Input: $\{S_i \in \mathbb{R}^{n_i \times q}\}$ (each S_i centered), integer k, and tolerance ϵ;
Output: $\{X_i \in \mathbb{O}^{n_i \times k}\}$ that maximizes $f(\{X_i\})$.

compute SVDs in (19);
pick an initial approximation $\widehat{X}_1^{(0)}$;
$\nu = 0$, $g = 0$;
repeat
  $g_0 = g$; $g = 0$;
  for $s = 1$ to ℓ **do**
    compute the next $\{\widehat{X}_s^{(\nu+1)}\}$ by solving (21), where either $D_s = D_s(\{\widehat{X}_i^{(\nu)}\}_{i \neq s})$ for Jacobi-style updating, or $D_s = D_s(\widehat{X}_1^{(\nu+1)}, \ldots, \widehat{X}_{s-1}^{(\nu+1)}, \widehat{X}_{s+1}^{(\nu)}, \ldots, \widehat{X}_\ell^{(\nu)})$ for Gauss-Seidel-style updating;
    $g = g + g_s$, where g_s is the computed optimal objective value of (21).
  end for
  $\nu = \nu + 1$;
until $|g - g_0| \leq \epsilon g$;
return $X_i = U_i \widehat{X}_i^{(\nu)}$ for $1 \leq i \leq \ell$.

Outline

1. Introduction to CCA
2. Orthogonal CCA (OCCA)
3. Submaximization Problem
4. Orthogonal Multiset CCA (OMCCA)
5. Applications
6. Summary

Application 1: Multi-label classification

Multi-class classification: assign an object (vector) $\boldsymbol{x}$ to one of n_c classes, often by attaching a label $y \in \{1, 2, \dots, n_c\}$.

Multi-label classification: assign an object (vector) $\boldsymbol{x}$ to one or more of n_c classes, often by attaching an indicator vector $\boldsymbol{y} \in \mathbb{R}^{n_c}$ of 0s and 1s in such a way that $\boldsymbol{x}$ belongs to class i if $\boldsymbol{y}_{(i)} = 1$ and doesn't otherwise.

$X \in \mathbb{R}^{n \times q}$ contains q vectors of size n, and $Y \in \mathbb{R}^{n_c \times q}$ consists of q corresponding indicator vectors. CCA for multi-label classification popularly treats X as one view and Y as the other.

We will use ML-kNN[1] as our backend multi-label classifier.

Table: Multi-label classification datasets

Dataset	Samples (q)	Attributes (n)	labels (n_c)
birds	645	260	19
emotions	593	72	6

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Table: Results on two datasets by 5 methods (40% for training and 60% for testing over 10 random splits). Best results are in bold.

dataset	method	OneError	Average_Precision
birds	OCCA-scf	**0.4964** $\pm$ **0.0201**	**0.5452** $\pm$ **0.0118**
	CCA	0.8110 $\pm$ 0.0302	0.3087 $\pm$ 0.0192
	LS-CCA	0.8110 $\pm$ 0.0302	0.3084 $\pm$ 0.0191
	OCCA-SSY	0.5978 $\pm$ 0.0269	0.4722 $\pm$ 0.0182
	ML-kNN	0.7101 $\pm$ 0.0136	0.3942 $\pm$ 0.0108
emotions	OCCA-scf	**0.3258** $\pm$ **0.0201**	**0.7640** $\pm$ **0.0118**
	CCA	0.3497 $\pm$ 0.0169	0.7443 $\pm$ 0.0126
	LS-CCA	0.3385 $\pm$ 0.0182	0.7553 $\pm$ 0.0154
	OCCA-SSY	0.3860 $\pm$ 0.0274	0.7190 $\pm$ 0.0172
	ML-kNN	0.3983 $\pm$ 0.0169	0.6960 $\pm$ 0.0085

- OneError: the average number of times the top-ranked label is not in the set of proper labels of the instance (the smaller the better)
- Average_Precision: the average precision of labels ranked above a particular label in the same label set. (the bigger the better)

Application 2: Multi-view feature extraction

1-nearest neighbor classifier for evaluating classification accuracy performance.

CCA methods with varying $k \in \{3, 4, 5, 6\}$ for `mfeat`, and $k \in \{3, 5, 10, 15, 20, 25, 30, 35, 40, 45, 50\}$ for other datasets.

Split data into training and testing with ratio 30/70. Results are based on the average of 10 randomly drawn splits.

Six variants of RCOMCCA in total based on different weighting rule. For the top-p weighting scheme, $p \in \{1, 3, 6\}$ is used, and best results are reported.

We compare with MCCA (Nielsen, 2002) and OMCCA-SS (Shen and Sun, 2015).

Table: Multi-view datasets

Dataset	Samples	Multiple views	classes
mfeat	2000	216;76;64;6;240;47	10
Caltech101-7	1474	254;512;1180;1008;64;1000	7
Caltech101-20	2386	254;512;1180;1008;64;1000	20

Table: Means and standard deviations of accuracy (Parameter k used by CCA methods to achieve the best accuracy is shown in the bracket).

	mfeat	Caltech101-7
view1	0.9513 ± 0.0053	0.9259 ± 0.0049
view2	0.7604 ± 0.0104	0.9443 ± 0.0051
view3	0.9293 ± 0.0043	0.9415 ± 0.0070
view4	0.6780 ± 0.0064	0.9287 ± 0.0105
view5	0.9630 ± 0.0025	0.7759 ± 0.0133
view6	0.7814 ± 0.0077	0.9152 ± 0.0059
MCCA	0.8679 ± 0.0073 (6)	0.8865 ± 0.0072 (15)
OMCCA-SS	0.8298 ± 0.0089 (6)	0.9493 ± 0.0024 (45)
RCOMCCA-G (uniform)	0.7634 ± 0.0134 (5)	0.8880 ± 0.0052 (50)
RCOMCCA-G (top-p)	$\mathbf{0.9696} \pm \mathbf{0.0035}$ (5)	$\mathbf{0.9664} \pm \mathbf{0.0060}$ (35)
RCOMCCA-G (tree)	0.9566 ± 0.0031 (6)	0.9392 ± 0.0043 (45)
RCOMCCA-J (uniform)	0.7540 ± 0.0121 (5)	0.8868 ± 0.0068 (30)
RCOMCCA-J (top-p)	0.9692 ± 0.0038 (5)	0.9649 ± 0.0029 (15)
RCOMCCA-J (tree)	0.9581 ± 0.0055 (6)	0.9474 ± 0.0041 (45)

Accuracy, CPU time and Training ratio

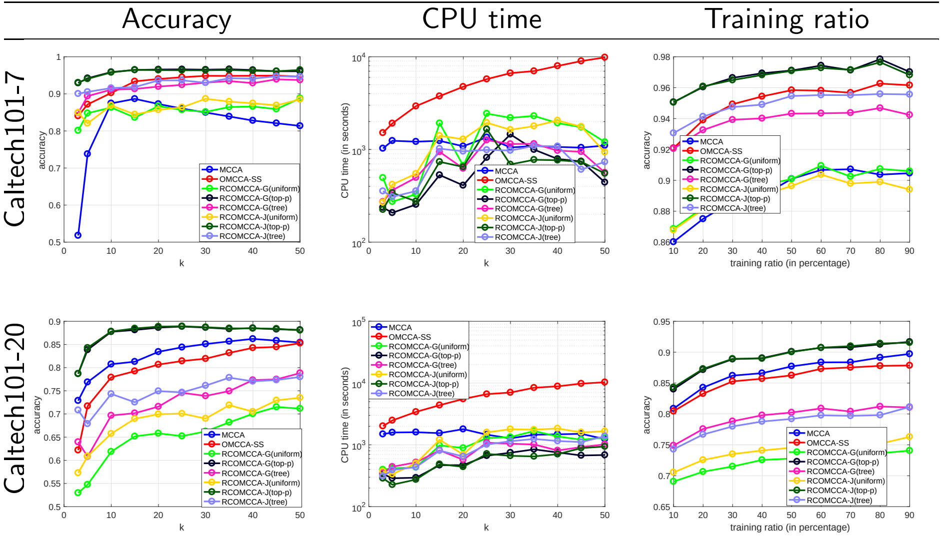

Figure: Accuracy and CPU time of MCCA methods on two datasets by varying the reduced dimension k and the training ratio.

Outline

Summary

- An OCCA-SCF algorithm for solving trace-fractional matrix optimization problem:

$$\max_{G\in\mathbb{O}^{n\times k}} \eta(G) \quad \text{with } \eta(G) := \frac{\operatorname{tr}(G^{\mathrm{T}}D)}{\sqrt{\operatorname{tr}(G^{\mathrm{T}}AG)}},$$

  where Stiefel manifold: $\mathbb{O}^{n\times k} = \{X \in \mathbb{R}^{n\times k} : X^{\mathrm{T}}X = I_k\}$.

- An alternating iterative method for solving Orthogonal Canonical Correlation Analysis (OCCA):

$$\max_{X\in\mathbb{O}^{n\times k},\, Y\in\mathbb{O}^{m\times k}} \frac{\operatorname{tr}(X^{\mathrm{T}}CY)}{\sqrt{\operatorname{tr}(X^{\mathrm{T}}AX)}\sqrt{\operatorname{tr}(Y^{\mathrm{T}}BY)}}.$$

- A new orthogonal multiset OCCA (OMCCA) model with integrated weights for each pair of views and trace-fractional objective for correlations between any two views.
- Applications to two real world applications: multi-label classification and multi-view feature extraction.

Related Reference

Leihong Zhang, Li Wang, Zhaojun Bai and Ren-Cang Li.
A Self-consistent-field Iteration for Orthogonal Canonical Correlation Analysis.
IEEE Transactions on Pattern Analysis and Machine Intelligence,
DOI: `10.1109/TPAMI.2020.3012541`, 2020.
(with a supplement of 13 pages for proofs)