Recent advances on Regularized Generalized Canonical Correlation Analysis

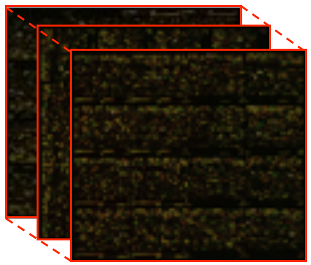
Arthur Tenenhaus

2013/05/16

Glioma Cancer Data

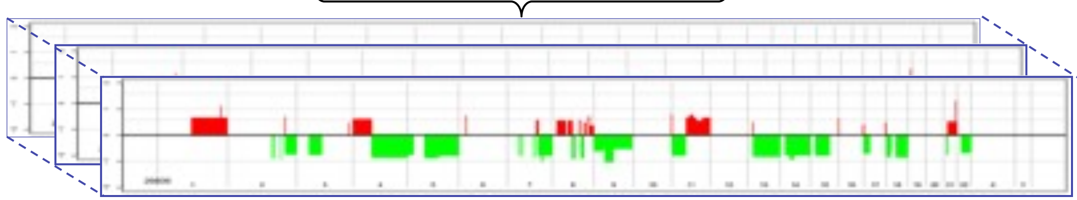
(Department of Pediatric Oncology of the Gustave Roussy Institute)

Transcriptomic data (X_1)



outcome (X_3)

	Gene 1	Gene 2	…	Gene 15201	CGH1	…	CGH 1909	Localization
Patient 1	0.18	-0.21		-0.73	0.00		-0.55	Hemisphere
Patient 2	1.15	-0.45		0.27	-0.30		0.00	Midline
Patient 3	1.35	0.17		0.22	0.33		0.64	DIPG
⋮								
⋮								
Patient 53	1.39	0.18	…	-0.17	0.00	…	0.43	Hemisphere

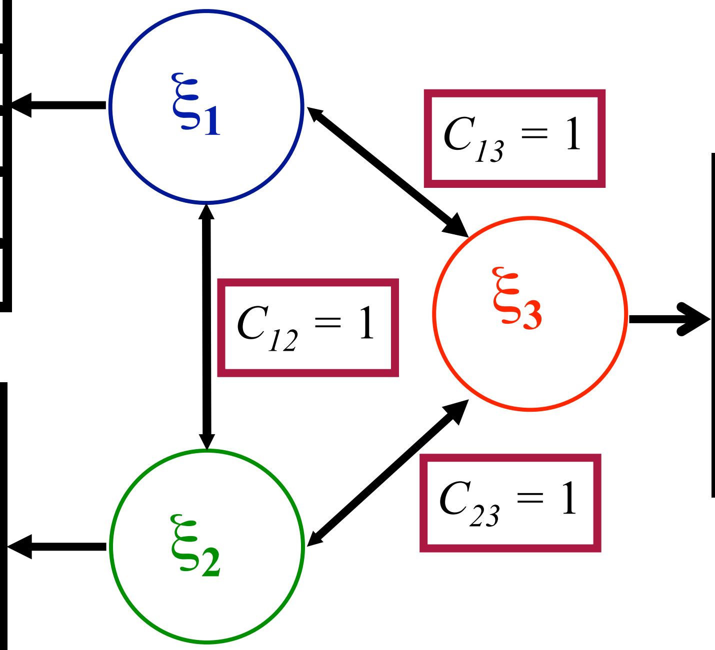


CGH data (X_2)

Glioma Cancer Data: from a multi-block viewpoint

(Department of Pediatric Oncology of the Gustave Roussy Institute)

	Gene 1	…	Gene 15201
Patient 1	0.18		-0.73
Patient 2	1.15		0.27
Patient 3	1.35		0.22
⋮			
Patient 53	1.39		-0.17



	Hemisphere	DIPG
Patient 1	1	0
Patient 2	0	0
Patient 3	0	1
⋮		
Patient 53	1	0

	CGH1	…	CGH 1909
Patient 1	0.00		-0.55
Patient 2	-0.30		0.00
Patient 3	0.33		0.64
⋮			
Patient 53	0.00		0.43

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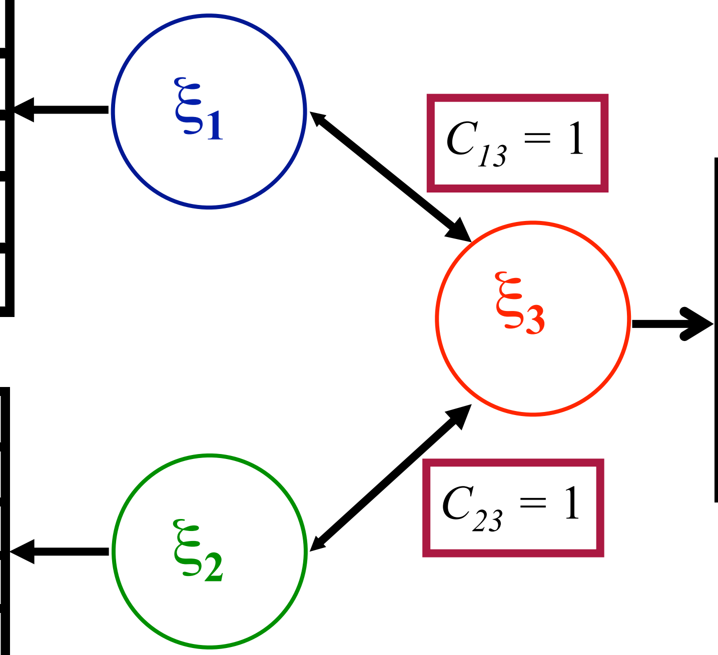

	Hemisphere	DIPG
Patient 1	1	0
Patient 2	0	0
Patient 3	0	1
⋮		
Patient 53	1	0

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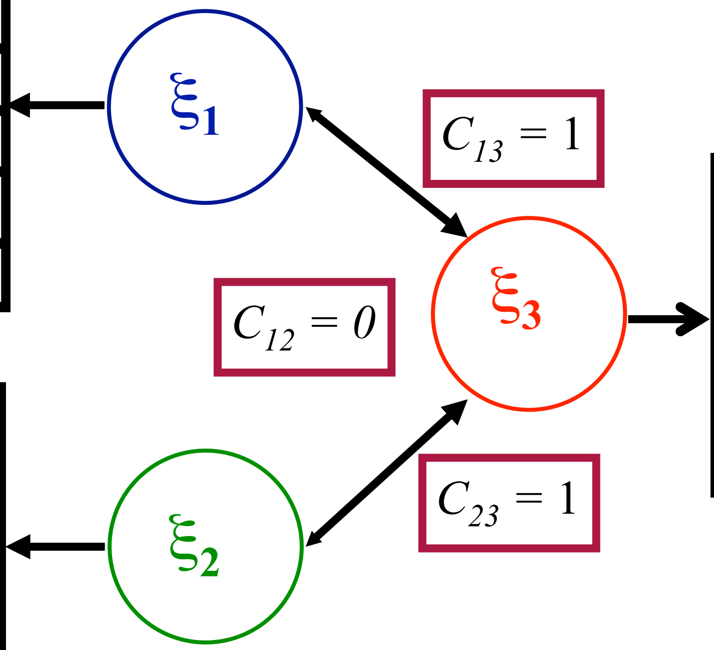

	Hemisphere	DIPG
Patient 1	1	0
Patient 2	0	0
Patient 3	0	1
⋮		
Patient 53	1	0

Block components

$$\mathbf{y}_1 = \mathbf{X}_1\mathbf{a}_1 = a_{11}\mathbf{Gene}_1 + \cdots + a_{1,15201}\mathbf{Gene}_{15201}$$

$$\mathbf{y}_2 = \mathbf{X}_2\mathbf{a}_2 = a_{21}\mathbf{CGH}_1 + \cdots + a_{2,1909}\mathbf{CGH}_{1909}$$

$$\mathbf{y}_3 = \mathbf{X}_3\mathbf{a}_3 = a_{31}\mathbf{Hemisphere} + a_{32}\mathbf{DIPG}$$

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$$\mathbf{y}_1 = \mathbf{X}_1\mathbf{a}_1 = a_{11}\mathbf{Gene}_1 + \cdots + a_{1,15201}\mathbf{Gene}_{15201}$$

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$$\mathbf{y}_3 = \mathbf{X}_3\mathbf{a}_3 = a_{31}\mathbf{Hemisphere} + a_{32}\mathbf{DIPG}$$

Block components should verified two properties at the same time:

(i) Block components well explain their own block.

(ii) Block components are as correlated as possible for connected blocks.

Some multi-block methods

SUMCOR (Horst, 1961) $\text{maximize} \sum_{j,k} \text{cor}(\mathbf{X_j a_j}, \mathbf{X_k a_k})$

SSQCOR (Mathes, 1993 ; Hanafi, 2004) $\text{maximize} \sum_{j,k} \text{cor}^2(\mathbf{X_j a_j}, \mathbf{X_k a_k})$

SABSCOR (Mathes, 1993 ; Hanafi, 2004) $\text{maximize} \sum_{j,k} |\text{cor}(\mathbf{X_j a_j}, \mathbf{X_k a_k})|$

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SABSCOR (Mathes, 1993 ; Hanafi, 2004)	$\text{maximize} \sum_{j,k} \lvert\text{cor}(\mathbf{X_j a_j}, \mathbf{X_k a_k})\rvert$
SUMCOV (Van de Geer, 1984)	$\underset{\text{all } \lVert a_j \rVert = 1}{\text{maximize}} \sum_{j,k} \text{cov}(\mathbf{X_j a_j}, \mathbf{X_k a_k})$
SSQCOV (Hanafi & Kiers, 2006)	$\underset{\text{all } \lVert a_j \rVert = 1}{\text{maximize}} \sum_{j,k} \text{cov}^2(\mathbf{X_j a_j}, \mathbf{X_k a_k})$
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$\text{cov}^2(\mathbf{X_j a_j}, \mathbf{X_k a_k}) = \text{var}(\mathbf{X_j a_j})\text{cor}^2(\mathbf{X_j a_j}, \mathbf{X_k a_k})\text{var}(\mathbf{X_j a_j})$

Some modified multi-block methods

$c_{jk} = 1$ if blocks are linked, 0 otherwise and $c_{jj} = 0$

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GENERALIZED CANONICAL CORRELATION ANALYSIS

$\sum_{j,k}$

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GENERALIZED CANONICAL COVARIANCE ANALYSIS

SABSCOV (Krämer, 2006) $\quad \underset{\text{all } \|a_j\|=1}{\text{maximize}} \sum_{j,k} c_{jk}\,|\text{cov}(\mathbf{X_j a_j}, \mathbf{X_k a_k})|$

$\text{cov}^2(\mathbf{X_j a_j}, \mathbf{X_k a_k}) = \text{var}(\mathbf{X_j a_j})\,\text{cor}^2(\mathbf{X_j a_j}, \mathbf{X_k a_k})\,\text{var}(\mathbf{X_j a_j})$

Covariance-based criteria

$c_{jk} = 1$ if blocks are linked, 0 otherwise and $c_{jj} = 0$

SUMCOR: $$\underset{\text{all } \mathrm{var}(\mathbf{X}_j\mathbf{a}_j)=1}{\text{maximize}} \sum_{j,k} c_{jk} \mathrm{cov}(\mathbf{X}_j\mathbf{a}_j, \mathbf{X}_k\mathbf{a}_k)$$

SSQCOR: $$\underset{\text{all } \mathrm{var}(\mathbf{X}_j\mathbf{a}_j)=1}{\text{maximize}} \sum_{j,k} c_{jk} \mathrm{cov}^2(\mathbf{X}_j\mathbf{a}_j, \mathbf{X}_k\mathbf{a}_k)$$

SABSCOR: $$\underset{\text{all } \mathrm{var}(\mathbf{X}_j\mathbf{a}_j)=1}{\text{maximize}} \sum_{j,k} c_{jk} \left|\mathrm{cov}(\mathbf{X}_j\mathbf{a}_j, \mathbf{X}_k\mathbf{a}_k)\right|$$

SUMCOV: $$\underset{\text{all } \|a_j\|=1}{\text{maximize}} \sum_{j,k} c_{jk} \mathrm{cov}(\mathbf{X}_j\mathbf{a}_j, \mathbf{X}_k\mathbf{a}_k)$$

SSQCOV: $$\underset{\text{all } \|a_j\|=1}{\text{maximize}} \sum_{j,k} c_{jk} \mathrm{cov}^2(\mathbf{X}_j\mathbf{a}_j, \mathbf{X}_k\mathbf{a}_k)$$

SABSCOV: $$\underset{\text{all } \|a_j\|=1}{\text{maximize}} \sum_{j,k} c_{jk} \left|\mathrm{cov}(\mathbf{X}_j\mathbf{a}_j, \mathbf{X}_k\mathbf{a}_k)\right|$$

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RGCCA optimization problem

$$\underset{\mathbf{a}_1,\mathbf{a}_2,\ldots,\mathbf{a}_J}{\text{argmax}} \sum_{j \neq k}^{J} c_{jk}\, g\left(\text{cov}(\mathbf{X}_j \mathbf{a}_j, \mathbf{X}_k \mathbf{a}_k)\right)$$

Subject to the constraints $(1-\tau_j)\text{var}(\mathbf{X}_j \mathbf{a}_j) + \tau_j \|\mathbf{a}_j\|^2 = 1, j = 1, \ldots, J$

where: $$c_{jk} = \begin{cases} 1 & \text{if } \mathbf{X_j} \text{ and } \mathbf{X_k} \text{ is connected} \\ 0 & \text{otherwise} \end{cases}$$

$$g = \begin{cases} \text{identity} & \text{(Horst sheme)} \\ \text{square} & \text{(Factorial scheme)} \\ \text{abolute value} & \text{(Centroid scheme)} \end{cases}$$

and: $\tau_j =$ Shrinkage constant between 0 and 1

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and: τ_j … …d 1

A monotone convergent algorithm related to this optimization problem will be described.

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$$\underset{\mathbf{a}_1,\mathbf{a}_2,\ldots,\mathbf{a}_J}{\operatorname{argmax}} \sum_{j \neq k}^{J} c_{jk}\, g\left(\operatorname{cov}(\mathbf{X}_j \mathbf{a}_j, \mathbf{X}_k \mathbf{a}_k)\right)$$

Subject to the constraints $(1-\tau_j)\operatorname{var}(\mathbf{X}_j \mathbf{a}_j) + \tau_j \|\mathbf{a}_j\|^2 = 1, j = 1, \ldots, J$

{1 if $\mathbf{X}_j$ and $\mathbf{X}_k$ is connected

Schäfer and Strimmer formula can be used for an optimal determination of the shrinkage constants

$g = \begin{cases} \text{identity} & \text{(Horst sheme)} \\ \text{square} & \text{(Factorial scheme)} \\ & \text{…e)} \end{cases}$

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and: … nd 1

Choice of the shrinkage constant τ_j (part 1)

$$\underset{\mathbf{a}_1,\mathbf{a}_2}{\operatorname{argmax}} \operatorname{cov}(\mathbf{X}_1\mathbf{a}_1, \mathbf{X}_2\mathbf{a}_2)$$

Subject to the constraints $(1-\tau_j)\operatorname{var}(\mathbf{X}_j\mathbf{a}_j) + \tau_j\|\mathbf{a}_j\|^2 = 1, j = 1,2$

Special cases

Method	Criterion	Constraints
PLS regression	Maximize $\operatorname{Cov}(\mathbf{X}_1\mathbf{a}_1, \mathbf{X}_2\mathbf{a}_2)$	$\|\mathbf{a}_1\| = \|\mathbf{a}_2\| = 1$
Canonical Correlation Analysis	Maximize $\operatorname{Cor}(\mathbf{X}_1\mathbf{a}_1, \mathbf{X}_2\mathbf{a}_2)$	$\operatorname{Var}(\mathbf{X}_1\mathbf{a}_1) = \operatorname{Var}(\mathbf{X}_2\mathbf{a}_2) = 1$
Redundancy analysis of X_1 with respect to X_2	Maximize $\operatorname{Cor}(\mathbf{X}_1\mathbf{a}_1, \mathbf{X}_2\mathbf{a}_2)\operatorname{Var}(\mathbf{X}_1\mathbf{a}_1)^{1/2}$	$\|\mathbf{a}_1\| = 1$ $\operatorname{Var}(\mathbf{X}_2\mathbf{a}_2) = 1$

Choice of the shrinkage constant τ_j (part 1)

$$\underset{\mathbf{a}_1,\mathbf{a}_2}{\text{argmax}}\ \text{cov}(\mathbf{X}_1\mathbf{a}_1, \mathbf{X}_2\mathbf{a}_2)$$

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Components $\mathbf{X}_1\mathbf{a}_1$ and $\mathbf{X}_2\mathbf{a}_2$ are well correlated.

Choice of the shrinkage constant τ_j (part 1)

$$\underset{\mathbf{a}_1,\mathbf{a}_2}{\text{argmax}}\ \text{cov}(\mathbf{X}_1\mathbf{a}_1, \mathbf{X}_2\mathbf{a}_2)$$

Subject to the constraints $(1-\tau_j)\text{var}(\mathbf{X}_j\mathbf{a}_j) + \tau_j\|\mathbf{a}_j\|^2 = 1, j = 1,2$

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Components $\mathbf{X}_1\mathbf{a}_1$ and $\mathbf{X}_2\mathbf{a}_2$ are well correlated.

1st component is stable

Choice of the shrinkage constant τ_j (part 1)

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Components $\mathbf{X_1a_1}$ and $\mathbf{X_2a_2}$ are well correlated.

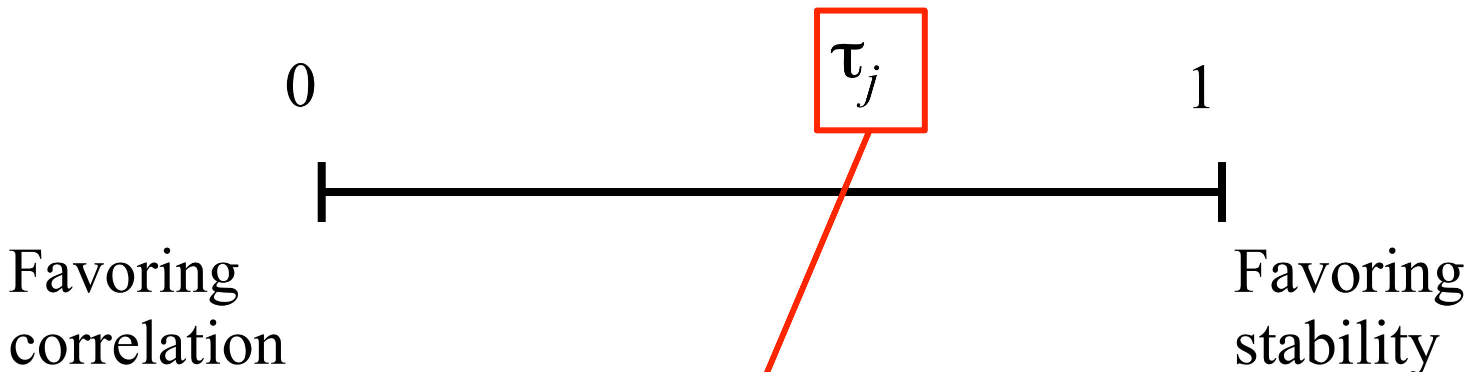
1st component is stable

No stability condition for 2nd component

Choice of the shrinkage constant τ_j (part 2)

$$\underset{\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_J}{\operatorname{argmax}} \sum_{j \neq k}^{J} c_{jk}\, g\left(\operatorname{cov}(\mathbf{X}_j \mathbf{a}_j, \mathbf{X}_k \mathbf{a}_k)\right)$$

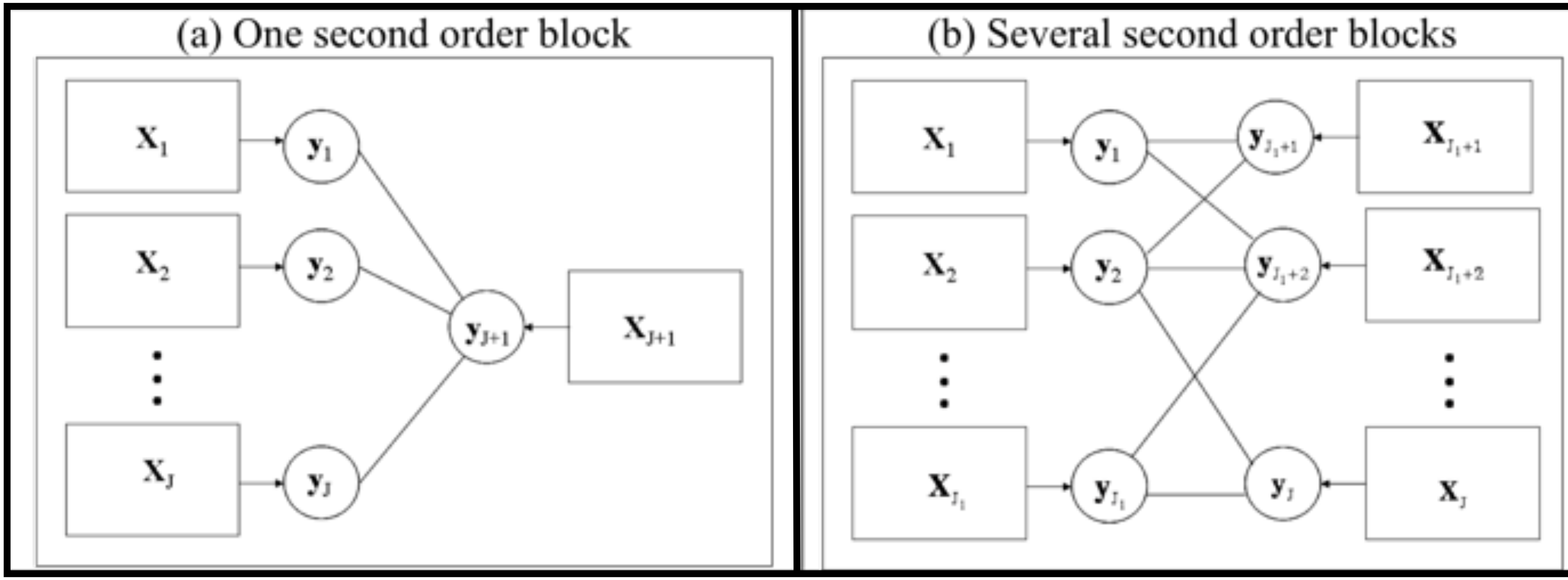
Subject to the constraints $(1 - \tau_j)\operatorname{var}(\mathbf{X}_j \mathbf{a}_j) + \tau_j \|\mathbf{a}_j\|^2 = 1, j = 1, \ldots, J$



Schäfer and Strimmer formula can be used for an optimal determination of the shrinkage constants

Choice of the design matrix C

Hierarchical models

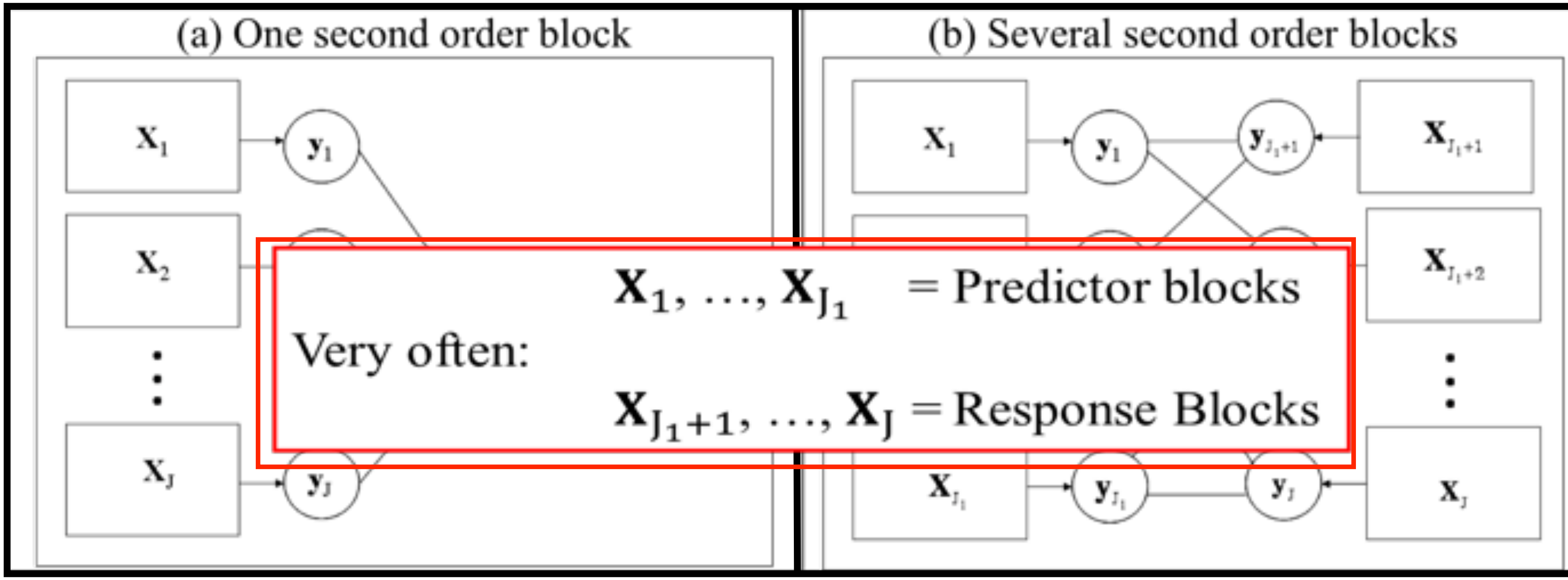


$$\begin{cases} \max_{\mathbf{a}_1,\mathbf{a}_2,\ldots,\mathbf{a}_J} \sum_{j \neq k}^{J} g\left(\text{cov}(\mathbf{X}_j\mathbf{a}_j, \mathbf{X}_{J+1}\mathbf{a}_{J+1})\right) \\ (1-\tau_j)\text{var}(\mathbf{X}_j\mathbf{a}_j) + \tau_j\|\mathbf{a}_j\|^2 = 1, j = 1, \ldots, J+1 \end{cases}$$

$$\begin{cases} \max_{\mathbf{a}_1,\mathbf{a}_2,\ldots,\mathbf{a}_J} \sum_{j=1}^{J_1} \sum_{k=J_1+1}^{J} c_{jk} g\left(\text{cov}(\mathbf{X}_j\mathbf{a}_j, \mathbf{X}_k\mathbf{a}_k)\right) \\ (1-\tau_j)\text{var}(\mathbf{X}_j\mathbf{a}_j) + \tau_j\|\mathbf{a}_j\|^2 = 1, j = 1, \ldots, J \end{cases}$$

Choice of the design matrix C

Hierarchical models



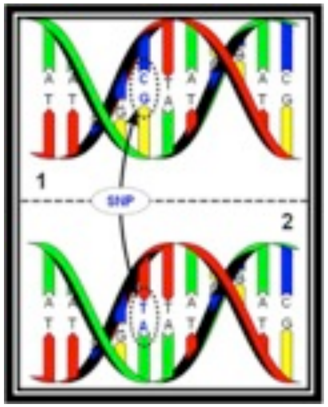
Very often: $\mathbf{X}_1, \ldots, \mathbf{X}_{J_1}$ = Predictor blocks

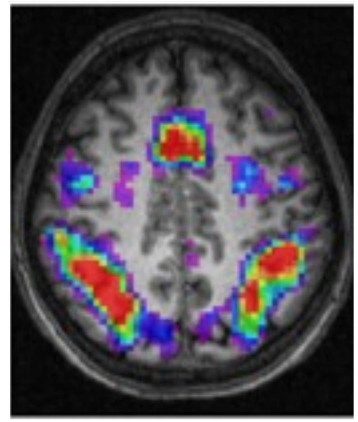
$\mathbf{X}_{J_1+1}, \ldots, \mathbf{X}_J$ = Response Blocks

$$\begin{cases} \max\limits_{\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_J} \sum\limits_{j \neq k}^{J} g\left(\operatorname{cov}(\mathbf{X}_j \mathbf{a}_j, \mathbf{X}_{J+1} \mathbf{a}_{J+1})\right) \\ (1-\tau_j)\operatorname{var}(\mathbf{X}_j \mathbf{a}_j) + \tau_j \|\mathbf{a}_j\|^2 = 1, j = 1, \ldots, J+1 \end{cases}$$

$$\begin{cases} \max\limits_{\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_J} \sum\limits_{j=1}^{J_1} \sum\limits_{k=J_1+1}^{J} c_{jk} g\left(\operatorname{cov}(\mathbf{X}_j \mathbf{a}_j, \mathbf{X}_k \mathbf{a}_k)\right) \\ (1-\tau_j)\operatorname{var}(\mathbf{X}_j \mathbf{a}_j) + \tau_j \|\mathbf{a}_j\|^2 = 1, j = 1, \ldots, J \end{cases}$$

Choice of the design for NeuroImaging-Genetic datasets





$p_1 \sim 10^6$ | $p_2 \sim 10^4$ | $p_3 \sim 10$

$n \sim 100$

X_1
DNA arrays (SNP)

$c_{12}=1$

X_2
Functional MRI

$c_{23}=1$

X_3
Developmental disorders - Reading difficulties - Basic numerical knowledge -…- Visuo-spatial abilities - Visuo-motor abilities

$c_{13}=0$

special cases of RGCCA (among others)

two-block case

PLS Regression	Wold S., Martens & Wold H. (1983): The multivariate calibration problem in chemistry solved by the PLS method. In Proc. Conf. Matrix Pencils, Ruhe A. & Kåstrøm B. (Eds), March 1982, Lecture Notes in Mathematics, Springer Verlag, Heidelberg, p. 286-293.
Redundancy analysis	Barker M. & Rayens W. (2003): Partial least squares for discrimination, *Journal of Chemometrics*, 17, 166-173.
Regularized CCA	Vinod H. D. (1976): Canonical ridge and econometrics of joint production. *Journal of Econometrics,* 4, 147–166.
Inter-battery factor analysis	Tucker L.R. (1958): An inter-battery method of factor analysis, *Psychometrika*, vol. 23, n°2, pp. 111-136.

multi-block case

MCOA	Chessel D. and Hanafi M. (1996): Analyse de la co-inertie de *K* nuages de points. *Revue de Statistique Appliquée*, 44, 35-60
SSQCOV	Hanafi M. & Kiers H.A.L. (2006): Analysis of K sets of data, with differential emphasis on agreement between and within sets, *Computational Statistics & Data Analysis*, 51, 1491-1508.
SUMCOR	Horst P. (1961): Relations among m sets of variables, *Psychometrika*, vol. 26, pp. 126-149.
SSQCOR	Kettenring J.R. (1971): Canonical analysis of several sets of variables, *Biometrika*, 58, 433-451
MAXDIFF	Van de Geer J. P. (1984): Linear relations among k sets of variables. *Psychometrik*a, 49, 70-94.
PLS path modeling (mode B)	Tenenhaus M., Esposito Vinzi V., Chatelin Y.-M., Lauro C. (2005): PLS path modeling. *Computational Statistics and Data Analysis,* 48, 159-205.
Generalized Orthogonal MCOA	Vivien M. & Sabatier R. (2003): Generalized orthogonal multiple co-inertia analysis (-PLS): new multiblock component and regression methods, *Journal of Chemometrics*, 17, 287-301.
Caroll's GCCA	Carroll, J.D. (1968): A generalization of canonical correlation analysis to three or more sets of variables, *Proc. 76th Conv. Am. Psych. Assoc.*, pp. 227-228.

Monotone convergent algorithm for the RGCCA criteria

$$\underset{\mathbf{a}_1,\mathbf{a}_2,\ldots,\mathbf{a}_J}{\operatorname{argmax}} \sum_{j \neq k}^{J} c_{jk}\, \mathrm{g}\left(\mathrm{cov}\left(\mathbf{X}_j \mathbf{a}_j, \mathbf{X}_k \mathbf{a}_k\right)\right)$$

Subject to the constraints $(1 - \tau_j)\mathrm{var}\left(\mathbf{X}_j \mathbf{a}_j\right) + \tau_j \|\mathbf{a}_j\|^2 = 1, j = 1, \ldots, J$

Monotone convergent algorithm for the RGCCA criteria

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Subject to the constraints $(1 - \tau_j)\mathrm{var}(\mathbf{X}_j \mathbf{a}_j) + \tau_j \|\mathbf{a}_j\|^2 = 1, j = 1, \ldots, J$

- Construct the Lagrangian function related to the optimization problem.

Monotone convergent algorithm for the RGCCA criteria

$$\underset{\mathbf{a}_1,\mathbf{a}_2,\ldots,\mathbf{a}_J}{\operatorname{argmax}} \sum_{j \neq k}^{J} c_{jk}\, \mathrm{g}\left(\operatorname{cov}(\mathbf{X}_j \mathbf{a}_j, \mathbf{X}_k \mathbf{a}_k)\right)$$

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- Construct the Lagrangian function related to the optimization problem.
- Cancel the derivative of the Lagrangian function with respect to each $\mathbf{a}_\mathbf{j}$.

Monotone convergent algorithm for the RGCCA criteria

$$\underset{\mathbf{a}_1,\mathbf{a}_2,\ldots,\mathbf{a}_J}{\operatorname{argmax}} \sum_{j \neq k}^{J} c_{jk}\, \mathrm{g}\left(\operatorname{cov}(\mathbf{X}_j \mathbf{a}_j, \mathbf{X}_k \mathbf{a}_k)\right)$$

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- Use the Wold's procedure to solve the stationary equations (≈ Gauss-Seidel algorithm).

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- Construct the Lagrangian function related to the optimization problem.
- Cancel the derivative of the Lagrangian function with respect to each $\mathbf{a}_\mathbf{j}$.
- Use the Wold's procedure to solve the stationary equations (≈ Gauss-Seidel algorithm).
- This procedure is monotonically convergent: the criterion increases at each step of the algorithm.

The RGCCA algorithm (primal version)

The RGCCA algorithm (primal version)

Initial step	→	$\mathbf{a}_j$

The RGCCA algorithm (primal version)

$$\mathbf{y}_j = \mathbf{X}_j \mathbf{a}_j$$

Outer Estimation
(explains the block)

$$(1-\tau_j)\mathrm{var}(\mathbf{X}_j\mathbf{a}_j) + \tau_j \|\mathbf{a}_j\|^2 = 1$$

Initial step → $\mathbf{a}_j$

The RGCCA algorithm (primal version)

$$\mathbf{y}_j = \mathbf{X}_j \mathbf{a}_j$$

Outer Estimation
(explains the block)

Initial step → $\mathbf{a}_j$

$$(1-\tau_j)\,\mathrm{var}(\mathbf{X}_j \mathbf{a}_j) + \tau_j \|\mathbf{a}_j\|^2 = 1$$

$$\mathbf{z}_j = \sum_{k \neq j} e_{jk} \mathbf{y}_k$$

Inner Estimation
(explains relation between block)

Choice of weights e_{jh}:

- Horst : $e_{jk} = c_{jk}$
- Centroid : $e_{jk} = c_{jk}\,\mathrm{sign}(\mathrm{cor}(\mathbf{y}_j, \mathbf{y}_k))$
- Factorial : $e_{jk} = c_{jk}\,\mathrm{cov}(\mathbf{y}_j, \mathbf{y}_k)$

$c_{jk} = 1$ if blocks are linked, 0 otherwise and $c_{jj} = 0$

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$$\mathbf{a}_j = \frac{\left((1-\tau_j)\frac{1}{\mathbf{n}}\mathbf{X}_j^t\mathbf{X}_j + \tau_j\mathbf{I}\right)^{-1}\mathbf{X}_j^t\mathbf{z}_j}{\sqrt{\mathbf{z}_j^t\mathbf{X}_j\left((1-\tau_j)\frac{1}{\mathbf{n}}\mathbf{X}_j^t\mathbf{X}_j + \tau_j\mathbf{I}\right)^{-1}\mathbf{X}_j^t\mathbf{z}_j}}$$

Dimension = $p_j \times p_j$

$c_{jk} = 1$ if blocks are linked, 0 otherwise and $c_{jj} = 0$

The RGCCA algorithm (primal version)

Initial step → $\mathbf{a}_j$

$$\mathbf{y}_\mathbf{j} = \mathbf{X}_\mathbf{j}\mathbf{a}_\mathbf{j}$$

Outer Estimation (explains the block)

$$(1-\tau_j)\mathrm{var}(\mathbf{X}_j\mathbf{a}_j)+\tau_j\|\mathbf{a}_j\|^2 = 1$$

$$\mathbf{z}_j = \sum_{k\neq j} e_{jk}\mathbf{y}_k$$

Inner Estimation (explains relation between block)

Iterate until convergence of the criterion

$$\mathbf{a}_\mathbf{j} = \frac{\left((1-\tau_j)\frac{1}{\mathbf{n}}\mathbf{X}_j^t\mathbf{X}_j+\tau_j\mathbf{I}\right)^{-1}\mathbf{X}_j^t\mathbf{z}_j}{\sqrt{\mathbf{z}_j^t\mathbf{X}_j\left((1-\tau_j)\frac{1}{\mathbf{n}}\mathbf{X}_j^t\mathbf{X}_j+\tau_j\mathbf{I}\right)^{-1}\mathbf{X}_j^t\mathbf{z}_j}}$$

Dimension = $p_j \times p_j$

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- Factorial : $e_{jk} = c_{jk}\,\mathrm{cov}(\mathbf{y}_j,\mathbf{y}_k)$

$c_{jk} = 1$ if blocks are linked, 0 otherwise and $c_{jj} = 0$

The RGCCA algorithm (dual version)

$$\mathbf{a}_j = \mathbf{X}_j^t \boldsymbol{\alpha}_j$$

Initial step → $\boldsymbol{\alpha}_j$

$$\mathbf{y}_j = \mathbf{X}_j \mathbf{X}_j^t \boldsymbol{\alpha}_j$$

Outer Estimation (explains the block)

$$\boldsymbol{\alpha}_j^t \left[\mathbf{X}_j \mathbf{X}_j^t \left(\tau_j \mathbf{I} + (1-\tau_j) \tfrac{1}{n} \mathbf{X}_j \mathbf{X}_j^t \right) \right] \boldsymbol{\alpha}_j = 1$$

$$\mathbf{z}_j = \sum_{k \neq j} e_{jk} \mathbf{y}_k$$

Inner Estimation (explains relation between block)

Choice of weights e_{jh}:

- Horst : $e_{jk} = c_{jk}$
- Centroid : $e_{jk} = c_{jk} \operatorname{sign}(\operatorname{cor}(\mathbf{y}_j, \mathbf{y}_k))$
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$c_{jk} = 1$ if blocks are linked, 0 otherwise and $c_{jj} = 0$

Iterate until convergence of the criterion

$$\boldsymbol{\alpha}_j = \frac{\left((1-\tau_j) \frac{1}{\mathbf{n}} \mathbf{X}_j \mathbf{X}_j^t + \tau_j \mathbf{I} \right)^{-1} \mathbf{z}_j}{\sqrt{\mathbf{z}_j^t \mathbf{X}_j \mathbf{X}_j^t \left((1-\tau_j) \frac{1}{\mathbf{n}} \mathbf{X}_j \mathbf{X}_j^t + \tau_j \mathbf{I} \right)^{-1} \mathbf{z}_j}}$$

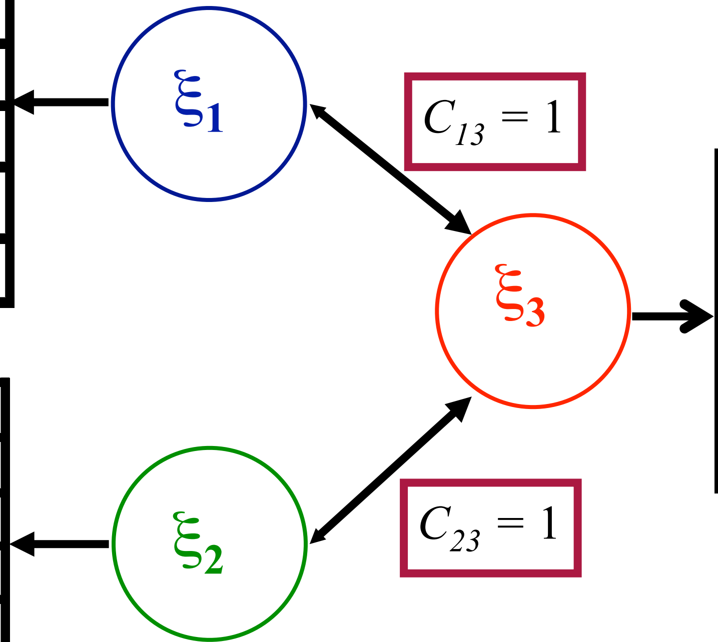
Dimension = $n \times n$

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 $\tau_3 = 0$

	Gene 1	…	Gene 15201
Patient 1	0.18		-0.73
Patient 2	1.15		0.27
Patient 3	1.35		0.22
⋮			
Patient 53	1.39		-0.17



	Hemisphere	DIPG
Patient 1	1	0
Patient 2	0	0
Patient 3	0	1
⋮		
Patient 53	1	0

	CGH1	…	CGH 1909
Patient 1	0.00		-0.55
Patient 2	-0.30		0.00
Patient 3	0.33		0.64
⋮			
Patient 53	0.00		0.43

High dimensional block settings $\Longrightarrow$ dual algorithm for RGCCA

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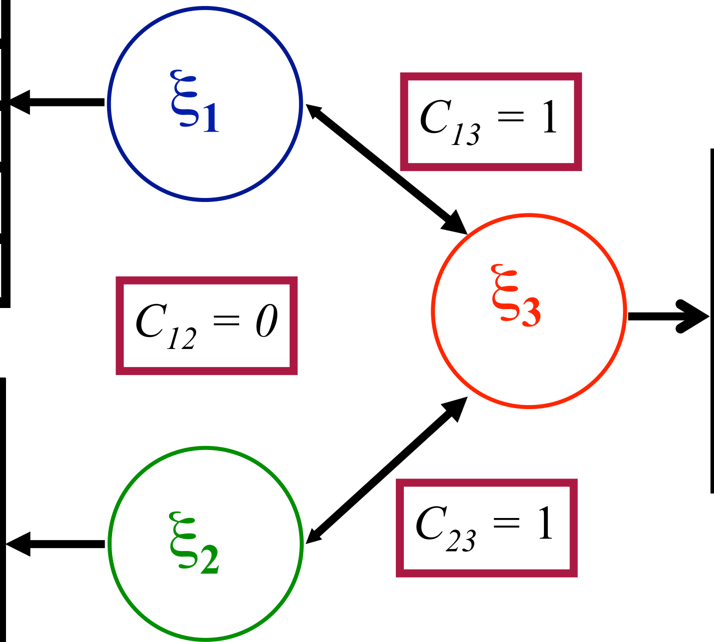

	Hemisphere	DIPG
Patient 1	1	0
Patient 2	0	0
Patient 3	0	1
⋮		
Patient 53	1	0

	CGH1	…	CGH 1909
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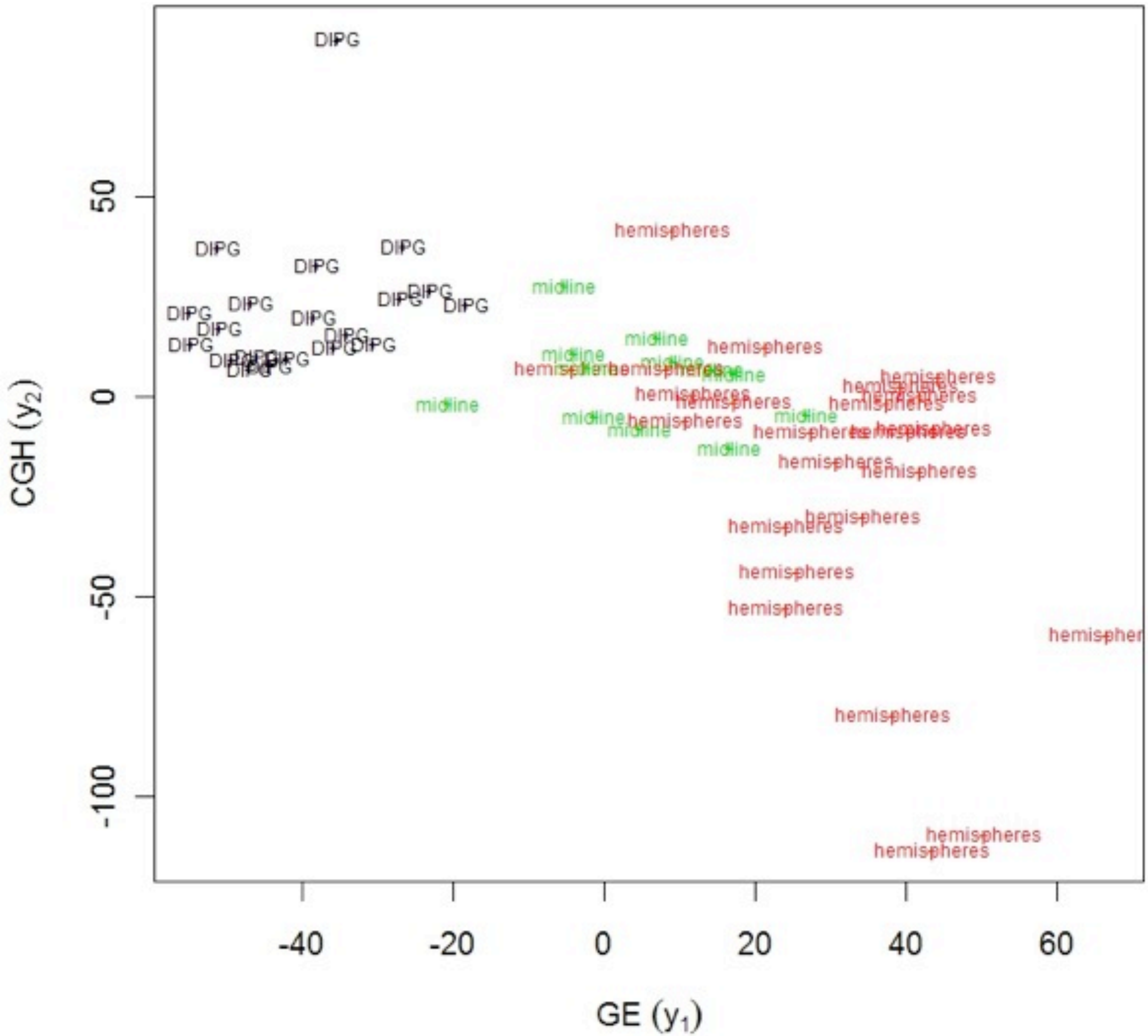
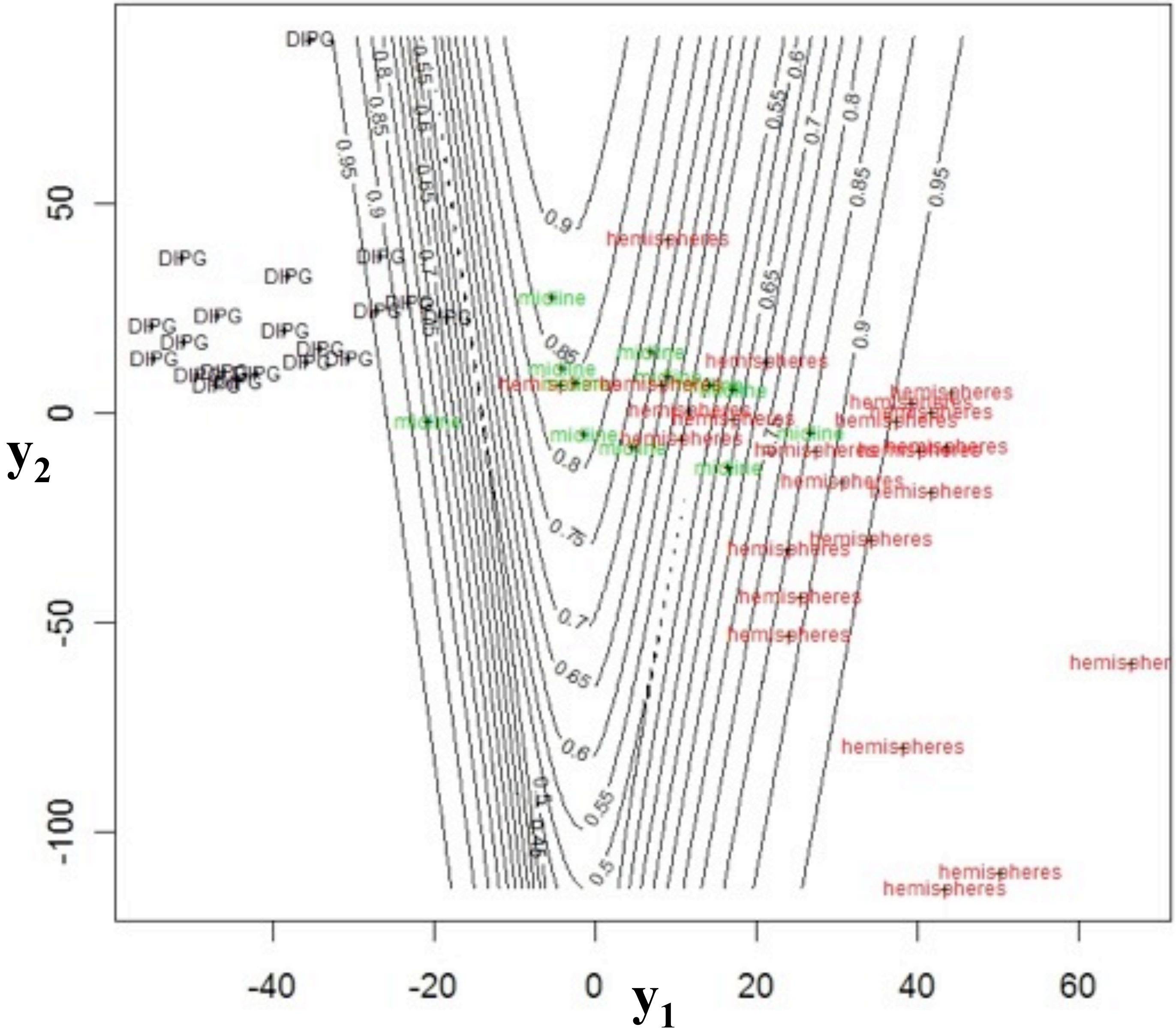
High dimensional block settings $\Longrightarrow$ dual algorithm for RGCCA


CGH (y_2)
GE (y_1)
50
0
-50
-100
-40
-20
0
20
40
60
DIPG
midline
hemispheres

Bayesian Discriminant Analysis of localization on y_1 and y_2



Predictive performance

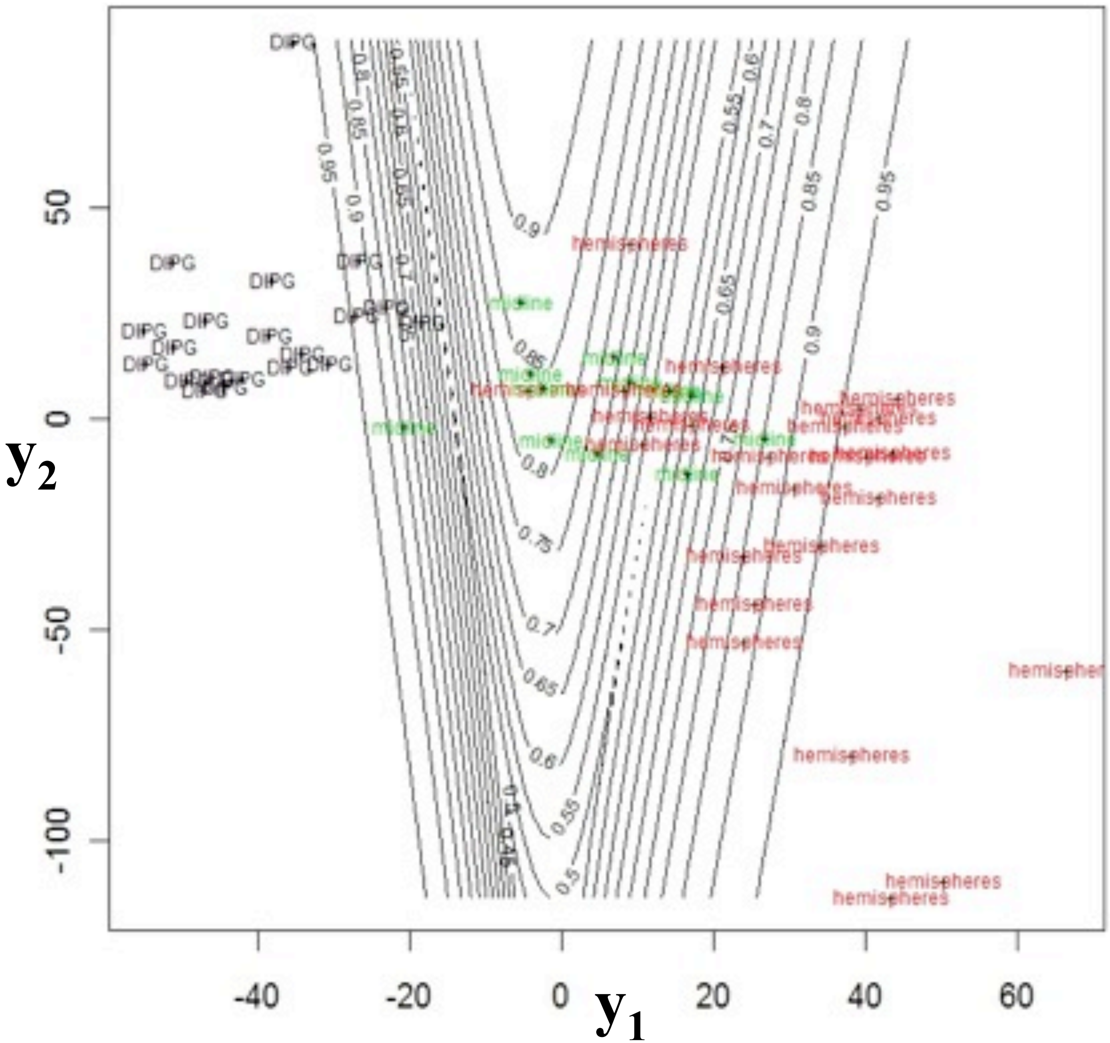


Table 1. Learning phase

Observed / Predicted	DIPG	Hemispheres	Midline
DIPG	20	0	1
Hemispheres	0	19	4
Midline	0	5	7

Accuracy = 82%

Table 2. Testing phase (leave-one-out)

Observed / Predicted	DIPG	Hemispheres	Midline
DIPG	18	1	1
Hemispheres	0	17	4
Midline	2	6	7

Accuracy = 75%

Block components

$$\mathbf{y}_1 = \mathbf{X_1 a_1} = a_{11}\mathbf{Gene_1} + \cdots + a_{1,15201}\mathbf{Gene_{15201}}$$

$$\mathbf{y}_2 = \mathbf{X_2 a_2} = a_{21}\mathbf{CGH_1} + \cdots + a_{2,15201}\mathbf{CGH_{15201}}$$

$$\mathbf{y_3} = \mathbf{X_3 a_3} = a_{31}\mathbf{Hemisphere} + a_{32}\mathbf{DIPG}$$

Block components

$$\mathbf{y}_1 = \mathbf{X_1 a_1} = a_{11}\mathbf{Gene_1} + \cdots + a_{1,15201}\mathbf{Gene_{15201}}$$

$$\mathbf{y}_2 = \mathbf{X_2 a_2} = a_{21}\mathbf{CGH_1} + \cdots + a_{2,15201}\mathbf{CGH_{15201}}$$

$$\mathbf{y_3} = \mathbf{X_3 a_3} = a_{31}\mathbf{Hemisphere} + a_{32}\mathbf{DIPG}$$

Block components should verified two properties at the same time:

(i) Block components well explain their own block.

(ii) Block components are as correlated as possible for connected blocks.

(iii) Block components are built from sparse $\mathbf{a}_j$

Variable selection for RGCCA

$$\underset{\mathbf{a}_1,\mathbf{a}_2,\ldots,\mathbf{a}_J}{\operatorname{argmax}} \sum_{j \neq k}^{J} c_{jk}\, g\left(\operatorname{cov}(\mathbf{X}_j \mathbf{a}_j, \mathbf{X}_k \mathbf{a}_k)\right)$$

Subject to the constraints $\begin{cases} \|\mathbf{a}_j\|_2^2 = 1, j = 1, \ldots, J \\ \|\mathbf{a}_j\|_1 \leq c_j, j = 1, \ldots, J \end{cases}$

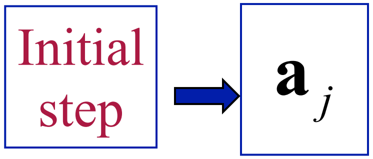
where: $c_{jk} = \begin{cases} 1 & \text{if } \mathbf{X}_\mathbf{j} \text{ and } \mathbf{X}_\mathbf{k} \text{ is connected} \\ 0 & \text{otherwise} \end{cases}$

$$g = \begin{cases} \text{identity} & \text{(Horst sheme)} \\ \text{square} & \text{(Factorial scheme)} \\ \text{abolute value} & \text{(Centroid scheme)} \end{cases}$$

and: $\tau_j =$ Shrinkage constant between 0 and 1

Sparse GCCA

Sparse GCCA



Sparse GCCA

$$\mathbf{y}_j = \mathbf{X}_j \mathbf{a}_j$$

Outer Estimation
(explains the block)

$$\|\mathbf{a}_j\|_2^2 = 1$$

Initial step

$$\mathbf{a}_j$$

Sparse GCCA

Initial step → $\mathbf{a}_j$

$$\mathbf{y}_j = \mathbf{X}_j \mathbf{a}_j$$

Outer Estimation
(explains the block)

$$\|\mathbf{a}_j\|_2^2 = 1$$

$$\mathbf{z}_j = \sum_{k \neq j} \mathbf{e}_{jk} \mathbf{y}_k$$

Inner Estimation (explains relation between block)

Choice of weights e_{jh}:

- Horst : $e_{jk} = c_{jk}$
- Centroid : $e_{jk} = c_{jk} \operatorname{sign}(\operatorname{cor}(\mathbf{y}_j, \mathbf{y}_k))$
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$c_{jk} = 1$ if blocks are linked, 0 otherwise and $c_{jj} = 0$

Sparse GCCA

Initial step → $\mathbf{a}_j$

$$\mathbf{y_j} = \mathbf{X_j a_j}$$

Outer Estimation (explains the block)

$$\|\mathbf{a_j}\|_2^2 = 1$$

$$\mathbf{z_j} = \sum_{\mathbf{k \neq j}} \mathbf{e_{jk} y_k}$$

Inner Estimation (explains relation between block)

Choice of weights e_{jh}:

- Horst : $e_{jk} = c_{jk}$
- Centroid : $e_{jk} = c_{jk}\,\mathrm{sign}\big(\mathrm{cor}(\mathbf{y}_j, \mathbf{y}_k)\big)$
- Factorial : $e_{jk} = c_{jk}\,\mathrm{cov}(\mathbf{y}_j, \mathbf{y}_k)$

$$\mathbf{a_j} = \frac{\mathbf{S}(\frac{1}{\mathbf{n}}\mathbf{X_j^t z_j}, \lambda_j)}{\left\|\mathbf{S}(\frac{1}{\mathbf{n}}\mathbf{X_j^t z_j}, \lambda_j)\right\|_2}$$

λ_j is chosen such that $\|\mathbf{a_j}\|_1 \le \kappa_j$

$$S(a, \lambda) = \mathrm{sign}(a)\max(0, |a| - \lambda)$$

$c_{jk} = 1$ if blocks are linked, 0 otherwise and $c_{jj} = 0$

Sparse GCCA

$$\mathbf{y}_j = \mathbf{X}_j \mathbf{a}_j$$

Outer Estimation
(explains the block)

$$\|\mathbf{a}_j\|_2^2 = 1$$

Initial step → $\mathbf{a}_j$

$$\mathbf{z}_j = \sum_{k \neq j} \mathbf{e}_{jk} \mathbf{y}_k$$

Inner Estimation (explains relation between block)

Iterate until convergence of the criterion

λ_j is chosen such that $\|\mathbf{a}_j\|_1 \le \kappa_j$

$$\mathbf{a}_j = \frac{\mathbf{S}(\frac{1}{\mathbf{n}}\mathbf{X}_j^t \mathbf{z}_j, \lambda_j)}{\left\| \mathbf{S}(\frac{1}{\mathbf{n}}\mathbf{X}_j^t \mathbf{z}_j, \lambda_j) \right\|_2}$$

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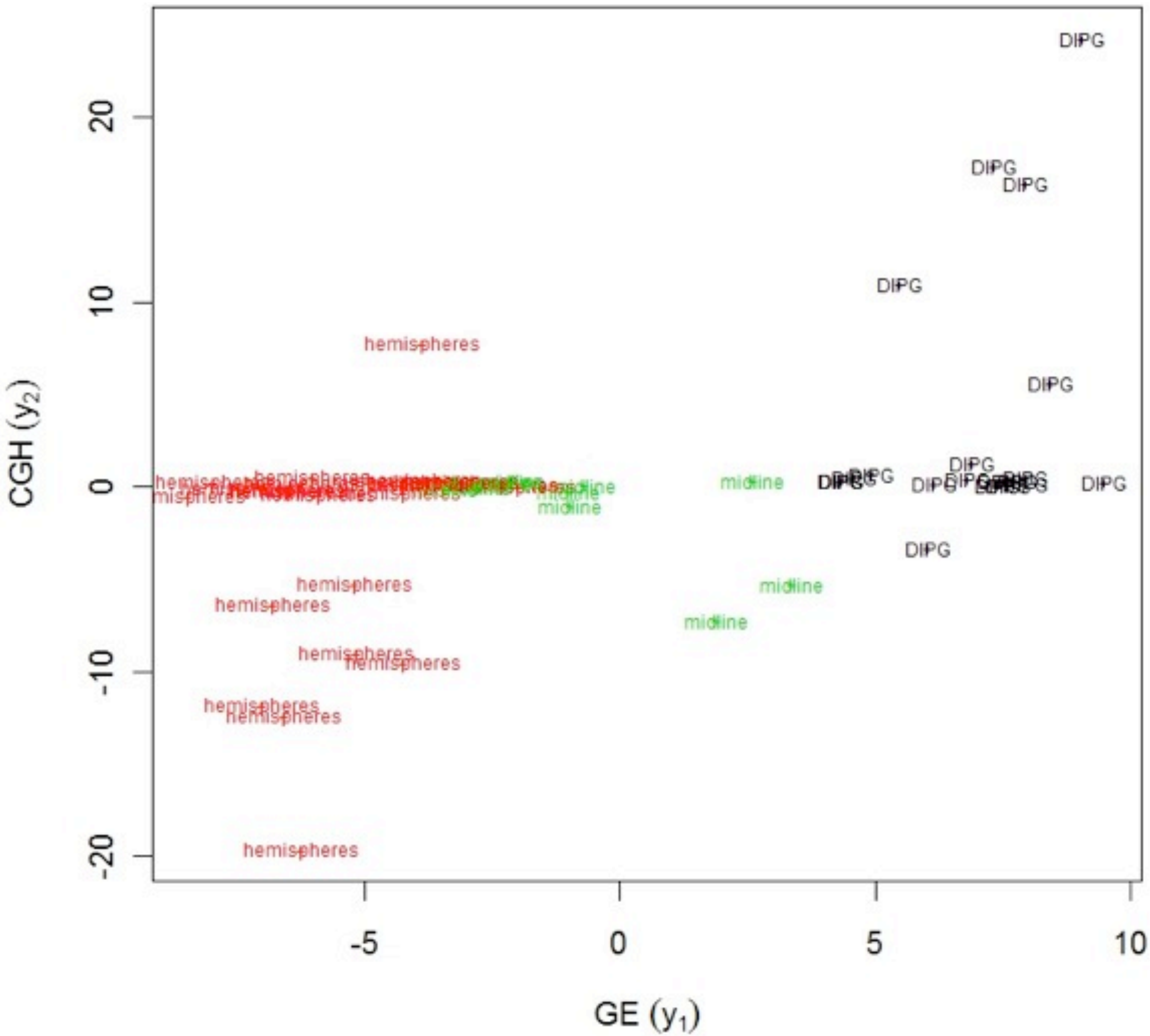

CGH (y_2)
GE (y_1)
20
10
0
-10
-20
-5
0
5
10
DIPG
hemispheres
midline

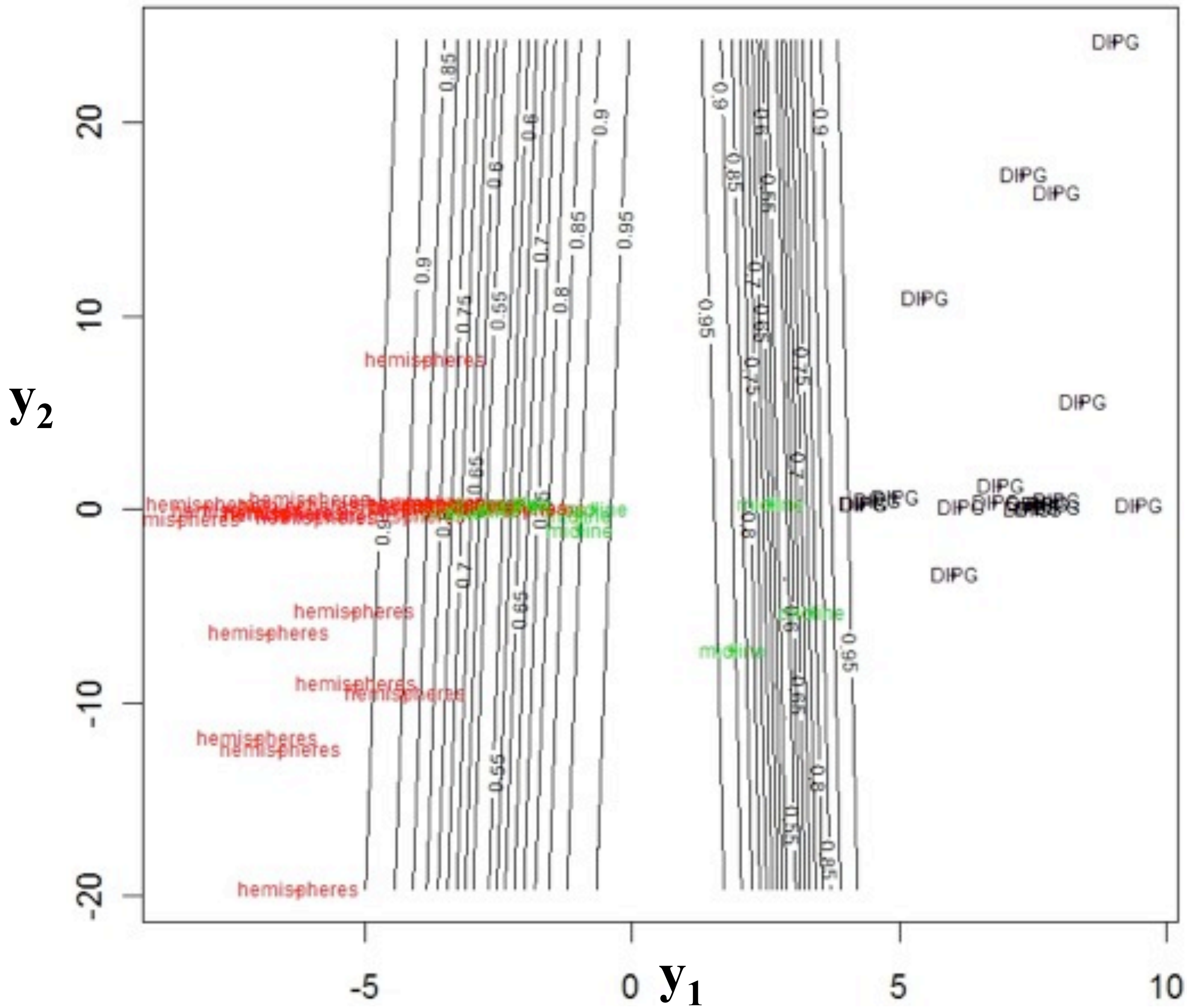
List of selected variables from GE data

FOXG1	PTPN9	CYP4Z1	ARFGAP3
ZFHX4	WNT5A	PI16	PDLIM4
EEPD1	COL10A1	TRIM43	VIPR2
GRID2	PBX3	BTC	ACADL
EMX1	TKTL1	PKNOX2	LAMB3
DLX2	LY6D	SERPINB10	DCAF6
ITM2C	CRYGD	TAAR2	NET1
SEMA3D	HOXA3	ZNF469	ELOVL2
PTHLH	KRTAP9-9	FAM196B	DAAM2
RASL12	LHX1	SLC22A3	CHCHD7
PPAPDC1A	ZNF483	HOXB2	FAIM
HCG4	NLRP7	SLC25A2	HOXA2
TRIM16L	ABI3BP	HES4	SPEF2
NR0B1	MCF2	SYT9	C8orf47
LHX2	SATB2	C2orf88	DLEC1
RNF182	HTR1D	CLDN3	FZD7
KIAA0556	LOXHD1	GLUD2	PLIN4
VAX2	IRX1	OMP	KAL1
ABP1	NRN1	KCND2	LRRC55
SFRP2	C14orf23	C17orf71	FAM89A
HERC3	IRX2	ADAMTS20	RSPH1
SPDEF	C1orf53	SLC1A6	AKR1C3
ONECUT2	GLIS1	SORD	C11orf86
OTX1	HELB	VPS37B	TBX15
OSR1	DLX1	NR2E1	SEMG2

List of selected variables from CGH data

KRAS	STK38L	BBS10	TMEM19
APOLD1	CAPRIN2	TSPAN11	HEBP1
CDKN2B	SOX5	GPRC5D	BHLHE41
CDKN2A	AMN1	GPRC5A	C12orf36
CNOT2	THAP2	DENND5B	RAB21
ABCC9	PYROXD1	NAP1L1	C12orf72
CAPS2	PHLDA1	KLHDC5	GSG1
IAPP	CSRP2	DDX47	C9orf53
PPFIBP1	KRR1	C12orf28	GLIPR1
NAV3	PTPRR	LDHB	PTPRB
SLCO1A2	TM7SF3	FAR2	E2F7
PTHLH	ZFC3H1	ST8SIA1	KIAA0528
ELK3	CCDC91	LRMP	LGR5
KIAA1467	KCNC2	EMP1	ZDHHC17
ETNK1	SLCO1B1	C12orf11	MRPS35
RAB3IP	BCAT1	OSBPL8	C12orf70
TMTC1	LYRM5	KCNJ8	TBC1D15
DDX11	RASSF8	TSPAN8	SSPN
GLIPR1L2	MED21	CASC1	
ITPR2	FGFR1OP2		

Bayesian Discriminant Analysis of localization on y_1 and y_2



Predictive performance

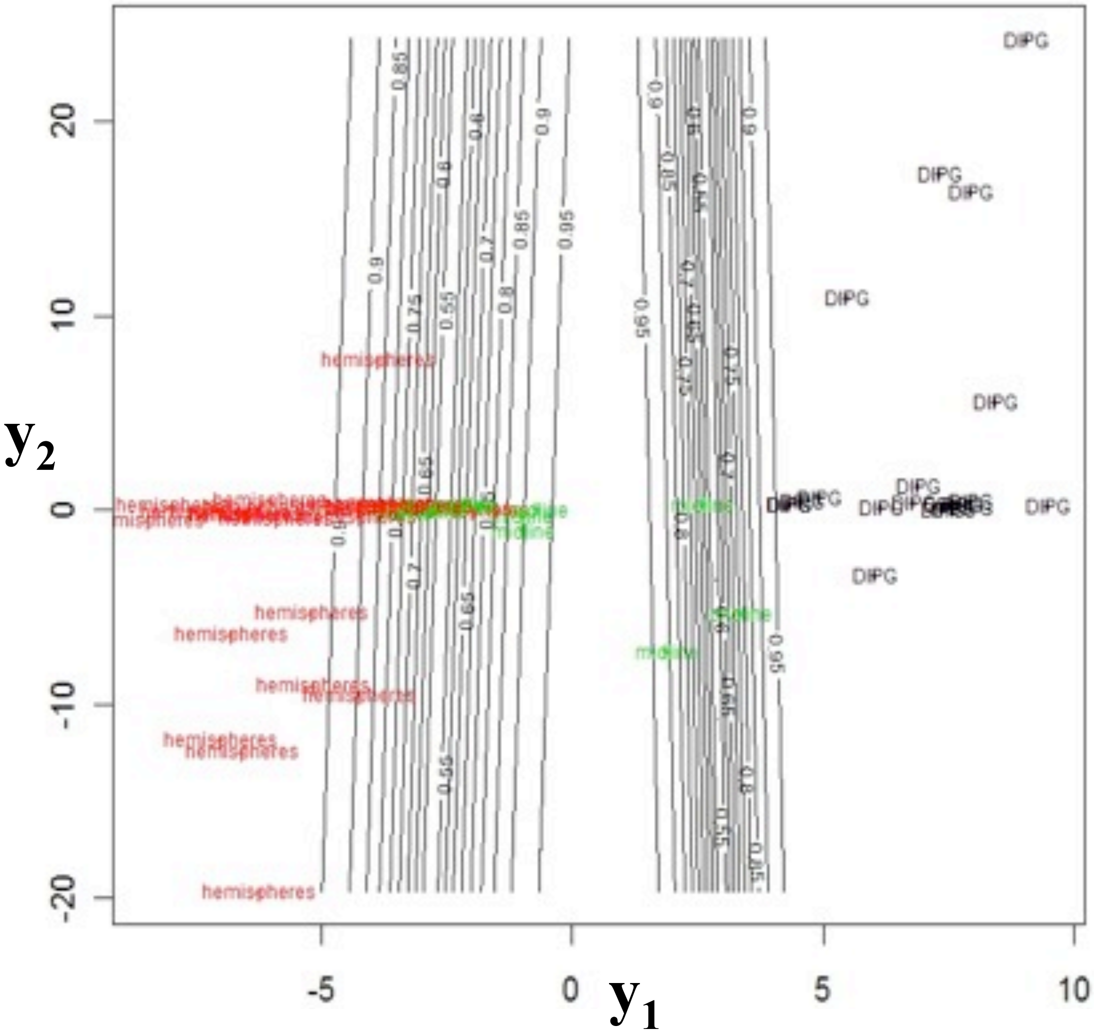


Table 1. Learning phase

Observed / **Predicted**	**DIPG**	**Hemispheres**	**Midline**
DIPG	20	0	1
Hemispheres	0	22	3
Midline	0	2	8

Accuracy = 89.2%

(82% non sparse)

Table 2. Testing phase (leave-one-out)

Observed / **Predicted**	**DIPG**	**Hemispheres**	**Midline**
DIPG	20	0	1
Hemispheres	0	20	3
Midline	0	4	8

Accuracy = 85.7%

(75% non sparse)

Conclusions

- Depending on the dimension of the blocks, you can use either the primal or the dual algorithm.

- The dual representation of the RGCCA algorithm allows:
    - Analysing high dimensional blocks.
    - recovering nonlinear relationship between blocks (choice of the kernel function).

- Sparse constraints are useful when the relevant variables are masked by (too many) noisy variables.

- Sparse constraints are useful when we want to identify a small number of significant variables which are active in the relationships between blocks.