The <u>Regularized Generalized Canonical</u> <u>Correlation Analysis (RGCCA) framework</u>

2025/04/10 @ Biopuces





Economic inequality and political instability Data from Russett (1964)

Economic inequality

Agricultural inequality

- **GINI :** Inequality of land distributions
- **FARM :** % farmers that own half of the land (> 50)
- **RENT :** % farmers that rent all their land

Industrial development

- **GNPR :** Gross national product per capita (\$ 1955)
- LABO : % of labor force employed in agriculture

Political instability

- **INST :** Instability of executive (45-61)
- ECKS : Nb of violent internal war incidents (46-61)
- **DEAT :** Nb of people killed as a result of civic group violence (50-62)
- **D-STAB :** Stable democracy
- **D-UNST :** Unstable democracy
- **DICT**: Dictatorship

Economic inequality and political instability (Data from Russett, 1964)



1 = Stable democracy

2 =Unstable democracy

3 = Dictatorship

Three data blocks

Path diagram

<u>Agricultural inequality</u> (\mathbf{X}_1)



Industrial development (\mathbf{X}_2)

<u>Political instability</u> (\mathbf{X}_3)

The philosophy of multiblock component methods



The philosophy of multiblock component methods



Block components should verify two properties at the same time:

- 1. Block components well explain their own block.
- 2. Block components are as correlated as possible for connected blocks.

Block components well explain their own block?

Principle of Principal Component Analysis(PCA)



Block components well explain their own block = find direction of high variance!

BLOCKS ARE PARTIALLY CONNECTED $c_{jk} = 1 \text{ if } \mathbf{X}_j \leftrightarrow \mathbf{X}_k, 0 \text{ otherwise}$ $\mathbf{X}_j \mathbf{X}_j \mathbf{X}_j$					
SUMCOR	$\max_{\operatorname{var}(\mathbf{X}_{j}\mathbf{w}_{j})=1} \sum_{j,k} c_{jk} \operatorname{cov}(\mathbf{X}_{j}\mathbf{w}_{j}, \mathbf{X}_{k}\mathbf{w}_{k})$				
SSQCOR	$\max_{\operatorname{var}(\mathbf{X}_{j}\mathbf{w}_{j})=1} \sum_{j,k} c_{jk} \operatorname{cov}^{2}(\mathbf{X}_{j}\mathbf{w}_{j}, \mathbf{X}_{k}\mathbf{w}_{k})$				
SABSCOR	$\max_{\operatorname{var}(\mathbf{X}_{j}\mathbf{w}_{j})=1} \sum_{j,k} \frac{c_{jk}}{c_{jk}} \operatorname{cov}(\mathbf{X}_{j}\mathbf{w}_{j}, \mathbf{X}_{k}\mathbf{w}_{k}) $				

RGCCA for multiblock analysis

$$\max_{\mathbf{w}_1,\ldots,\mathbf{w}_J} h(\mathbf{w}_1,\ldots,\mathbf{w}_J) = \sum_{j,k}^J c_{jk} g\left(\operatorname{cov}(\mathbf{X}_j \mathbf{w}_j, \mathbf{X}_k \mathbf{w}_k)\right)$$

s.t.
$$(1 - \tau_j)$$
var $(\mathbf{X}_j \mathbf{w}_j) + \tau_j \|\mathbf{w}_j\|_2^2 = 1, j = 1, ..., J$

•
$$c_{jk} = 1$$
 if $\mathbf{X}_j \leftrightarrow \mathbf{X}_k$, 0 otherwise

•
$$g =$$
 any convex function – e.g.
$$\begin{cases} g(x) = x & (\text{Horst sheme}) \\ g(x) = x^2 & (\text{Factorial scheme}) \\ g(x) = |x| & (\text{Centroid scheme}) \end{cases}$$

• $0 \le \tau_j \le 1$ continuum between correlation and covariance

Girka F, Camenen E, Caroline P, Gloaguen A, Guillemot V, Le Brusquet L, Tenenhaus A (2023): RGCCA Package. http://cran.project.org/web/packages/RGCCA/index.html

Tenenhaus A, Philippe C, Frouin V (2015) Kernel generalized canonical correlation analysis, Computational Statistics & Data Analysis, vol. 90, pp. 114-131. Tenenhaus A, Tenenhaus M (2011) Regularized generalized canonical correlation analysis, vol. 76, pp. 257-284, Psychometrika.

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RGCCA for multiblock analysis

$$\max_{\mathbf{w}_{1},...,\mathbf{w}_{J}} h(\mathbf{w}_{1},...,\mathbf{w}_{J}) = \sum_{j,k}^{J} c_{jk} g\left(\operatorname{cov}(\mathbf{X}_{j}\mathbf{w}_{j},\mathbf{X}_{k}\mathbf{w}_{k})\right)$$

s.t. $\mathbf{w}_{j}^{\mathsf{T}}\left((1-\tau_{j})n^{-1}\mathbf{X}_{j}^{\mathsf{T}}\mathbf{X}_{j} + \tau_{j}\mathbf{I}_{p_{j}}\right)\mathbf{w}_{j} = 1, j = 1, ..., J$

Two key ingredients:

(i) Block relaxation

(ii) Majorization by Minorization (MM)

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Block relaxation: from w^s to w^{s+1}

.

$$\mathbf{w}^{s} = \left(\mathbf{w}_{1}^{s}, \mathbf{w}_{2}^{s}, \dots, \mathbf{w}_{J}^{s}\right)$$

$$\underset{\mathbf{w}_{1},\mathbf{w}_{1}^{\mathsf{T}}\mathsf{M}_{1}\mathbf{w}_{1}=1}{\operatorname{argmax}} h(\mathbf{w}_{1},\mathbf{w}_{2}^{s},\ldots,\mathbf{w}_{J}^{s}) \longrightarrow \mathbf{w}_{1}^{s+1}$$

 $\rightarrow \mathbf{w}_2^{s+1}$



 $\rightarrow \mathbf{w}_{J}^{s+1}$



Primal/dual update for RGCCA

Primal update

$$\mathbf{w}_{j}^{s+1} = \frac{\left((1-\tau_{j})n^{-1}\mathbf{X}_{j}^{t}\mathbf{X}_{j}+\tau_{j}\mathbf{I}_{p_{j}}\right)^{-1}\mathbf{X}_{j}^{\mathsf{T}}\mathbf{z}_{j}^{s}}{\left(\mathbf{z}_{j}^{s^{\mathsf{T}}}\mathbf{X}_{j}\left((1-\tau_{j})n^{-1}\mathbf{X}_{j}^{t}\mathbf{X}_{j}+\tau_{j}\mathbf{I}_{p_{j}}\right)^{-1}\mathbf{X}_{j}^{\mathsf{T}}\mathbf{z}_{j}^{s}\right)^{1/2}}$$

Dual update



Properties of the RGCCA algorithm for multiblock data

► Monotone convergence: $h(\mathbf{w}_1^{s+1}, ..., \mathbf{w}_J^{s+1}) \ge h(\mathbf{w}_1^s, ..., \mathbf{w}_J^s)$.

In addition, assuming uniqueness of the solution of the MM step, the following properties hold:

- The sequence $\{\mathbf{w}^s\}$ is asymptotically regular: $\lim_{s\to\infty} ||\mathbf{w}^{s+1} \mathbf{w}^s|| = 0$.
- At convergence, a stationary point is obtained.

Tenenhaus M, Tenenhaus A, Groenen P.J.F, (2017) Regularized generalized canonical correlation analysis: A framework for sequential multiblock component methods, Psychometrika, doi: 10.1007/s11336-017-9573-x Girka F, Camenen E, Caroline P, Gloaguen A, Guillemot V, Le Brusquet L, Tenenhaus A (2023): RGCCA Package. http://cran.project.org/web/packages/RGCCA/index.html

RGCCA as a general framework for multiblock analysis

Methods	g(x)	$ au_j$ or s_j	С	Orthogonality
Canonical correlation analysis		$\tau_1 = \tau_2 = 0$		
сса				
Inter-battery factor analysis or		$\tau_1 = \tau_2 = 1$		
PLS regression				
ifa/pls				
sparse PLS regression		$\frac{1}{\sqrt{p_1}} < s_1 \le 1;$		
spls		$\frac{1}{\sqrt{22}} < s_2 \le 1$	(0 1)	
Redundancy analysis	x	$ \sqrt{p_2} \tau_2 = 0 $ $ \tau_1 = 1 \; ; \; au_2 = 0 $	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	Comp
ra				
Regularized redundancy		$0 \le \tau_1 \le 1$; $\tau_2 = 0$		
analysis				
rgcca				
Regularized canonical		$0 \le \tau_1 \le 1$;		
correlation analysis		$0 \le \tau_2 \le 1$		
rgcca			I	I

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RGCCA as a general framework for multiblock analysis

Methods	g(x)	$ au_{j}$	С	Orthogonality
SUMCOR sumcor SSQCOR ssqcor SABSCOR sabscor SUMCOV-1 sumcov-1 MAXBET maxbet SSQCOV-1 ssqcov-1 MAXBET-B maxbet-b SABSCOV-1 sabscov-1 SABSCOV-2 sabscov-2	$ x \\ x^{2} \\ x \\ x \\ x \\ x^{2} \\ x^{2} \\ x^{2} \\ x \\ x^{2} $	$\tau_j = 0$ $\tau_j = 0$ $\tau_j = 0$ $\tau_j = 1$ $\tau_j = 1$ $\tau_j = 1$ $\tau_j = 1$ $\tau_j = 1$ $\tau_j = 1$ $\tau_j = 1$	$ \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 1 & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 1 \\ 1 & \cdots & 1 & 1 \end{pmatrix} $	Comp Comp Comp Weight Comp Weight Comp Comp
SUMCOV-2 sumcov-2 MAXDIFF maxdiff SSQCOV-2 ssqcov-2 MAXDIFF-B maxdiff-b	$egin{array}{c} x \ x \ x^2 \ x^2 \ x^2 \end{array}$	$\tau_j = 1$ $\tau_j = 1$ $\tau_j = 1$ $\tau_j = 1$	$\begin{pmatrix} 0 & 1 & \cdots & 1 \\ 1 & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 1 \\ 1 & \cdots & 1 & 0 \end{pmatrix}$	Comp Weight Comp Weight
PLS path modeling - mode B rgcca DIABLO sgcca Regularized Generalized Canonical Correlation	x g g	$\tau_j = 0$ $\frac{1}{\sqrt{p_j}} \le s_j \le 1$ $0 \le \tau_j \le 1$	$c_{jk} \neq 0$ for two connected blocks	Comp Comp Comp/Weight
Analysis rgcca Sparse Generalized Canonical Correlation Analysis sgcca	g	$\frac{1}{\sqrt{p_j}} \le s_j \le 1$		Comp/Weight

The Russett dataset

<u>Agricultural inequality</u> (\mathbf{X}_1)



Industrial development (\mathbf{X}_2)

<u>Political instability</u> (\mathbf{X}_3)

RGCCA on Russett data Block-weight vectors with $\tau_i = 1$ and $g(x) = x^2$

 $\max_{\mathbf{w}_1, \mathbf{w}_2, \mathbf{w}_3} \operatorname{cov}^2(\mathbf{X}_1 \mathbf{w}_1, \mathbf{X}_3 \mathbf{w}_3) + \operatorname{cov}^2(\mathbf{X}_2 \mathbf{w}_2, \mathbf{X}_3 \mathbf{w}_3) \text{ s.t. } \|\mathbf{w}_j\| = 1, j = 1, 2, 3$



Block-weight vectors













Bootstrap sample #1









Bootstrap samle #2





Bootstrap sample #B



 \Rightarrow The weight is likely to be considered as significantly different from 0.

 \Rightarrow The weight is unlikely to be considered as significantly different from 0.

From these distributions, we can derive nonparametric confidence intervals $[q_{0.025}, q_{0.975}]$

Bootstrap confidence intervals





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Data vizualization



Greece: Colonels' dictatorship 1967-1974 Chili: Pinochet's military regime 1973-1990 Argentine: Military dictartorship 1976-1983 Brasil: Branco's military dictatorship 1964-1985

Higher-level block components

$$\mathbf{w}_{1}^{(1)}, \dots, \mathbf{w}_{J}^{(1)} = \operatorname*{argmax}_{\mathbf{w}_{1},\dots,\mathbf{w}_{J}} \sum_{j,k}^{J} c_{jk} g\left(\operatorname{cov}(\mathbf{X}_{j} \mathbf{w}_{j}, \mathbf{X}_{k} \mathbf{w}_{k})\right) \text{ s. t. } \mathbf{w}_{j}^{\top} \mathbf{M}_{j} \mathbf{w}_{j} = 1, j = 1, \dots, J$$

Higher level block components are obtained by considering the following optimization problem:

$$\mathbf{w}_{1}^{(2)}, \dots, \mathbf{w}_{J}^{(2)} = \underset{\mathbf{w}_{1}, \dots, \mathbf{w}_{J}}{\operatorname{argmax}} \sum_{j,k}^{J} c_{jk} g\left(\operatorname{cov}(\mathbf{X}_{j}\mathbf{w}_{j}, \mathbf{X}_{k}\mathbf{w}_{k})\right) \text{ s.t. } \begin{array}{l} \mathbf{w}_{j}^{\mathsf{T}}\mathbf{M}_{j}\mathbf{w}_{j} = 1, j = 1, \dots, J \\ \mathbf{y}_{j}^{(1)^{\mathsf{T}}}\mathbf{X}_{j}\mathbf{w}_{j} = 0, j = 1, \dots, J \end{array}$$
$$\Rightarrow \text{ Solved by deflation } \begin{array}{l} \mathbf{w}_{j}^{\mathsf{T}}\mathbf{M}_{j}\mathbf{w}_{j} = 1, j = 1, \dots, J \\ \mathbf{y}_{j}^{(1)^{\mathsf{T}}}\mathbf{X}_{j}\mathbf{w}_{j} = 0, j = 1, \dots, J \end{array}$$

Higher-level block components



Choice of the shrinkage constant : τ_j (analytical formula)

$$\max_{\mathbf{v}_{1},...,\mathbf{w}_{J}} h(\mathbf{w}_{1},...,\mathbf{w}_{J}) = \sum_{j,k}^{J} c_{jk} g\left(\operatorname{cov}(\mathbf{X}_{j}\mathbf{w}_{j},\mathbf{X}_{k}\mathbf{w}_{k})\right)$$
s.t.
$$\mathbf{w}_{j}^{\mathsf{T}}\left((1-\tau_{j})n^{-1}\mathbf{X}_{j}^{\mathsf{T}}\mathbf{X}_{j}+\tau_{j}\mathbf{I}_{p_{j}}\right)\mathbf{w}_{j} = 1, j = 1, ..., J$$

$$0 \qquad 1$$
Favoring correlation
$$\tau_{j} \qquad \operatorname{Favoring}_{\text{correlation}} \qquad \tau_{j} \qquad \operatorname{Favoring}_{\text{stability}}$$
Schäfer & Strimmer formula can be used for an optimal determination of the shrinkage constants





Permutation #1





Permutation #2











The best set of parameters is associated with the highest z-value

Determination of τ_i by permutation



Supervised RGCCA



Supervised RGCCA



Standard Cross-Validation (K-Fold, LOO) can be performed to tune hyperparameters.
Choice of the shrinkage parameter: τ_j (Cross-validation)

Leitmotiv: a good model should predict efficiently samples not used for its construction.











Model selection by cross validation: au^*



Model selection by cross-validation



Consensus space with RGCCA

The goal is to find jointly a global component **y** and block components $\mathbf{y}_1 = \mathbf{X}_1 \mathbf{w}_1, ..., \mathbf{y}_J = \mathbf{X}_J \mathbf{w}_J$.

• The global block component is obtained by considering the following optimization problem

$$\max_{\mathbf{w}_{1},...,\mathbf{w}_{J+1}} \sum_{j=1}^{J} g\left(\operatorname{cov}(\mathbf{X}_{j} \mathbf{w}_{j}, \mathbf{X}_{J+1} \mathbf{w}_{J+1}) \right) \text{ s. t. } \mathbf{w}_{j}^{\mathsf{T}} \mathbf{M}_{j} \mathbf{w}_{j} = 1 \text{ , } \forall j$$

• <u>Important result</u>: The optimal global component is obtained as linear combination of the variable of the so-called superblock defined as: $X_{J+1} = [X_1 | ... | X_J]$

RGCCA as a general framework for multiblock analysis

Methods	g(x)	$ au_{j}$	\mathbf{C}	Orthogonality
Generalized CCA	x^2	$\tau_j = 0, j = 1, \dots, J + 1$		Comp
gcca/maxvar/maxvar-b		2		
(mixed) Generalized CCA	x^2	$ au_j = 0, j = 1, \dots, J_1;$		Comp
rgcca		$\tau_j = 1, j = J_1 + 1, \dots, J$		
Multiple co-inertia	x^2	$ au_{j} = 1, j = 1, \dots, J$;	$(0 \cdots 0 1)$	Weight
analysis mcoa/mcia		$\tau_{J+1} = 0$		
Multiple factor analysis	x^2	$\tau_j = 1, j = 1, \dots, J + 1$:	Comp
mfa		-	$0 \cdots 0 1$	
Consensus PCA(1)	x	$ au_j = 1, j = 1, \dots, J;$	$\begin{pmatrix} 1 & \cdots & 1 & 0 \end{pmatrix}$	Comp
cpca-1		$\tau_{J+1} = 0$		
Consensus PCA(2)	x^2	$ au_j = 1, j = 1, \dots, J;$		Comp
cpca-2/maxvar-a		$\tau_{J+1} = 0$		
Hierarchical PCA	x^4	$ au_j = 1, j = 1, \ldots, J$;		Comp
hpca/cpca-4		$\tau_{J+1} = 0$		

Consensus space of Russett (sample plot)



Consensus space of Russett (correlation circle)



Consensus space of Russett (biplot)





Glioma Cancer Data: from an RGCCA viewpoint

(Department of Pediatric Oncology of the Gustave Roussy Institute)

RGCCA with factorial scheme - $\tau_1 = 1$, $\tau_2 = 1$ and $\tau_3 = 0$



High dimensional block settings \Rightarrow dual algorithm for RGCCA



Multiblock component methods with sparsity



Block components should verified three properties at the same time:

- 1. Block components well explain their own block.
- 2. Block components are as correlated as possible for connected blocks.
- 3. Block components are built from sparse w_j

RGCCA for multiblock analysis

$$\max_{\mathbf{w}_{1},...,\mathbf{w}_{J}} \sum_{j,k}^{J} c_{jk} g\left(\operatorname{cov}(\mathbf{X}_{j} \mathbf{w}_{j}, \mathbf{X}_{k} \mathbf{w}_{k})\right)$$

s.t. $\left\|\mathbf{w}_{j}\right\|_{2}^{2} = 1 \quad \& \quad \left\|\mathbf{w}_{j}\right\|_{1} \leq s_{j} = 1, ..., J$

Tenenhaus A., Philippe C., Guillemot V, et al..(2014). Variable Selection for Generalized Canonical Correlation Analysis, Biostatistics, 15 (3): 569-583 Tenenhaus A. and Guillemot V. (2017): RGCCA Package. <u>http://cran.project.org/web/packages/RGCCA/index.html</u>

Block components

 $\mathbf{y}_1 = \mathbf{X}_1 \mathbf{w}_1 = w_{11} \mathbf{Gene}_1 + \dots + w_{1,15201} \mathbf{Gene}_{15201}$

$$\mathbf{y}_2 = \mathbf{X}_2 \mathbf{w}_2 = w_{21} \mathbf{C} \mathbf{G} \mathbf{H}_1 + \dots + w_{2,1909} \mathbf{C} \mathbf{G} \mathbf{H}_{1909}$$

$$\mathbf{y}_3 = \mathbf{X}_3 \mathbf{w}_3 = w_{31}$$
Hemisphere + w_{32} DIPG

Block components should verify three properties at the same time:

- (i) Block components explain their block well.
- (ii) Block components are as correlated as possible for connected blocks.

(iii) Block components are built from sparse w_j

Block relaxation: from w^s to w^{s+1}



THE CORNER: SGCCA ON GLIOMA DATA



High dimensional block settings \Rightarrow sparse GCCA





How to handle multiway data in RGCCA





The COMA project

(Brain and Spine Institute, La pitié Salpêtrière Hospital)



COMA project

Contribution of the voxels and the modalities to predict the long term recovery of patients after traumatic brain injury can be studied separately.



Discriminating voxels within the white matter bundles

Influence of spatial positions: \mathbf{w}_1^K

Modality	\mathbf{w}_1^K
FA	0.9887
MD	0.0036
\mathbf{L}_{1}	0.0046
L _t	0.0031

MGCCA optimization problem



Block relaxation: from w^s to w^{s+1}

$$\begin{split} \mathbf{w}^{s} &= \left(\mathbf{w}_{1}^{s}, \mathbf{w}_{2}^{s}, ..., \mathbf{w}_{j}^{s}\right) \qquad \underset{\|\mathbf{w}_{1}\|_{2}=1 \& \|\mathbf{w}_{1}\|_{2} \leq s_{1}}{\operatorname{argmax}} h\left(\mathbf{w}_{1}, \mathbf{w}_{2}^{s}, ..., \mathbf{w}_{j}^{s}\right) \qquad \longrightarrow \mathbf{w}_{1}^{s+1} \\ &\underset{\|\mathbf{w}_{2}\|_{2}=1 \& \|\mathbf{w}_{2}\|_{1} \leq s_{2}}{\operatorname{argmax}} h\left(\mathbf{w}_{1}^{s+1}, \mathbf{w}_{2}, \mathbf{w}_{3}^{s}, ..., \mathbf{w}_{j}^{s}\right) \qquad \longrightarrow \mathbf{w}_{2}^{s+1} \\ &\underset{\|\mathbf{w}_{j}\|_{2}=1 \& \|\mathbf{w}_{j}\|_{1} \leq s_{j}}{\operatorname{argmax}} h\left(\mathbf{w}_{1}^{s+1}, ..., \mathbf{w}_{j-1}^{s+1}, \mathbf{w}_{j}, \mathbf{w}_{j+1}^{s}, ..., \mathbf{w}_{j}^{s}\right) \qquad \longrightarrow \mathbf{w}_{j}^{s+1} \\ &\underset{\|\mathbf{w}_{j}\|_{2}=1 \& \|\mathbf{w}_{j}\|_{1} \leq s_{j}}{\operatorname{argmax}} h\left(\mathbf{w}_{1}^{s+1}, ..., \mathbf{w}_{j-1}^{s+1}, \mathbf{w}_{j}\right) \qquad \longrightarrow \mathbf{w}_{j}^{s+1} \\ &\underset{\|\mathbf{w}_{j}\|_{2}=1 \& \|\mathbf{w}_{j}\|_{1} \leq s_{j}}{\operatorname{argmax}} h\left(\mathbf{w}_{1}^{s+1}, ..., \mathbf{w}_{j-1}^{s+1}, \mathbf{w}_{j}\right) \qquad \longrightarrow \mathbf{w}_{j}^{s+1} \\ &\underset{\|\mathbf{w}_{j}\|_{2}=1 \& \|\mathbf{w}_{j}\|_{1} \leq s_{j}}{\operatorname{argmax}} h\left(\mathbf{w}_{1}^{s+1}, ..., \mathbf{w}_{j-1}^{s+1}, \mathbf{w}_{j}\right) \qquad \longrightarrow \mathbf{w}_{j}^{s+1} \\ &\underset{\|\mathbf{w}_{j}\|_{2}=1 \& \|\mathbf{w}_{j}\|_{1} \leq s_{j}}{\operatorname{argmax}} h\left(\mathbf{w}_{1}^{s+1}, ..., \mathbf{w}_{j-1}^{s+1}, \mathbf{w}_{j}\right) \qquad \longrightarrow \mathbf{w}_{j}^{s+1} \\ &\underset{\|\mathbf{w}_{j}\|_{2}=1 \& \|\mathbf{w}_{j}\|_{1} \leq s_{j}}{\operatorname{argmax}} h\left(\mathbf{w}_{1}^{s+1}, ..., \mathbf{w}_{j-1}^{s+1}, \mathbf{w}_{j}\right) \qquad \longrightarrow \mathbf{w}_{j}^{s+1} \\ &\underset{\|\mathbf{w}_{j}\|_{2}=1 \& \|\mathbf{w}_{j}\|_{1} \leq s_{j}}{\operatorname{argmax}} h\left(\mathbf{w}_{1}^{s+1}, ..., \mathbf{w}_{j-1}^{s+1}, \mathbf{w}_{j}\right) \qquad \longrightarrow \mathbf{w}_{j}^{s+1} \\ &\underset{\|\mathbf{w}_{j}\|_{2}=1 \& \mathbf{w}_{j}\|_{1} \leq s_{j}}{\operatorname{argmax}} h\left(\mathbf{w}_{1}^{s+1}, ..., \mathbf{w}_{j-1}^{s+1}, \mathbf{w}_{j}\right) \qquad \longrightarrow \mathbf{w}_{j}^{s+1} \\ &\underset{\|\mathbf{w}_{j}\|_{2}=1 \& \mathbf{w}_{j}\|_{1} \leq s_{j}}{\operatorname{argmax}} h\left(\mathbf{w}_{1}^{s+1}, ..., \mathbf{w}_{j-1}^{s+1}, \mathbf{w}_{j}\right) \qquad \longrightarrow \mathbf{w}_{j}^{s+1} \\ &\underset{\|\mathbf{w}_{j}\|_{2}=1 \& \mathbf{w}_{j}\|_{1} \leq s_{j}}{\operatorname{argmax}} h\left(\mathbf{w}_{j}\|_{1} \leq s_{j}\right) \qquad \longrightarrow \mathbf{w}_{j}^{s+1} \\ &\underset{\|\mathbf{w}_{j}\|_{2}=1 \& \mathbf{w}_{j}\|_{1} \leq s_{j}}{\operatorname{argmax}} h\left(\mathbf{w}_{j}\|_{1} \leq s_{j}\right) \qquad \longrightarrow \mathbf{w}_{j}^{s+1} \\ &\underset{\|\mathbf{w}_{j}\|_{2}=1 \& \mathbf{w}_{j}\|_{1} \leq s_{j}}{\operatorname{argmax}} h\left(\mathbf{w}_{j}\|_{1} \leq s_{j}\right) \end{cases}$$

$$\mathbf{w}_j^{S+1} = \mathbf{w}_j^K \otimes \mathbf{w}_j^J$$

where \mathbf{w}_{j}^{K} and \mathbf{w}_{j}^{J} are obtained as the first left and right singular vector of a certain matrix of dimension $K_{j} \times J_{j}$

$$\mathbf{w}^{s+1} = \left(\mathbf{w}_1^{s+1}, \mathbf{w}_2^{s+1}, \dots, \mathbf{w}_J^{s+1}\right)$$

Consensus space with RGCCA

$$\max_{\mathbf{w}_{1},\ldots,\mathbf{w}_{J+1}}\sum_{j=1}^{J}\left(\operatorname{cov}(\mathbf{X}_{j}\mathbf{w}_{j},\mathbf{X}_{J+1}\mathbf{w}_{J+1})\right)^{m} \text{ s. t. } \mathbf{w}_{j}^{\mathsf{T}}\mathbf{M}_{j}\mathbf{w}_{j}=1, \forall j$$

The superblock component \mathbf{y}_{J+1} is proportional to:

$$\mathbf{y}_{J+1} \propto \mathbf{X}_{J+1} \mathbf{M}_{J+1}^{-1} \mathbf{X}_{J+1}^{\top} \sum_{j=1}^{J} \left(\operatorname{cov}(\mathbf{y}_{j}, \mathbf{y}_{J+1}) \right)^{m-1} \mathbf{y}_{j}$$
When $\mathbf{M}_{J+1} = n^{-1} \mathbf{X}_{J+1}^{\top} \mathbf{X}_{J+1}$, it reduces to
$$\mathbf{y}_{J+1} \propto \sum_{j=1}^{J} \left(\operatorname{cov}(\mathbf{y}_{j}, \mathbf{y}_{J+1}) \right)^{m-1} \mathbf{y}_{j} \qquad \text{weighted sums of block components}$$

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Consensus space with RGCCA

$$\max_{\mathbf{w}_{1},\dots,\mathbf{w}_{J}} \sum_{j=1}^{J} \operatorname{cov}(\mathbf{X}_{j}\mathbf{w}_{j}, \mathbf{X}_{J+1}\mathbf{w}_{J+1})^{m} \quad \text{s.t.} \begin{cases} \|\mathbf{w}_{j}\| = \dots = \|\mathbf{w}_{J}\| = 1\\ \operatorname{var}(\mathbf{X}_{J+1}\mathbf{w}_{J+1}) = 1 \end{cases}$$
$$m = 1 \qquad m = 2 \qquad m = 4\\ \mathbf{y}_{J+1} \propto \sum_{j=1}^{J} \mathbf{y}_{j} \qquad \mathbf{y}_{J+1} \propto \sum_{j=1}^{J} \operatorname{cov}(\mathbf{y}_{j}, \mathbf{y}_{J+1}) \mathbf{y}_{j} \qquad \mathbf{y}_{J+1} \propto \sum_{j=1}^{J} \operatorname{cov}(\mathbf{y}_{j}, \mathbf{y}_{J+1})^{2} \mathbf{y}_{j}$$

Fairness and block selection behavior

Will a solution be accepted as a good one even if it is dominated by only a few of the J sets, ignoring the other sets? Or do we require that all J sets have equal share in the solution? (Van de Geer, 1984)

The stationary equations of CPCA(m) give some information:

$$\mathbf{y}_{J+1} \propto \mathbf{X}_{J+1} \mathbf{M}_{J+1}^{-1} \mathbf{X}_{J+1}^{\mathsf{T}} \sum_{j=1}^{J} \left(\operatorname{cov}(\mathbf{y}_{j}, \mathbf{y}_{J+1}) \right)^{m-1} \mathbf{y}_{j}$$
 weighted sums of block components

The influence of the various blocks \mathbf{X}_j on the solution is related to the scale of the block component \mathbf{y}_k and to the weights $\operatorname{cov}(\mathbf{y}_j, \mathbf{y}_{J+1})^{m-1}$.

Fairness and block selection behavior

weighted sums of block components

$$\mathbf{y}_{J+1} \propto \mathbf{X}_{J+1} \mathbf{M}_{J+1}^{-1} \mathbf{X}_{J+1}^{\mathsf{T}} \sum_{j=1}^{J} \left(\operatorname{cov}(\mathbf{y}_{j}, \mathbf{y}_{J+1}) \right)^{m-1} \mathbf{y}_{j} \checkmark$$

► Methods with equal block component scales are fairer than methods with unequal block component scales

 \Rightarrow Correlation-based methods are fairer than covariancebased methods

Methods with equal weights are fairer than methods with unequal weights.

 \Rightarrow Using g(x) = x or g(x) = |x| scheme functions lead to fair methods. Block selection behavior is favored by using the scheme function $g(x) = x^m$ where *m* is a positive even integer.

The core optimization of sGCCA

Proposition. Consider the optimization problem

$$\max_{\mathbf{w}_{j}} \frac{1}{n} \mathbf{w}_{j}^{\mathsf{T}} \mathbf{X}_{j}^{\mathsf{T}} \mathbf{z}_{j} \quad \text{subject to} \quad \left\| \mathbf{w}_{j} \right\|_{2} = 1 \& \left\| \mathbf{w}_{j} \right\|_{1} \le s_{j}$$

The solution satisfies $\mathbf{w}_j = \frac{S(\frac{1}{n}\mathbf{X}_j^{\mathsf{T}}\mathbf{z}_j,\lambda_j)}{\|S(\frac{1}{n}\mathbf{X}_j^{\mathsf{T}}\mathbf{z}_j,\lambda_j)\|_2}$, with S corresponds to soft-thresholding operator and $\lambda_j = 0$ if this results in $\|\mathbf{w}_j\|_1 \le s_j$; otherwise, s_j is chosen so that $\|\mathbf{u}_1\|_1 = s_j$.

Proof. (with subgradient)

First, we rewrite the optimization problem using Lagrange multipliers:

$$\mathcal{L} = \frac{1}{n} \mathbf{w}_j^{\mathsf{T}} \mathbf{X}_j^{\mathsf{T}} \mathbf{z}_j - \lambda_2 \left(\left\| \mathbf{w}_j \right\|_2^2 - 1 \right) - \lambda_1 \left(\left\| \mathbf{w}_j \right\|_1 - s_j \right)$$

The core optimization of sGCCA

Considering the partial subgradient of the Lagrangian function with respect to \mathbf{w}_i yields :

$$\partial_{\mathbf{w}_j} \mathcal{L} = \frac{1}{n} \mathbf{X}_j^{\mathsf{T}} \mathbf{z}_j - 2\lambda_{2j} \mathbf{w}_j - \lambda_{1j} \mathbf{\gamma}_j, \qquad j = 1, \dots, J$$

where the kth element γ_{jk} of $\mathbf{\gamma}_j$ is the subgradient of $\sum_{k=1}^{p_j} |w_{jk}|$ with respect to w_{jk} , defined as:

$$\gamma_{jk} = \begin{cases} \operatorname{sign}(w_{jk}) \text{ if } w_{jk} \neq 0\\ [-1;1] \quad \text{ if } w_{jk} = 0 \end{cases}$$

Therefore, we obtain:

$$\partial_{w_{jk}} \mathcal{L} = \begin{cases} \frac{1}{n} \mathbf{x}_{jk}^{\mathsf{T}} \mathbf{z}_j - 2\lambda_{2j} w_{jk} - \lambda_{1j} \operatorname{sign}(w_{jk}) & \text{if } w_{jk} \neq 0 \\ \\ \left[\frac{1}{n} \mathbf{x}_{jk}^{\mathsf{T}} \mathbf{z}_j - \lambda_{1j}; \frac{1}{n} \mathbf{x}_{jk}^{\mathsf{T}} \mathbf{z}_j + \lambda_{1j} \right] & \text{if } w_{jk} = 0 \end{cases}$$

The core optimization of sGCCA

$$\partial_{w_{jk}} \mathcal{L} = \begin{cases} \frac{1}{n} \mathbf{x}_{jk}^{\mathsf{T}} \mathbf{z}_j - 2\lambda_{2j} w_{jk} - \lambda_{1j} \operatorname{sign}(w_{jk}) & \text{if } w_{jk} \neq 0 \\ \\ \left[\frac{1}{n} \mathbf{x}_{jk}^{\mathsf{T}} \mathbf{z}_j - \lambda_{1j}; \frac{1}{n} \mathbf{x}_{jk}^{\mathsf{T}} \mathbf{z}_j + \lambda_{1j} \right] & \text{if } w_{jk} = 0 \end{cases}$$

At the optimum, we must have $0 \in \partial_{\mathbf{w}_j} \mathcal{L}$ and we get:

$$\begin{cases} \frac{1}{n} \mathbf{x}_{jk}^{\mathsf{T}} \mathbf{z}_j - 2\lambda_{2j} w_{jk} - \lambda_{1j} \operatorname{sign}(w_{jk}) = 0 & \text{if } w_{jk} \neq 0 \\ \\ \left| \frac{1}{n} \mathbf{x}_{jk}^{\mathsf{T}} \mathbf{z}_j \right| < \lambda_{1j} & \text{if } w_{jk} = 0 \end{cases}$$
The core optimization of sGCCA

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$$\begin{cases} \frac{1}{n} \mathbf{x}_{jk}^{\mathsf{T}} \mathbf{z}_{j} - 2\lambda_{2j} w_{jk} - \lambda_{1j} \operatorname{sign}(w_{jk}) = 0 & \text{if } w_{jk} \neq 0 \\ \\ \left| \frac{1}{n} \mathbf{x}_{jk}^{\mathsf{T}} \mathbf{z}_{j} \right| < \lambda_{1j} & \text{if } w_{jk} = 0 \end{cases}$$

From sign $\left(\frac{1}{n}\mathbf{x}_{jk}^{\mathsf{T}}\mathbf{z}_{j}\right) = \operatorname{sign}(w_{jk})$ $w_{jk} = \begin{cases} \frac{1}{2\lambda_{2j}} \left(\frac{1}{n} \mathbf{x}_{jk}^{\mathsf{T}} \mathbf{z}_j - \lambda_{1j} \operatorname{sign} \left(\frac{1}{n} \mathbf{x}_{jk}^{\mathsf{T}} \mathbf{z}_j \right) \right) & \text{if } w_{jk} \neq 0 \\ \\ 0 & \text{if } \left| \frac{1}{n} \mathbf{x}_{jk}^{\mathsf{T}} \mathbf{z}_j \right| < \lambda_{1j} \end{cases}$ $w_{jk} = \begin{cases} \frac{1}{2\lambda_{2j}} \operatorname{sign}\left(\frac{1}{n} \mathbf{x}_{jk}^{\mathsf{T}} \mathbf{z}_{j}\right) \left(\left|\frac{1}{n} \mathbf{x}_{jk}^{\mathsf{T}} \mathbf{z}_{j}\right| - \lambda_{1j}\right) & \text{if } w_{jk} \neq 0\\\\ 0 & \text{if } \left|\frac{1}{n} \mathbf{x}_{jk}^{\mathsf{T}} \mathbf{z}_{j}\right| < \lambda_{1j} \end{cases}$

The core optimization of sGCCA

$$w_{jk} = \begin{cases} \frac{1}{2\lambda_{2j}} \operatorname{sign}\left(\frac{1}{n} \mathbf{x}_{jk}^{\mathsf{T}} \mathbf{z}_{j}\right) \left(\left|\frac{1}{n} \mathbf{x}_{jk}^{\mathsf{T}} \mathbf{z}_{j}\right| - \lambda_{1j}\right) & \text{if } w_{jk} \neq 0\\\\0 & \text{if } \left|\frac{1}{n} \mathbf{x}_{jk}^{\mathsf{T}} \mathbf{z}_{j}\right| < \lambda_{1j} \end{cases}$$

$$w_{jk} = \frac{1}{2\lambda_{2j}} \operatorname{sign}\left(\frac{1}{n} \mathbf{x}_{jk}^{\mathsf{T}} \mathbf{z}_{j}\right) \max\left(0, \left|\frac{1}{n} \mathbf{x}_{jk}^{\mathsf{T}} \mathbf{z}_{j}\right| - \lambda_{1j}\right)$$

where λ_{1j} is chosen such that $\|\mathbf{w}_j\|_1 = s_j$ (e.g. binary search) and λ_2 such that $\|\mathbf{w}_j\|_2 = 1$.

$$\mathbf{w}_{j} = \frac{\mathcal{S}\left(\frac{1}{n}\mathbf{X}_{j}^{\mathsf{T}}\mathbf{z}_{j}, \lambda_{1j}\right)}{\left\|\mathcal{S}\left(\frac{1}{n}\mathbf{X}_{j}^{\mathsf{T}}\mathbf{z}_{j}, \lambda_{1j}\right)\right\|_{2}}, \qquad j = 1, \dots, J$$