Regularized Generalized Canonical Correlation Analysis (RGCCA), a flexible framework for multiblock (and multiway) data analysis: case study on a cohort of Major Depressive Disorder (MDD) patients and controls

Arnaud Gloaguen, Jimmy Vandel

1. Introduction of the case study

2. Unsupervised analysis with one-block:
Principal Component Analysis (PCA)

3. Unsupervised analysis with two-blocks:
Partial Least Squares (PLS) and Canonical Correlation Analysis (CCA)

4. Unsupervised analysis with $\boldsymbol{L}$-blocks:
Regularized Generalized Canonical Correlation Analysis (RGCCA)

5. Supervised analysis with RGCCA

6. Variable selection in RGCCA:
Sparse Generalized Canonical Correlation Analysis (SGCCA)

7. The flexible Optimization Framework of RGCCA

→ 7.1 The general principal

→ 7.2 Extension to multi-way analysis

→ 7.3 From Sequential to Global

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Case Study: Major Depressive Disorder (MDD)

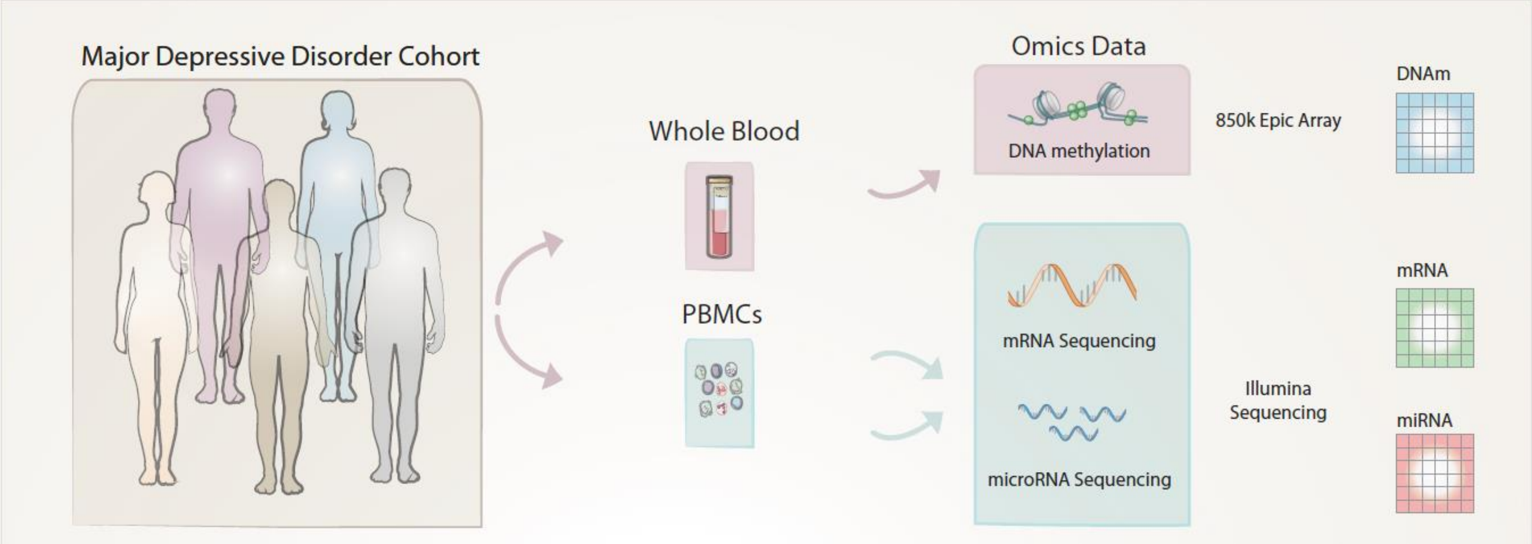
a

Cohort Description

Sex	n .max	Group	mean.Age	mean.BMI	mean.HDRS	n (mRNA)	n (miRNA)	n (DNAm)
Female	55	Control	45	23.97	1.44	55 (100%)	51 (92.7%)	50 (90.9%)
	50	Patient	42	24	23.16	50 (100%)	39 (78%)	39 (78%)
Male	34	Control	45	24.02	1.18	34 (100%)	34 (100%)	31 (91.1%)
	30	Patient	43	25.51	23.47	30 (100%)	30 (100%)	28 (93.3%)
Total	**169**							

b

Data Collection



Taken from Amazigh Mokhtari's PhD manuscript.

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      CD4               CD8                MO                 B                  NK                 GR
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Relative to blood cell composition (T cells subsets, monocytes, B cells, NK cells and granulocytes) inferred from DNAm.

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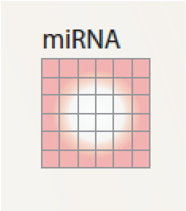

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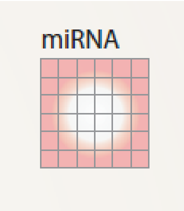

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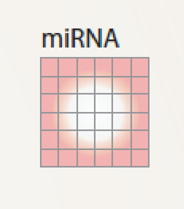

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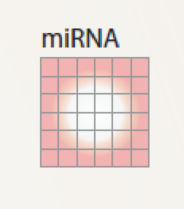

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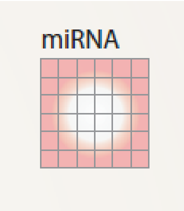

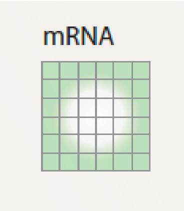

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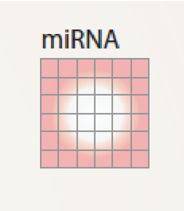

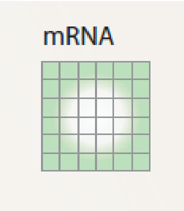

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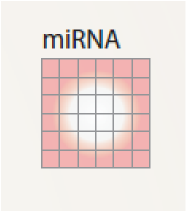

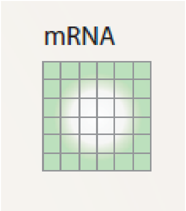

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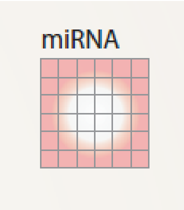

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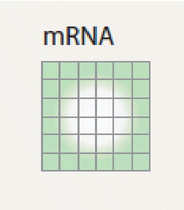

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$MAD = median(|x_i - median(\mathbf{x})|)$, it is a robust estimation of the standard deviation.

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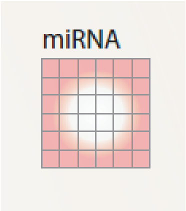

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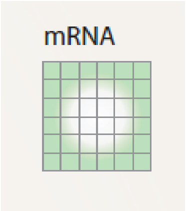

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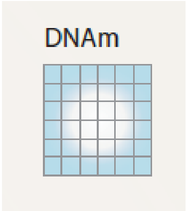

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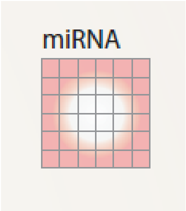

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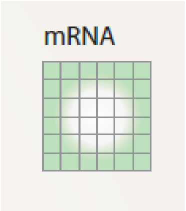

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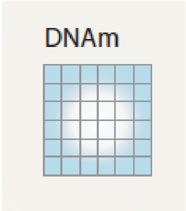

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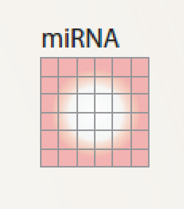

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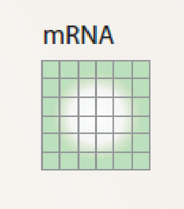

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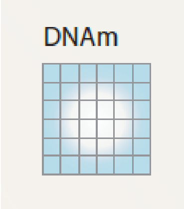

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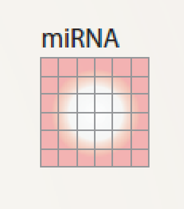

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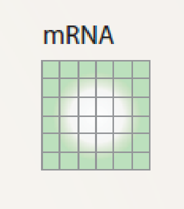

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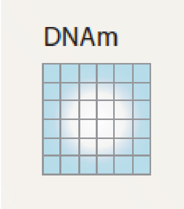

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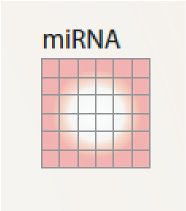

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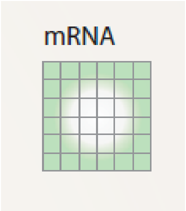

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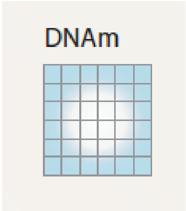

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Finally: individuals common to ALL omics data are kept.

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If the variables are strongly linked ➔ $RSS_0 \gg RSS_1$ ➔ $F \sim \frac{RSS_0}{RSS_1} \times (n-2) \gg n-2$

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$$F = \frac{(RSS_0 - RSS_1)}{1} \times \frac{(n-2)}{RSS_1} = \frac{(\sum_i (y_i - \beta_0)^2 - \sum_i (y_i - \beta_0 - \beta_1 x_i)^2)}{1} \times \frac{(n-2)}{\sum_i (y_i - \beta_0 - \beta_1 x_i)^2}$$

It is possible to show that F follows an F-distribution of 1 and $n-2$ degrees of freedom.

If the variables are strongly linked ➔ $RSS_0 \gg RSS_1$ ➔ $F \sim \frac{RSS_0}{RSS_1} \times (n-2) \gg n-2$ ➔ The test is likely to be rejected.

If the variables are NOT strongly linked ➔ $RSS_0 \sim RSS_1$

ChAMP's representation: F-test

In order to evaluate the link between two continuous variables y_i and x_i, the following model is used:

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i$$

Where β_0 is the intercept, β_1 is the coefficient associated with x_i and $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$.

The following test is used:
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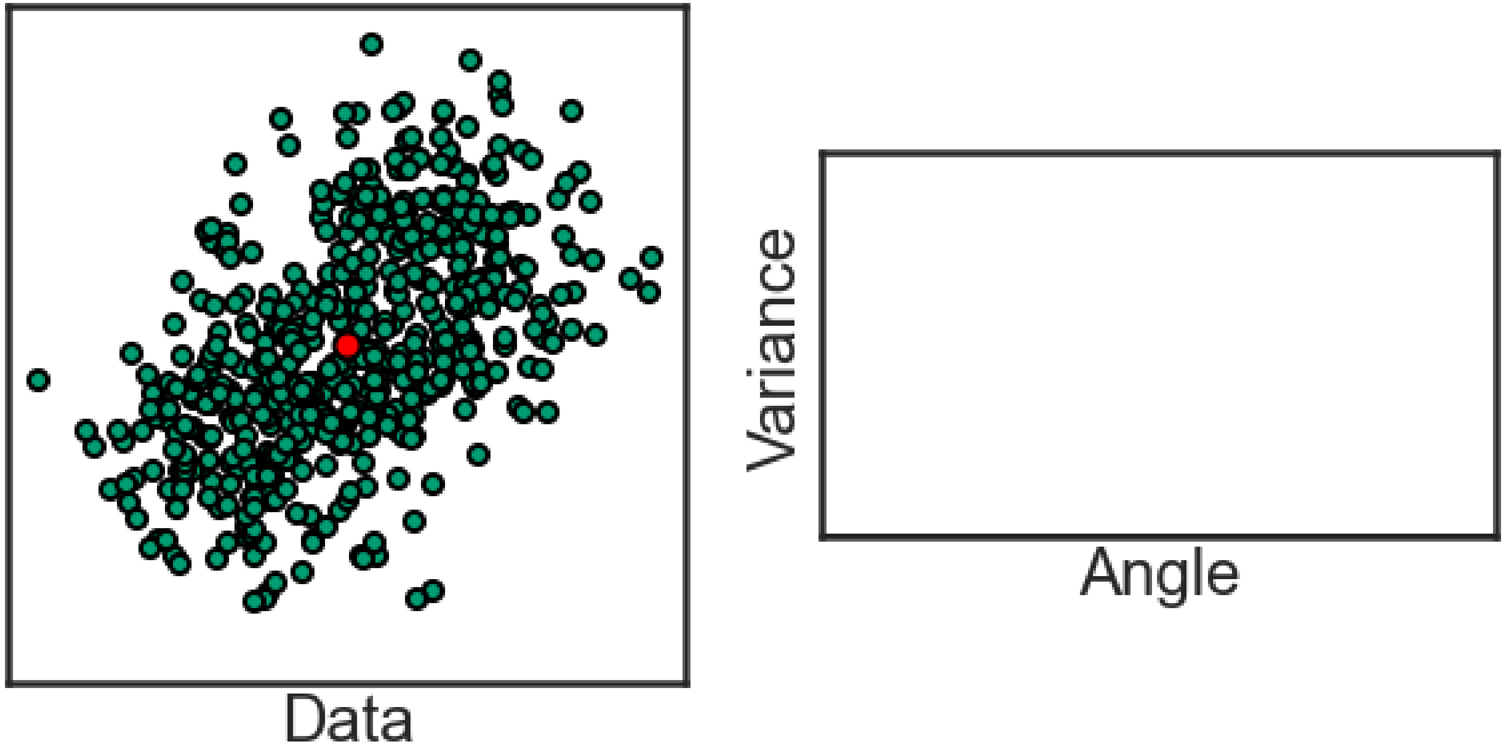
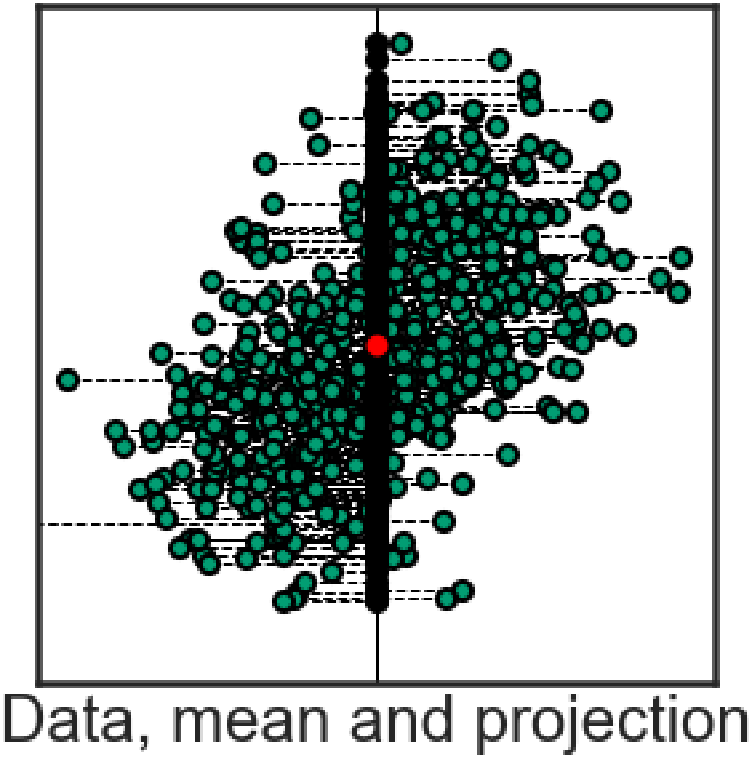
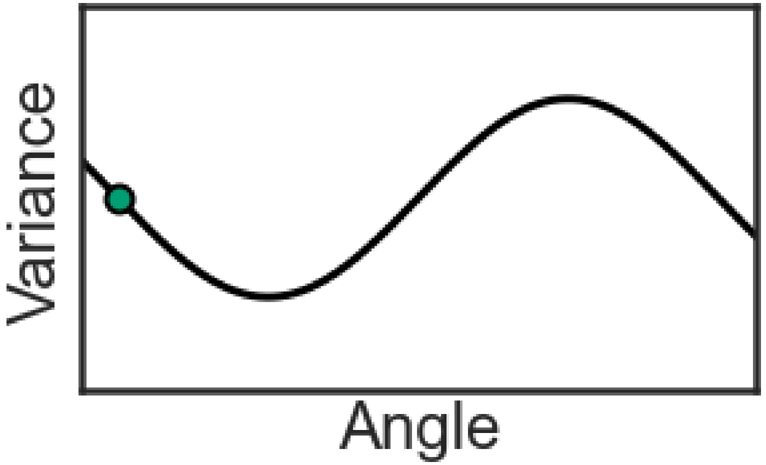
If the variables are NOT strongly linked ➔ $RSS_0 \sim RSS_1$ ➔ $F \sim 0$ ➔ The test is likely to be accepted.

Principle of Principal Component Analysis (PCA)



Principle of Principal Component Analysis (PCA)





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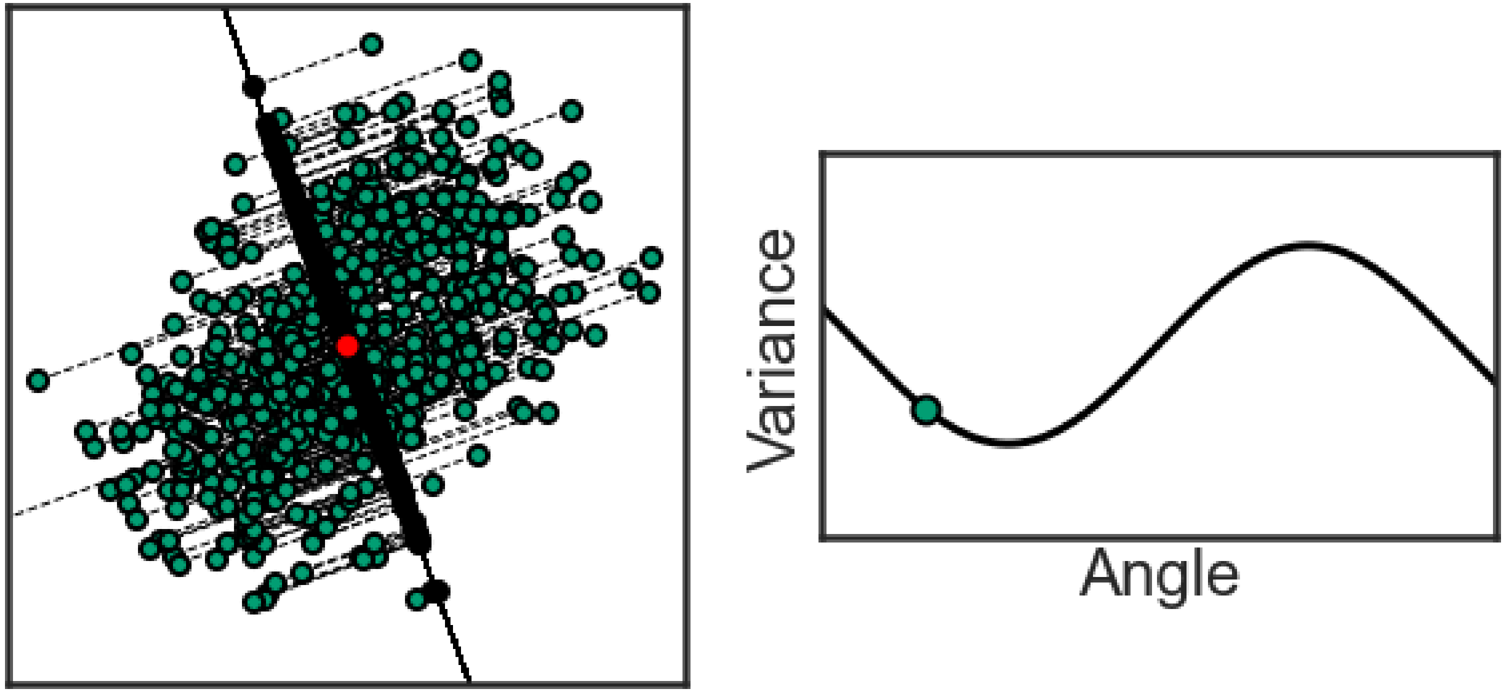
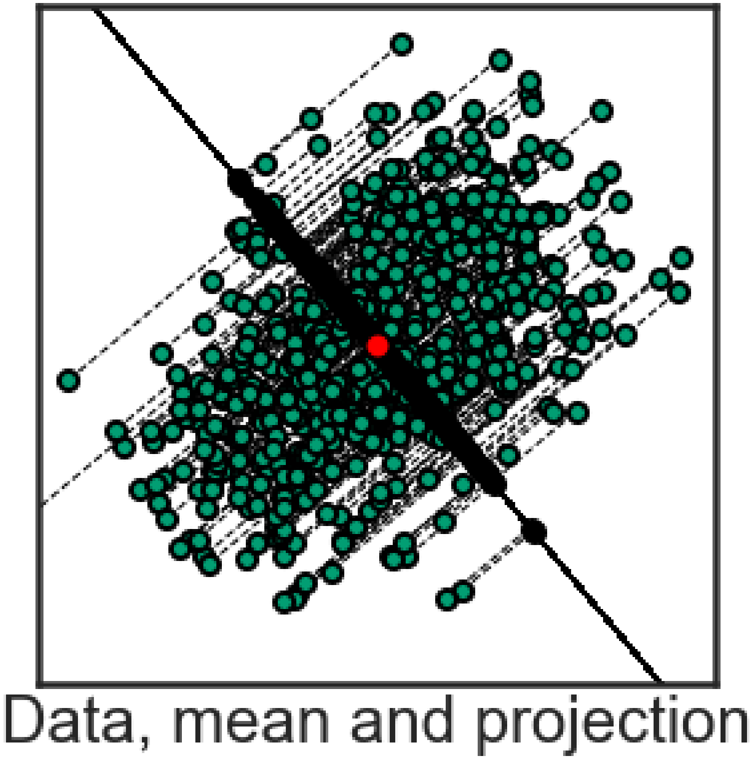
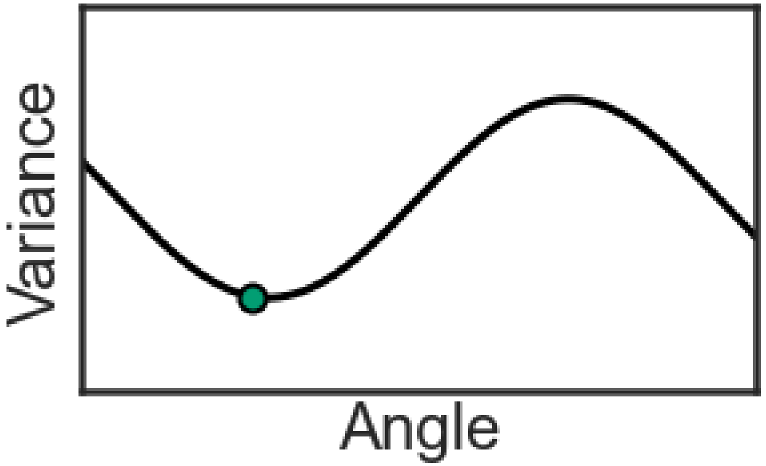


Data, mean and projection

Principle of Principal Component Analysis (PCA)





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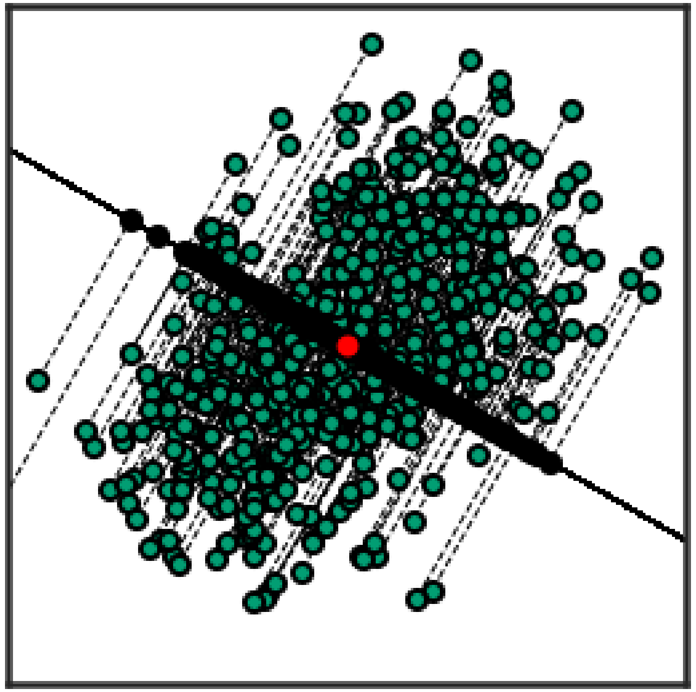

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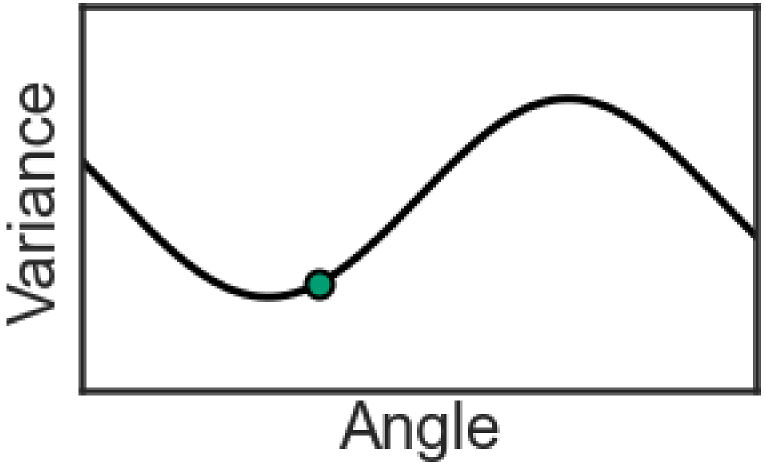

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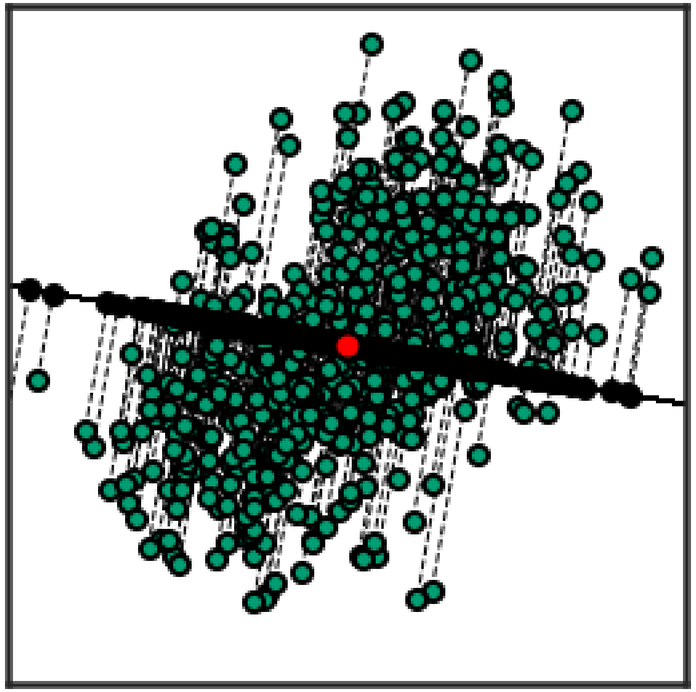

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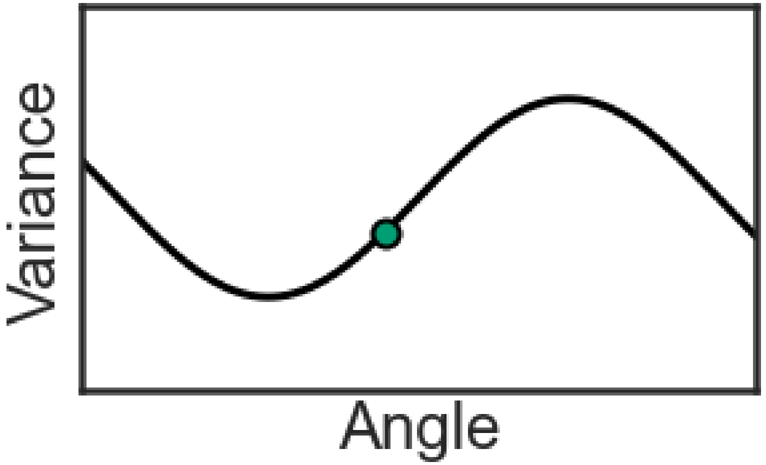

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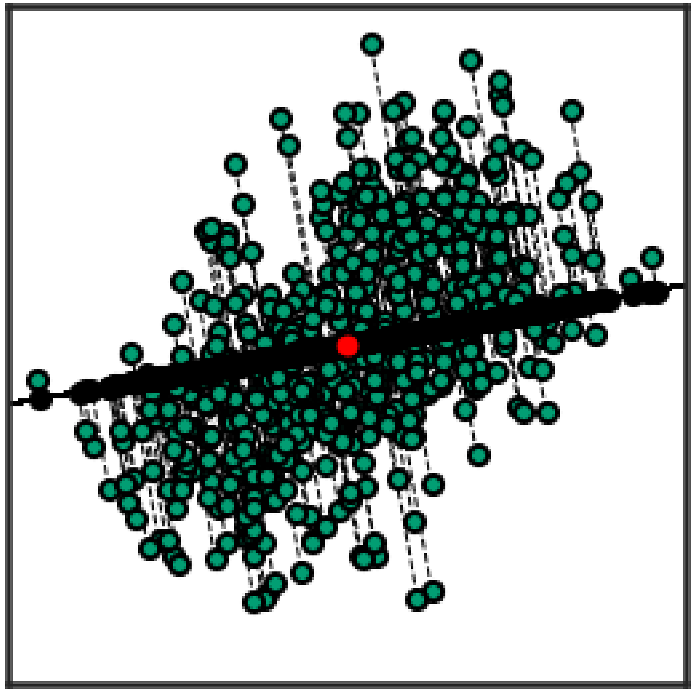

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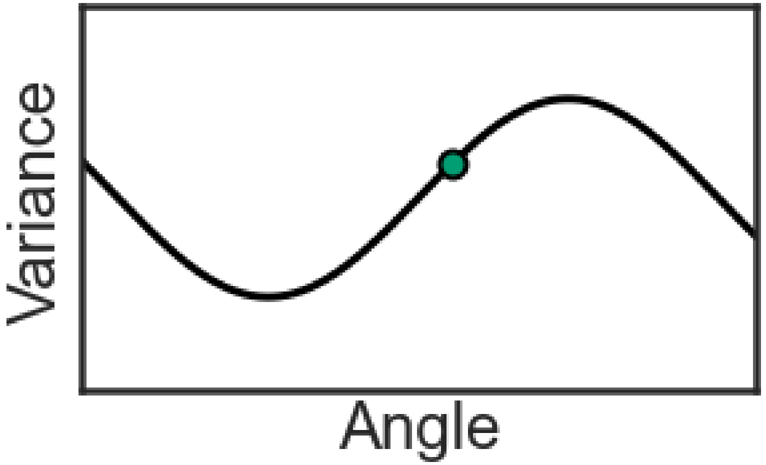

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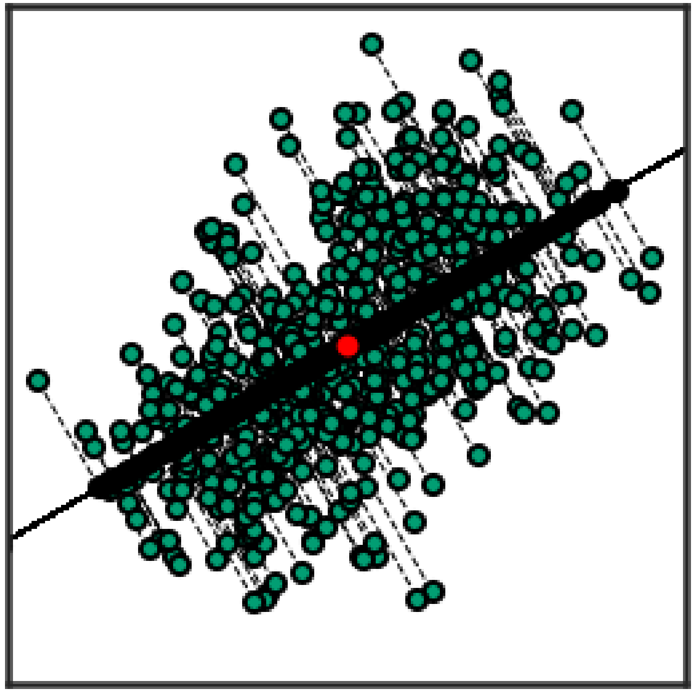

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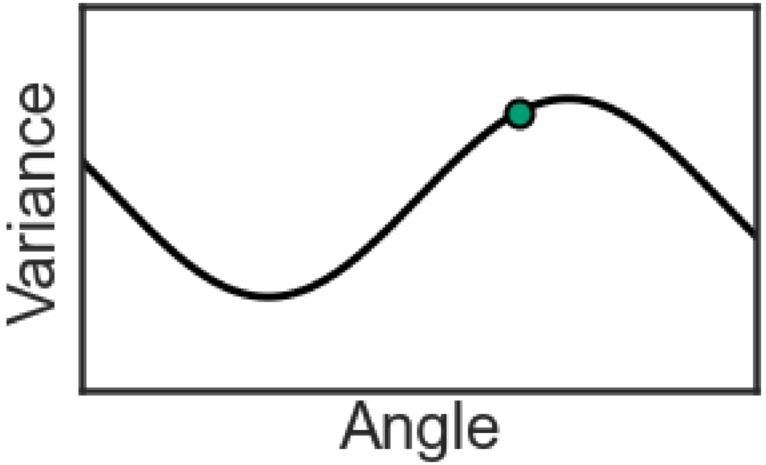

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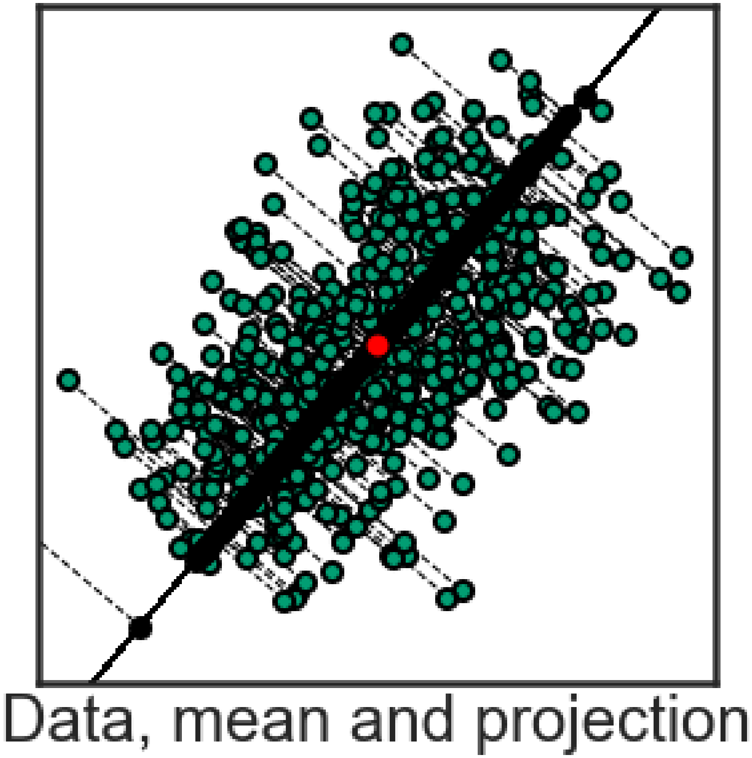

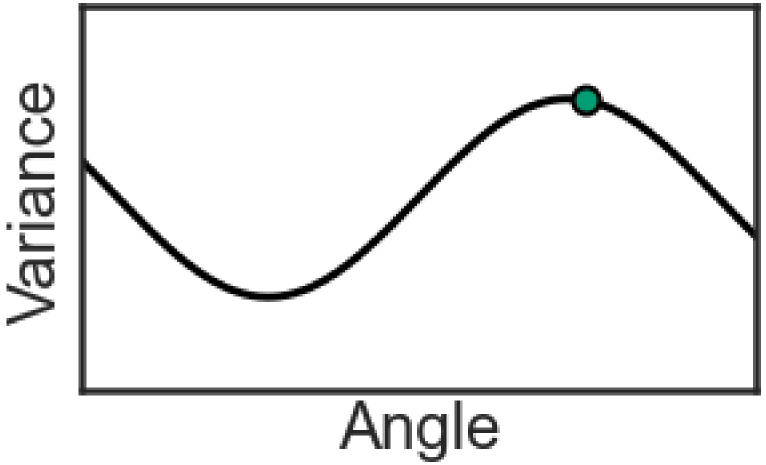

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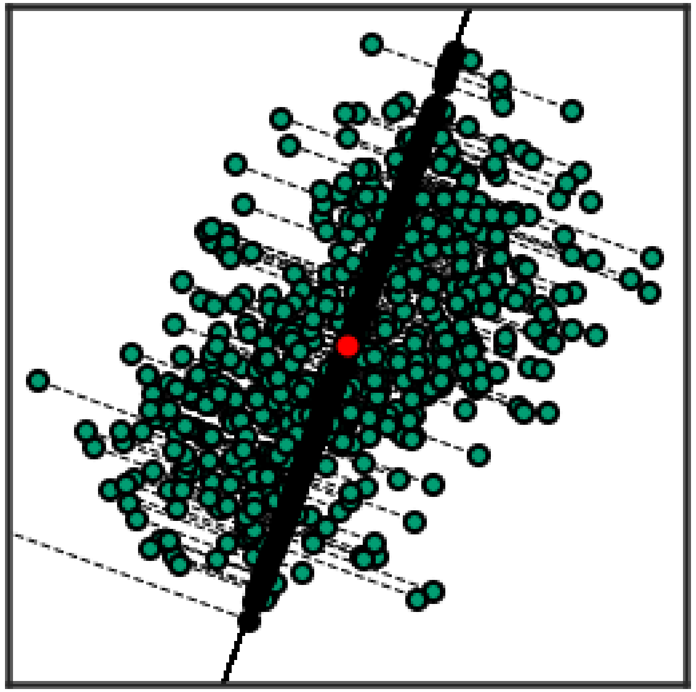

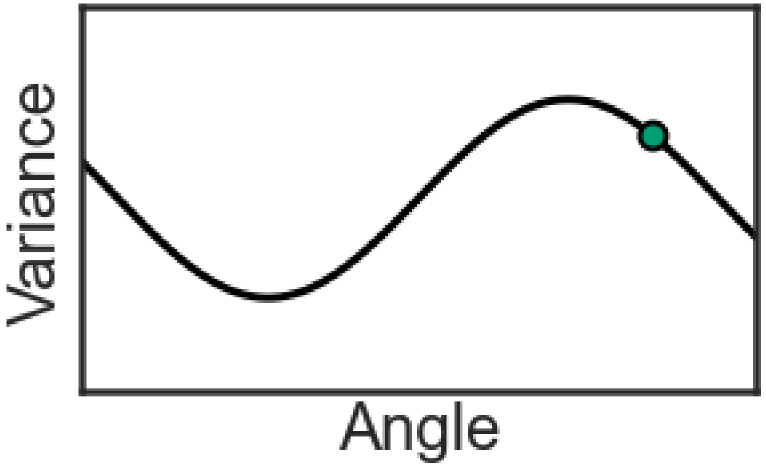

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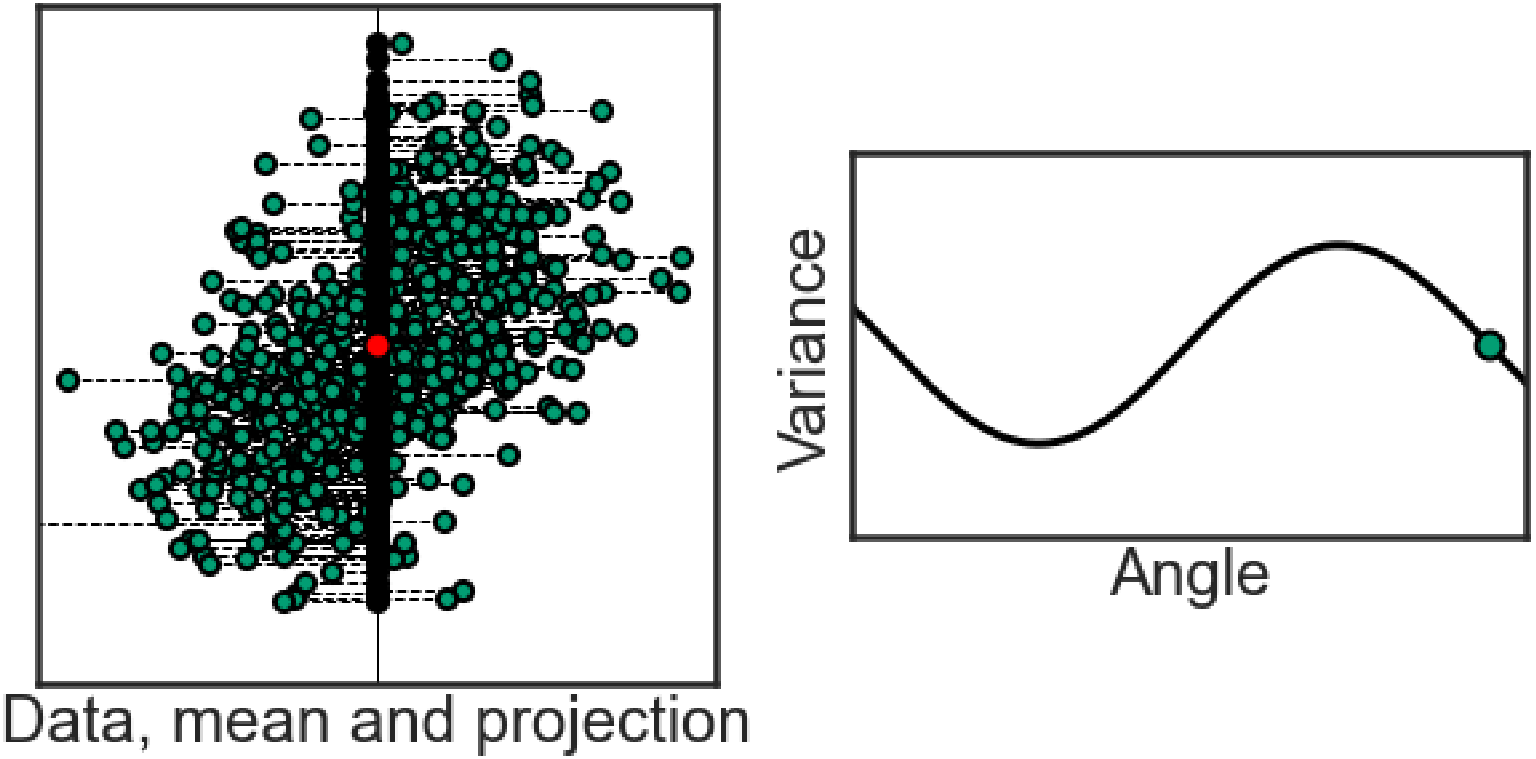

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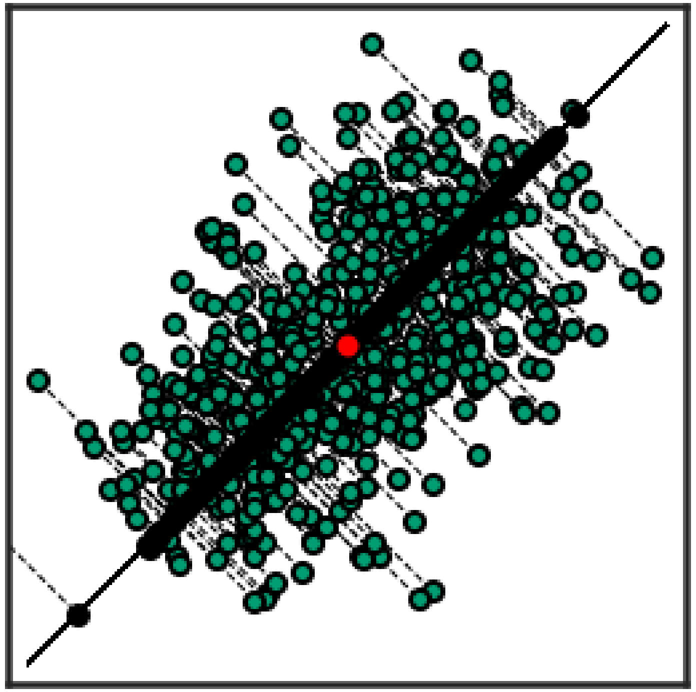

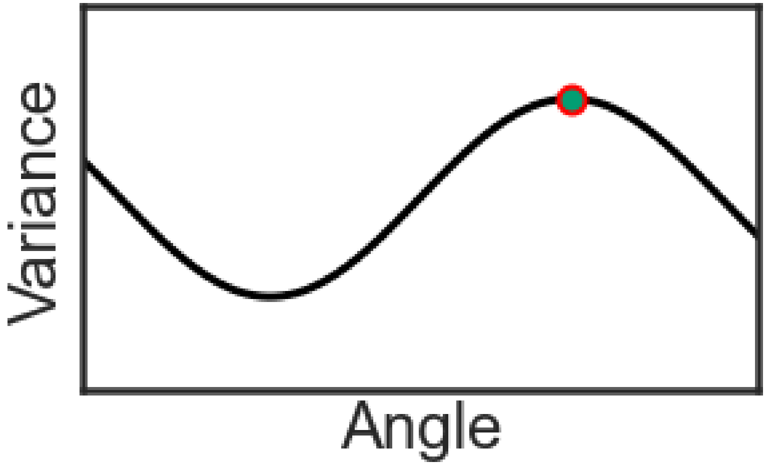

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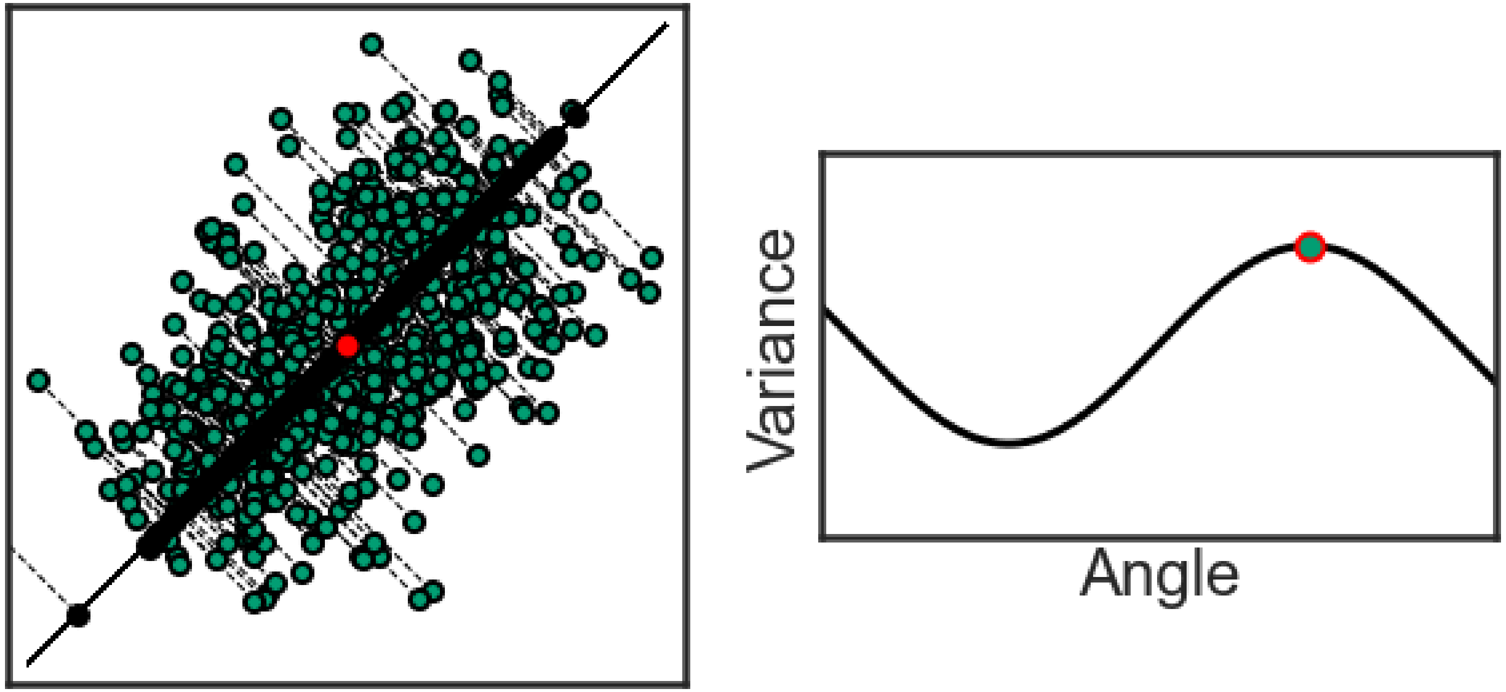

Principal direction (main axis)

How can we estimate this projection ?

Courtesy to Arthur Tenenhaus, Laurent Le Busquet and Julien Bect.

Total Variance

Total Variance

$$\mathbf{X} = \begin{pmatrix} x_{11} & \cdots & x_{1p} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{np} \end{pmatrix}$$

Total Variance

$$\mathbf{X} = \overbrace{\begin{pmatrix} x_{11} & \cdots & x_{1p} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{np} \end{pmatrix}}^{p \text{ variables}}$$

Total Variance

n individuals/subjects

$$\begin{array}{c} p \text{ variables} \\ \mathbf{X} = \begin{pmatrix} x_{11} & \cdots & x_{1p} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{np} \end{pmatrix} \end{array}$$

Total Variance

n individuals/subjects

p variables

$$\mathbf{X} = \begin{pmatrix} x_{11} & \cdots & x_{1p} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{np} \end{pmatrix} = \begin{pmatrix} \mathbf{x}_1^\top \\ \mathbf{x}_2^\top \\ \vdots \\ \mathbf{x}_n^\top \end{pmatrix}$$

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Total Variance (TV)

Total Variance

n individuals/subjects

p variables

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$$\text{Total Variance (TV)} = \sum_{j=1}^{p} \text{Variance}\left(\text{Variable}_\mathrm{j}\right)$$

Total Variance

n individuals/subjects

p variables

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$$\text{Total Variance (TV)} = \sum_{j=1}^{p} \text{Variance}\left(\text{Variable}_\mathrm{j}\right) = \frac{1}{n}\sum_{j=1}^{p}\sum_{i=1}^{n}\left(x_{ij} - \overline{x_j}\right)^2$$

Total Variance

n individuals/subjects

p variables

$$\mathbf{X} = \begin{pmatrix} x_{11} & \cdots & x_{1p} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{np} \end{pmatrix} = \begin{pmatrix} \mathbf{x}_1^\top \\ \mathbf{x}_2^\top \\ \vdots \\ \mathbf{x}_n^\top \end{pmatrix} \text{ where } \mathbf{x}_\mathrm{i} = \begin{pmatrix} x_{i1} \\ x_{i2} \\ \vdots \\ x_{ip} \end{pmatrix}$$

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$$= \frac{1}{n}\sum_{i=1}^{n}\left\| \begin{pmatrix} x_{i1} \\ x_{i2} \\ \vdots \\ x_{ip} \end{pmatrix} - \begin{pmatrix} \overline{x_1} \\ \overline{x_2} \\ \vdots \\ \overline{x_p} \end{pmatrix} \right\|_2^2$$

Total Variance

n individuals/subjects

p variables

$$\mathbf{X} = \begin{pmatrix} x_{11} & \cdots & x_{1p} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{np} \end{pmatrix} = \begin{pmatrix} \mathbf{x}_1^\top \\ \mathbf{x}_2^\top \\ \vdots \\ \mathbf{x}_n^\top \end{pmatrix} \text{ where } \mathbf{x}_\mathrm{i} = \begin{pmatrix} x_{i1} \\ x_{i2} \\ \vdots \\ x_{ip} \end{pmatrix}$$

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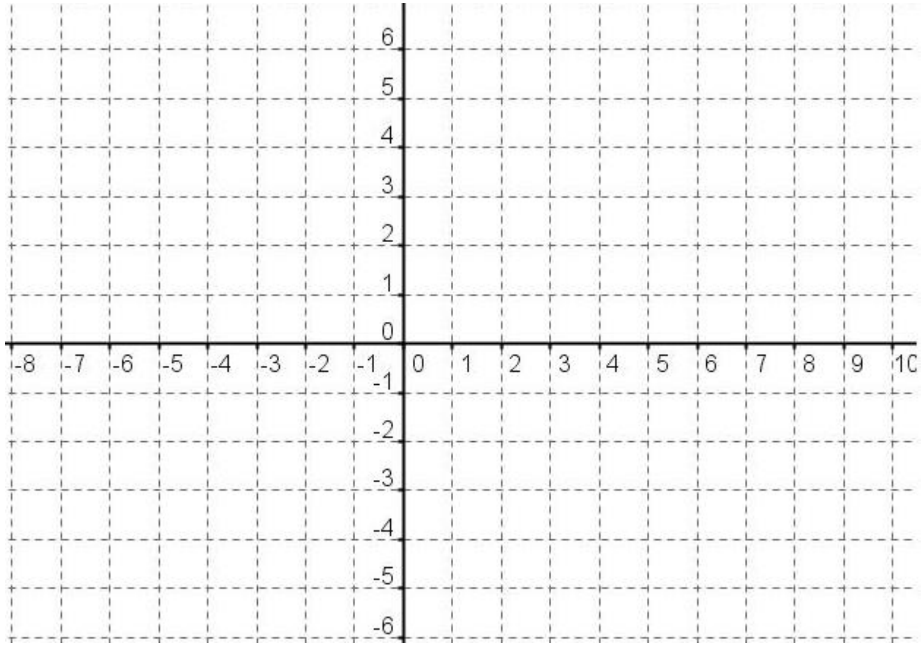
Here, we suppose that every variable is centered $\Rightarrow \text{TV} = \frac{1}{n}\sum_{i=1}^{n}\|\mathbf{x}_\mathrm{i}\|_2^2$

Total Variance – Example in 2D



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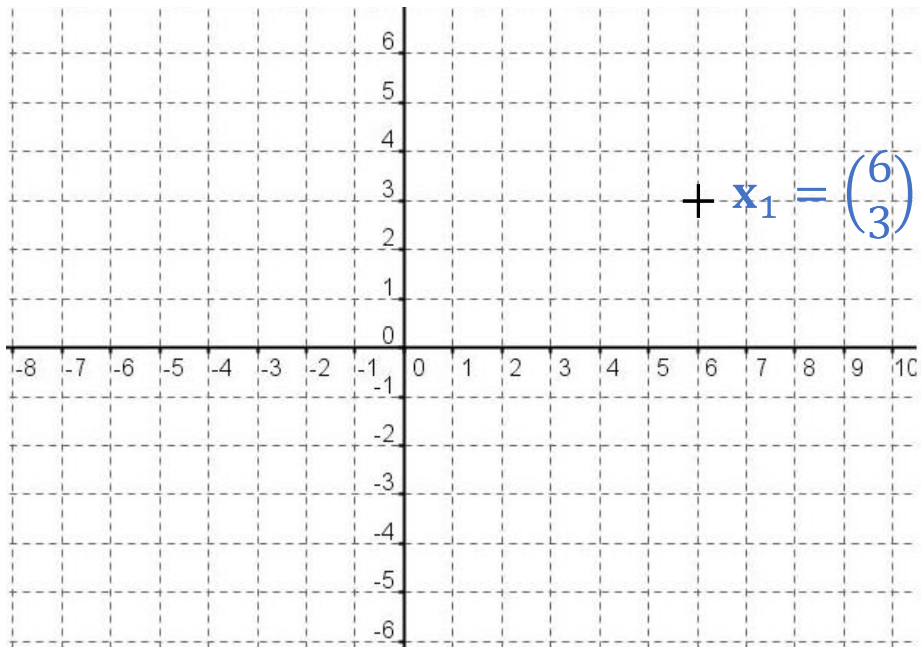

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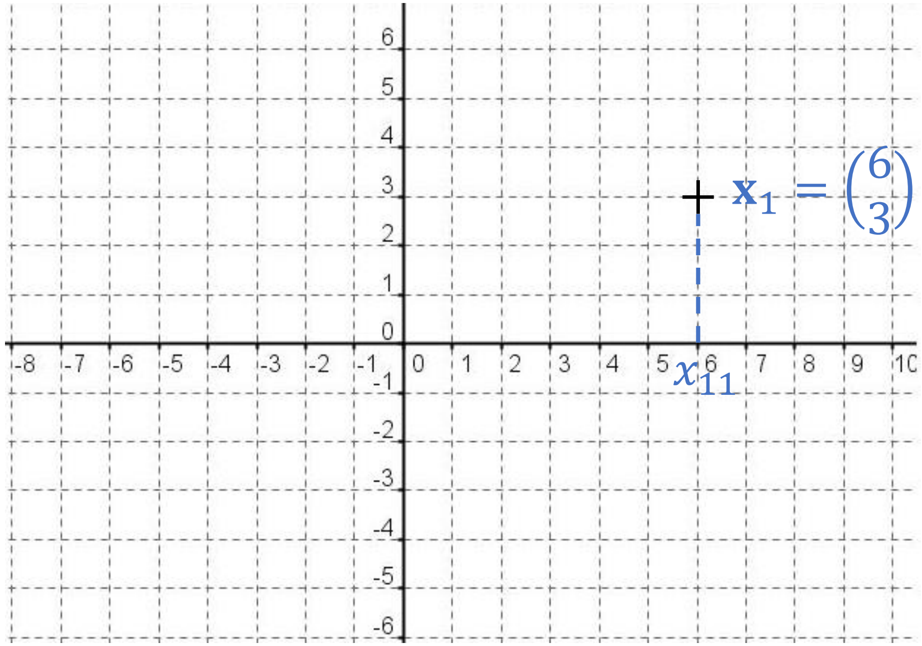

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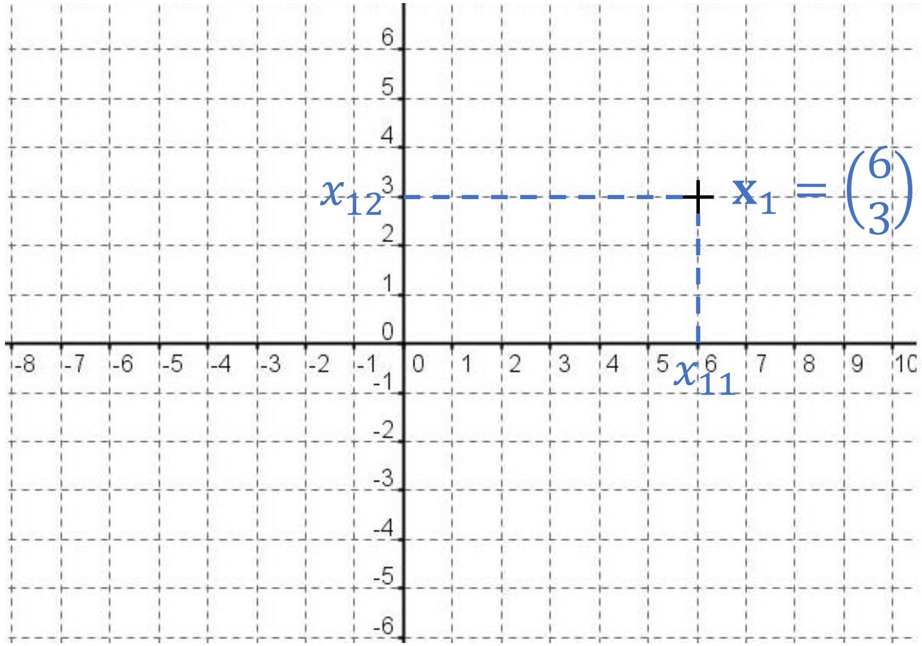
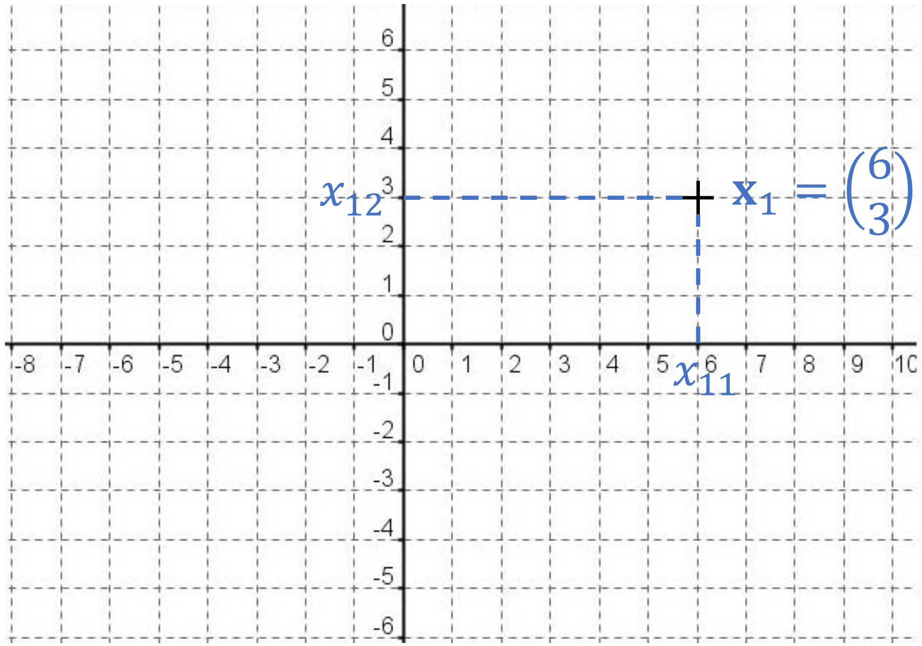


Total Variance – Example in 2D

$$\|\mathbf{x}_1\|_2 = \sqrt{x_{11}^2 + x_{12}^2}$$



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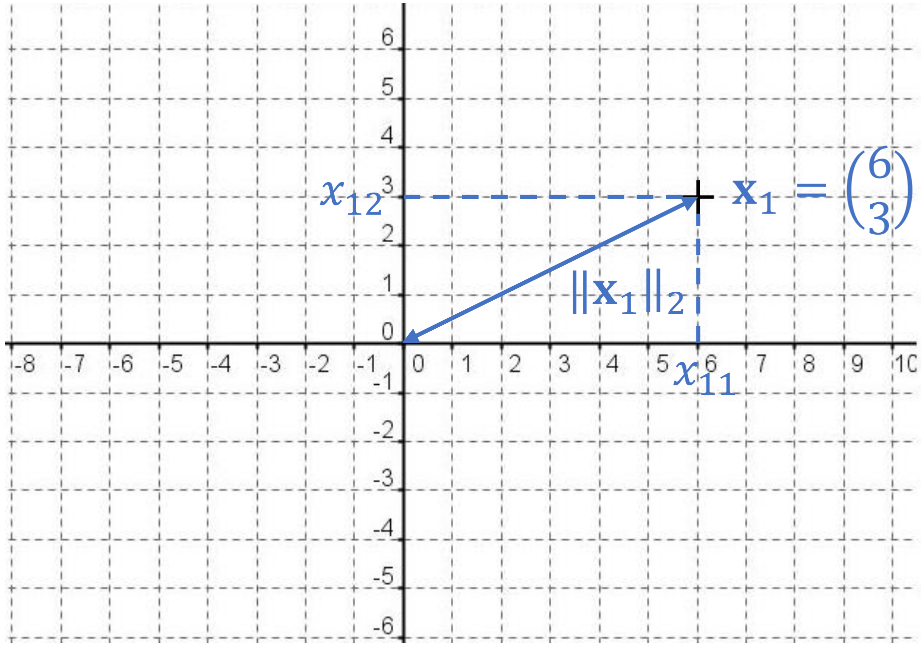

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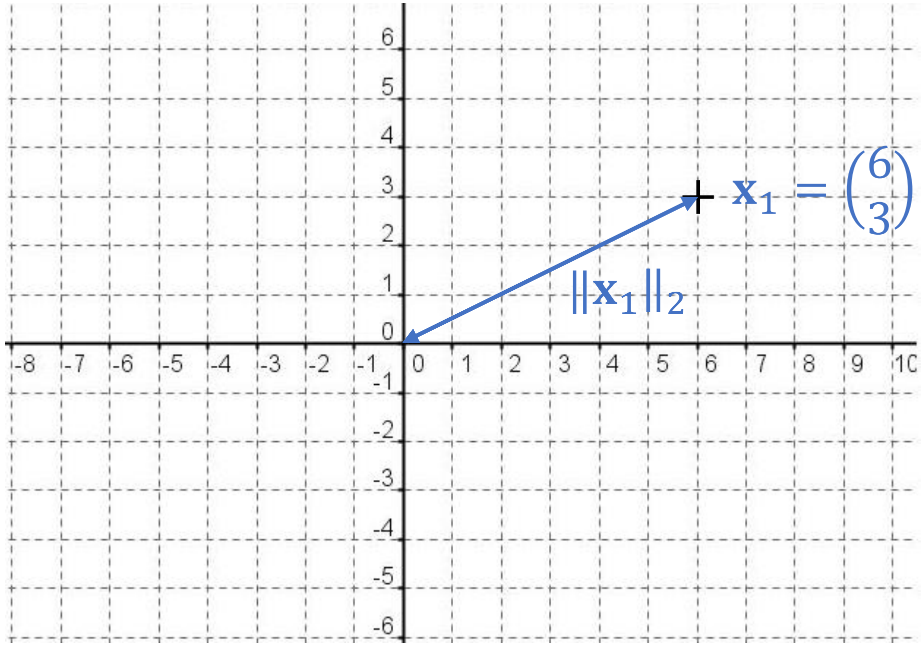
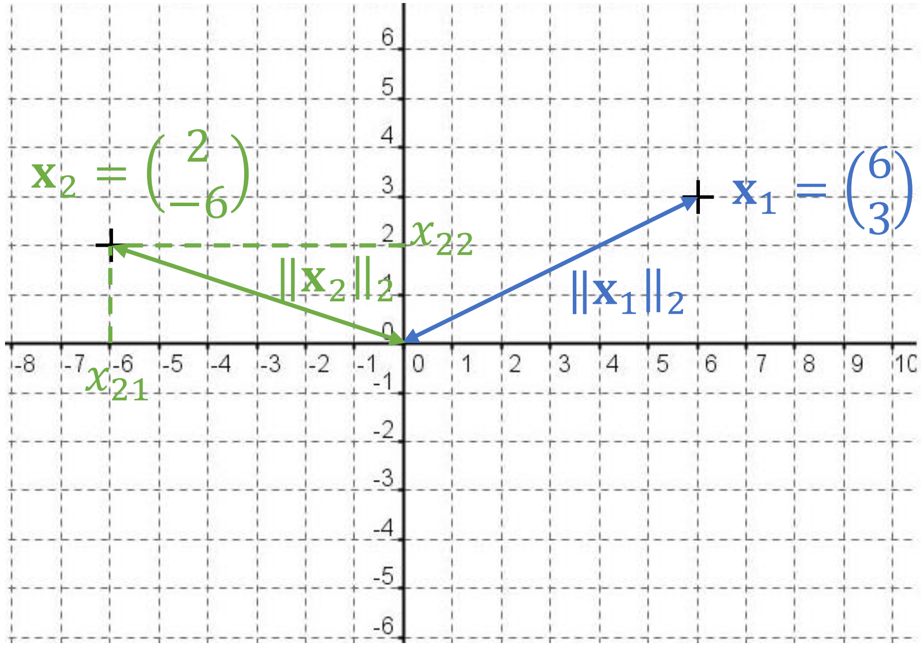


Total Variance – Example in 2D

$$\|\mathbf{x}_1\|_2 = \sqrt{x_{11}^2 + x_{12}^2} \qquad \|\mathbf{x}_2\|_2 = \sqrt{x_{21}^2 + x_{22}^2}$$



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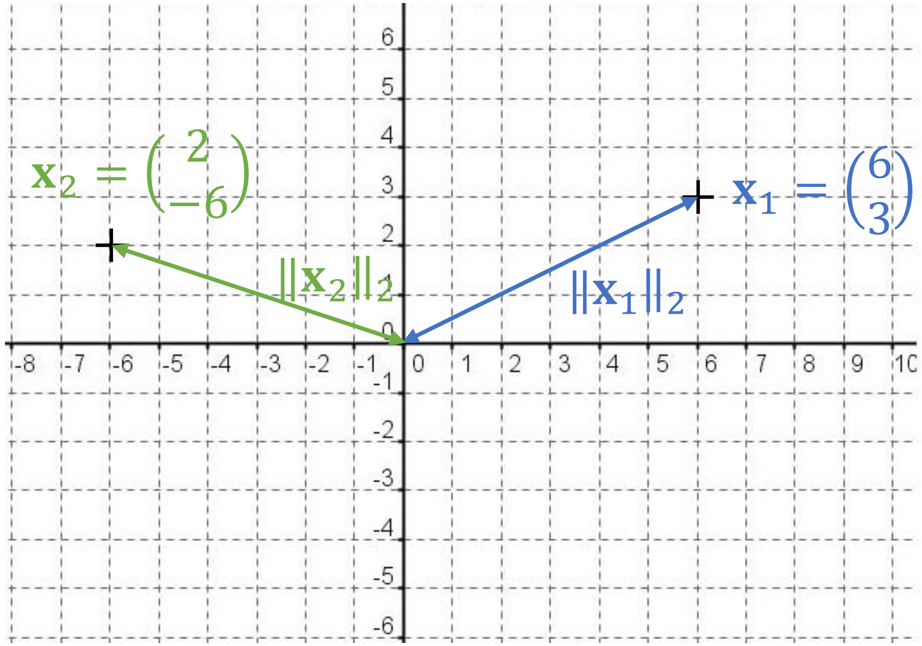

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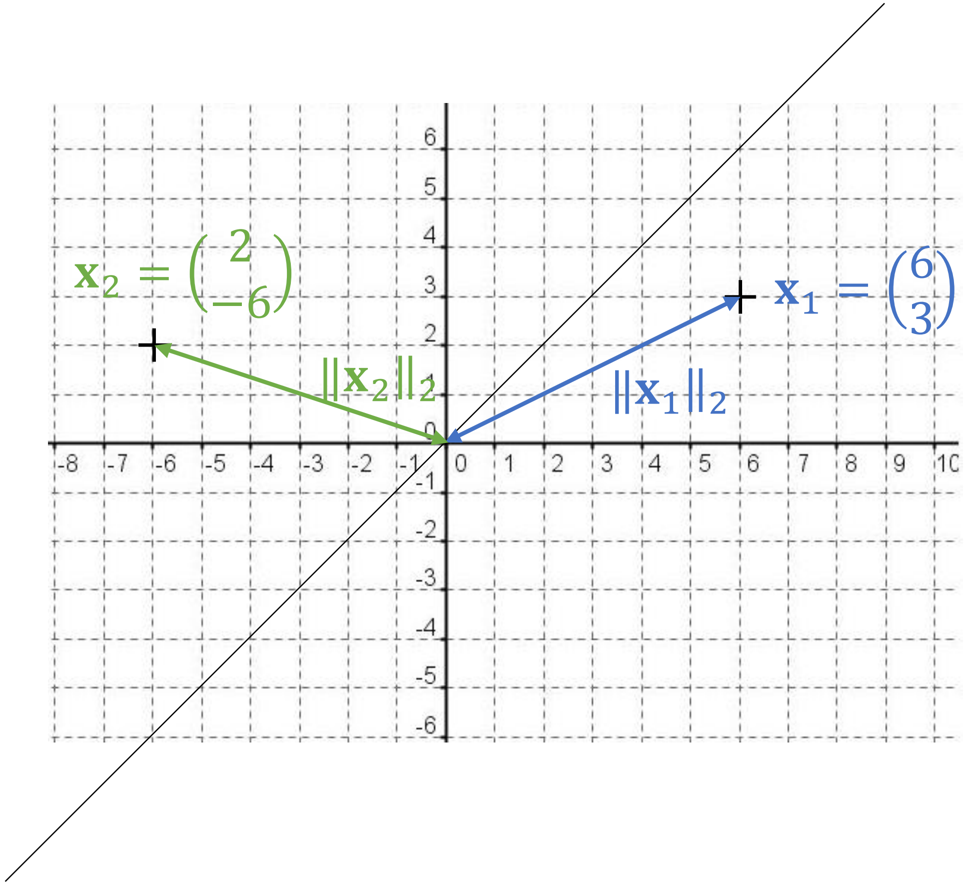

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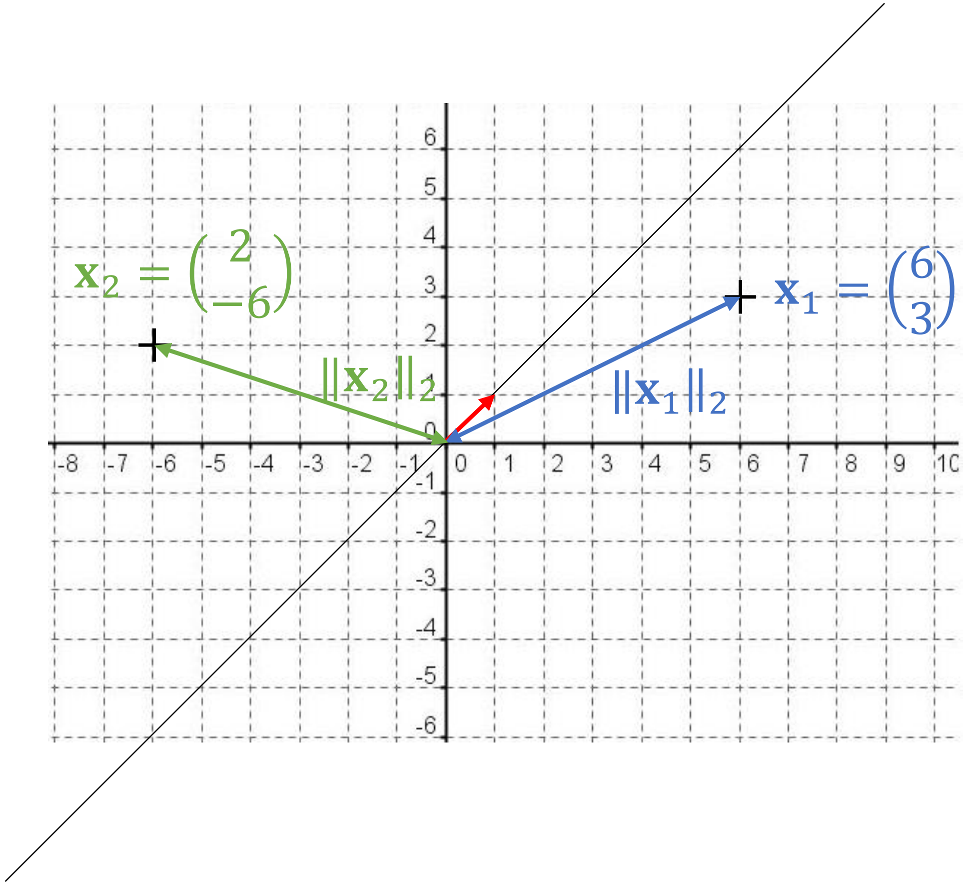

$\|\mathbf{x}_1\|_2 = \sqrt{x_{11}^2 + x_{12}^2}$

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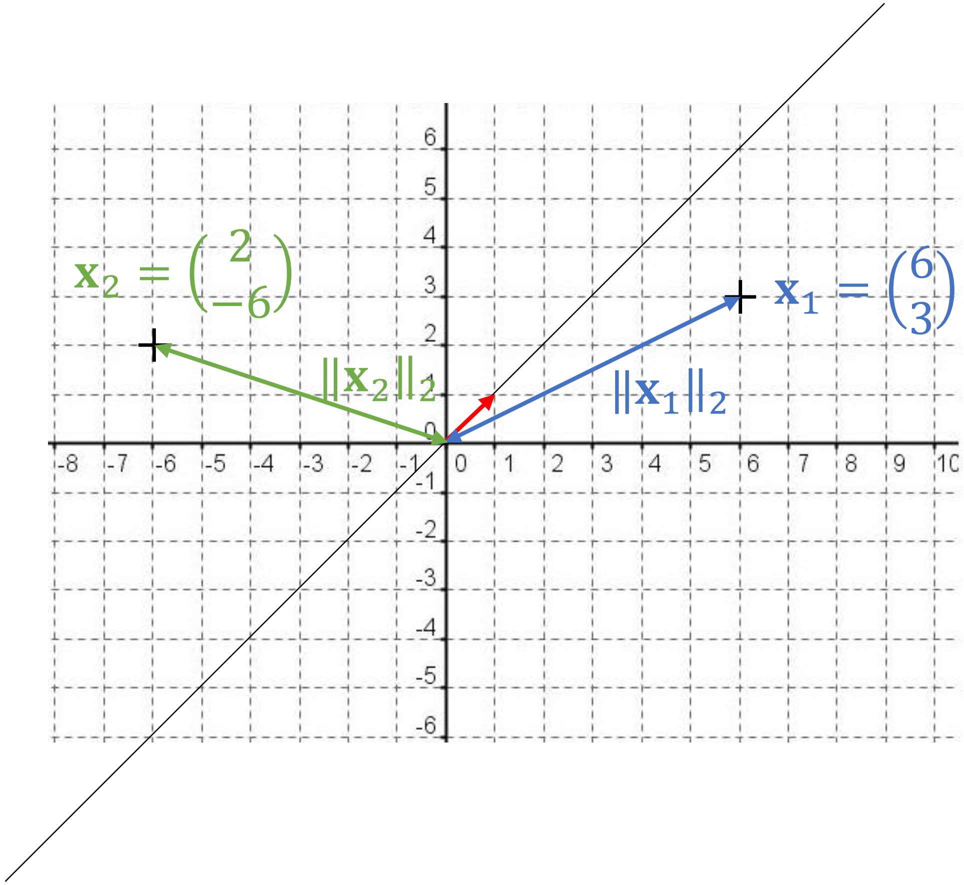
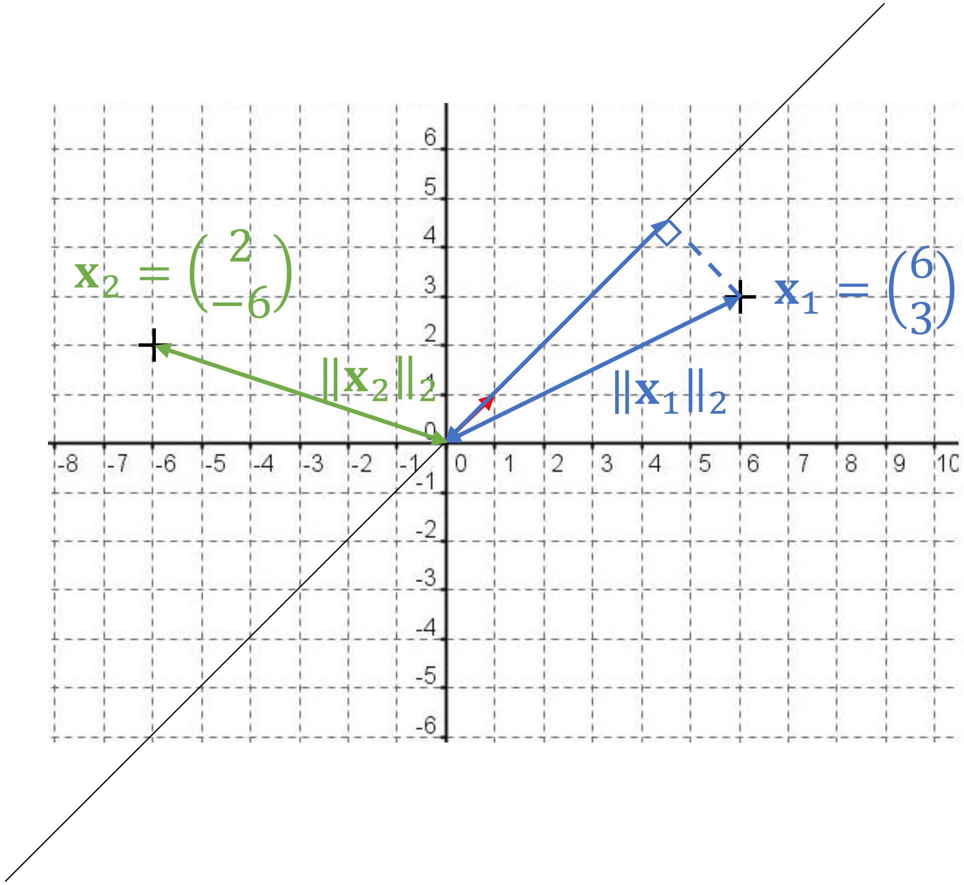
Total Variance – Example in 2D



$\|\mathbf{x}_1\|_2 = \sqrt{x_{11}^2 + x_{12}^2}$ $\|\mathbf{x}_2\|_2 = \sqrt{\mathrm{x}_{21}^2 + \mathrm{x}_{22}^2}$

Director vector $\mathbf{w} = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$. We can see that $\|\mathbf{w}\|_2 = 1$.

Total Variance – Example in 2D



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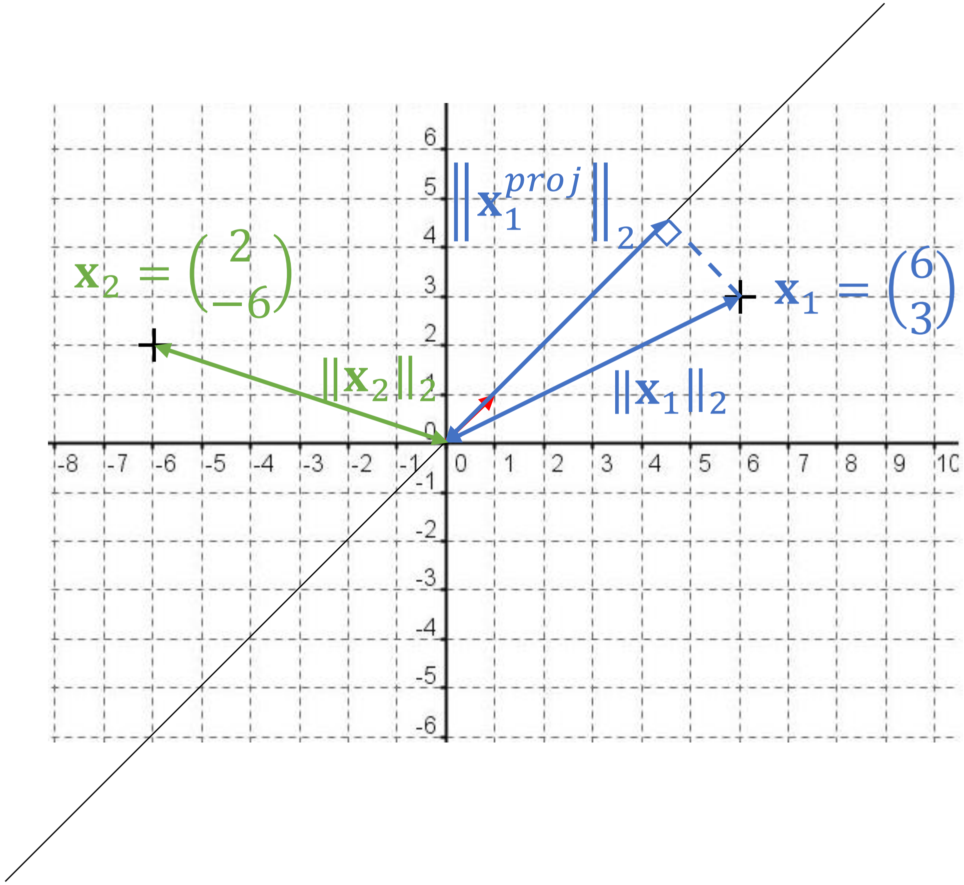
Total Variance – Example in 2D



$\|\mathbf{x}_1\|_2 = \sqrt{x_{11}^2 + x_{12}^2}$ $\|\mathbf{x}_2\|_2 = \sqrt{\mathrm{x}_{21}^2 + \mathrm{x}_{22}^2}$

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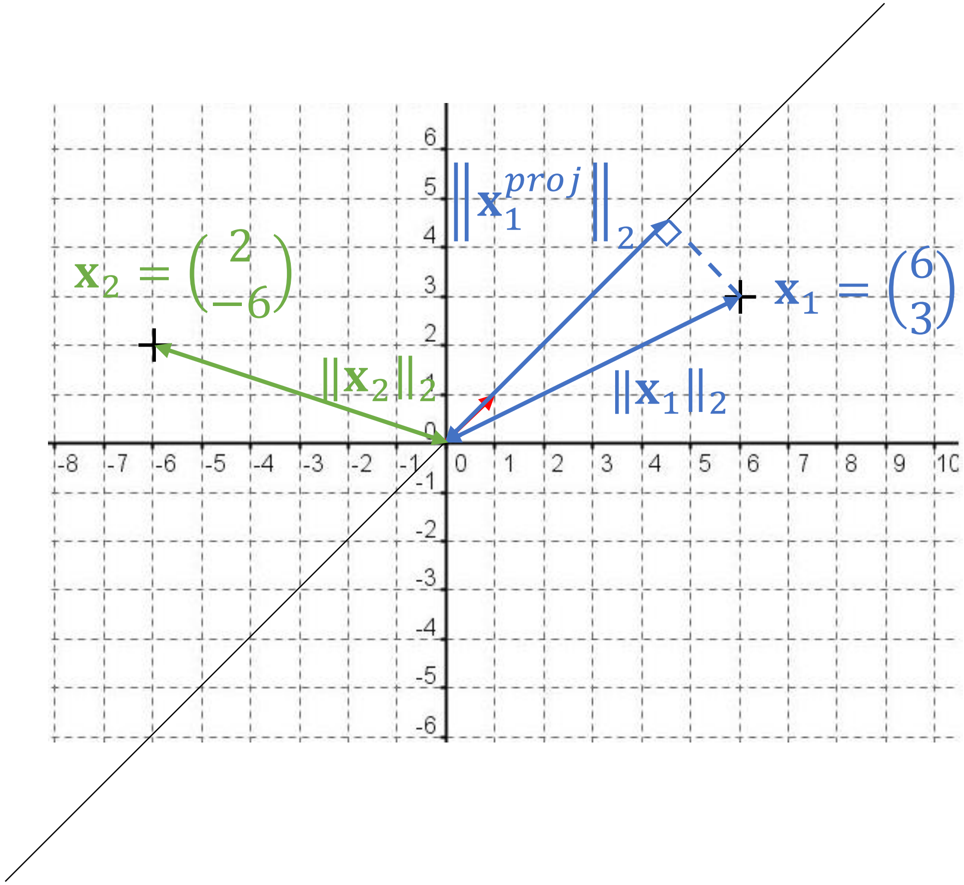

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$\mathbf{x}_1^\top \mathbf{w}$

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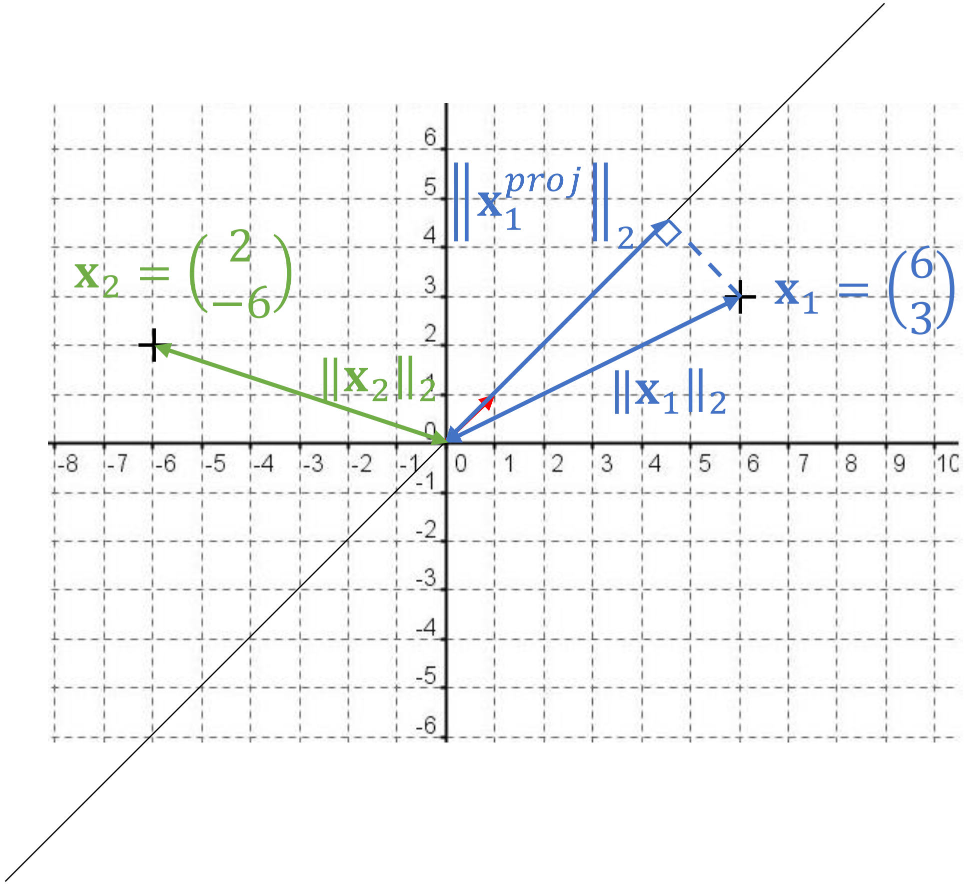

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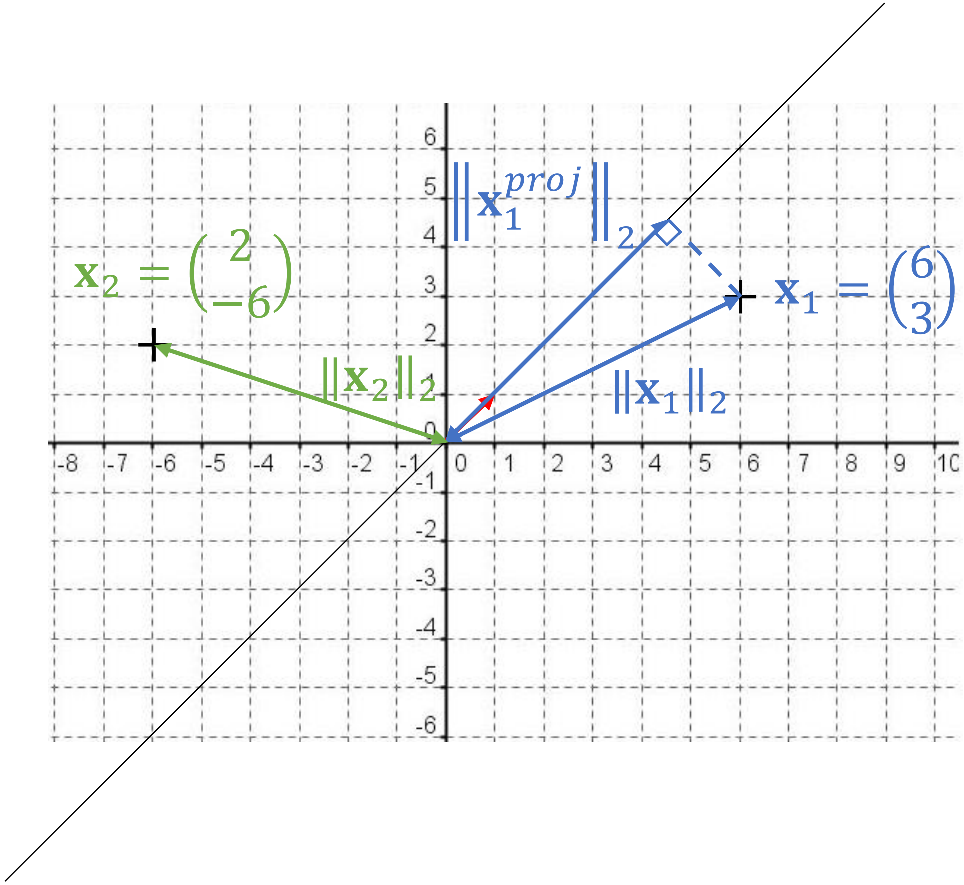
$\mathbf{x}_1^\top \mathbf{w} = (x_{11} \quad x_{12}) \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$

Total Variance – Example in 2D



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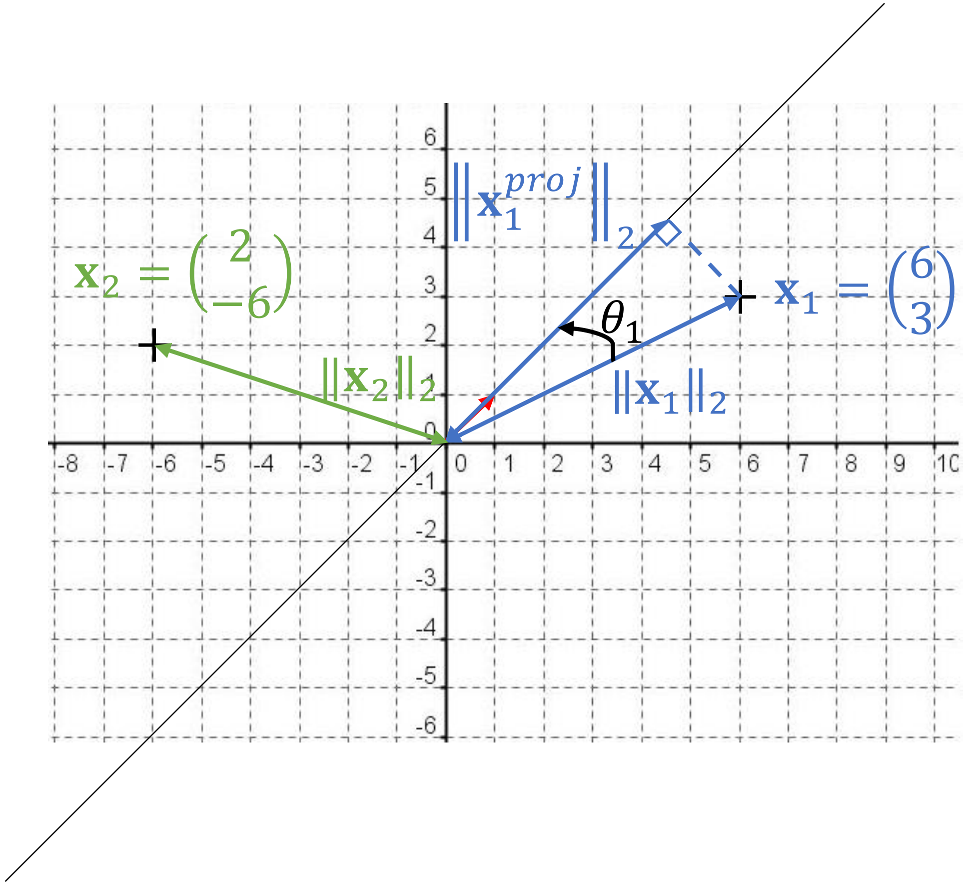

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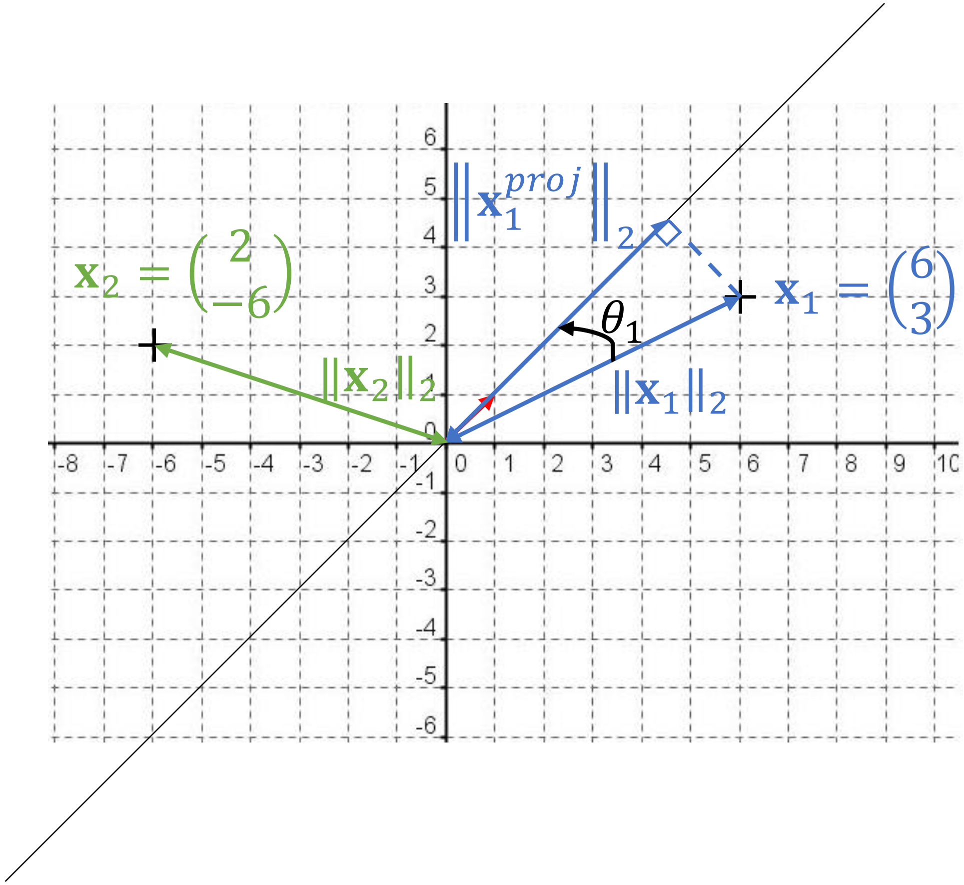
$$= \|\mathbf{x}_1\|_2 \|\mathbf{w}\|_2 \cos(\theta_1)$$

Total Variance – Example in 2D



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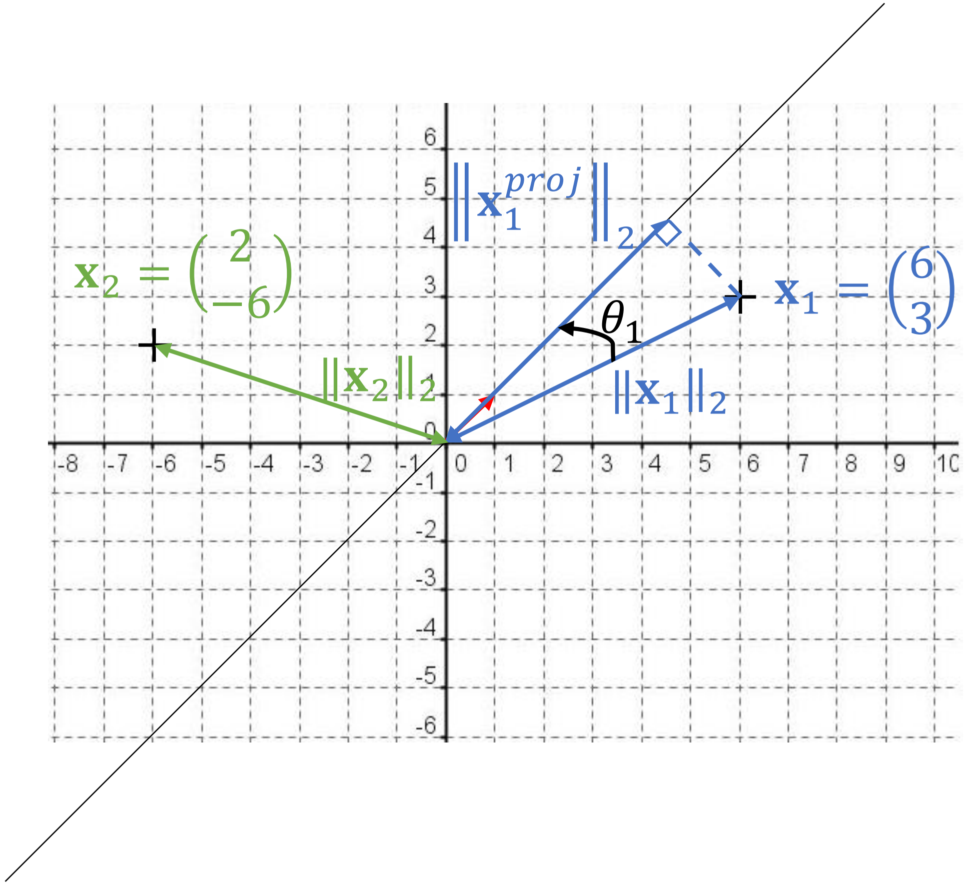

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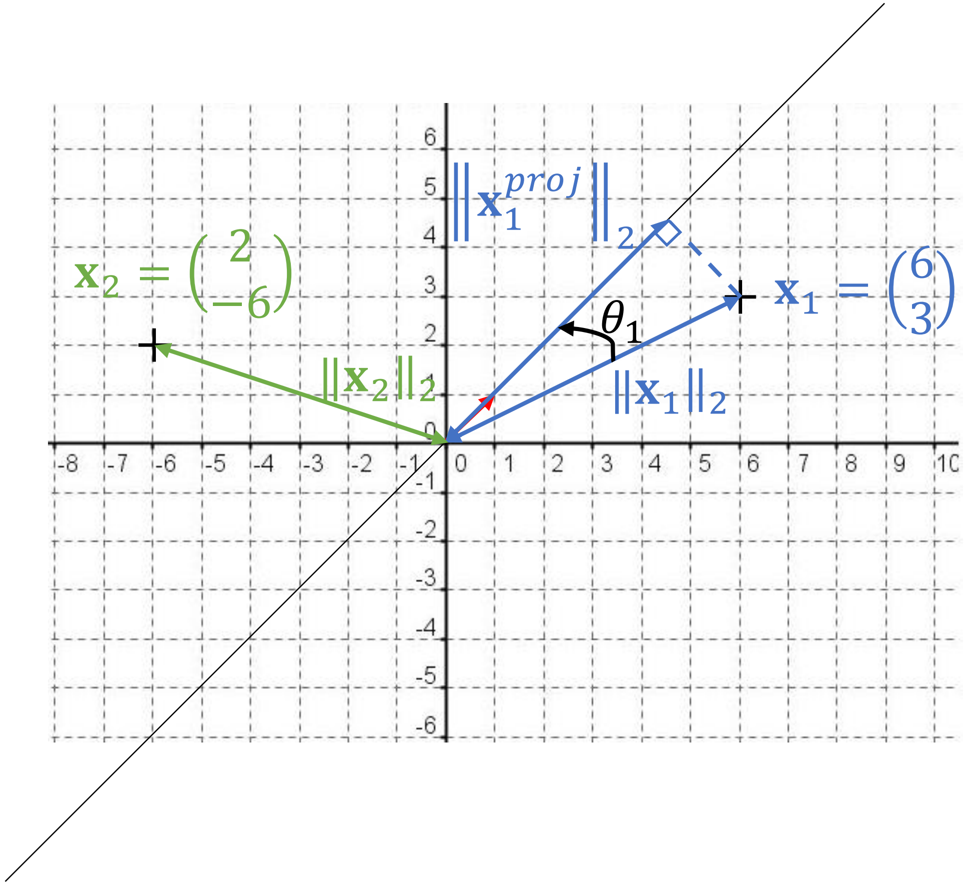

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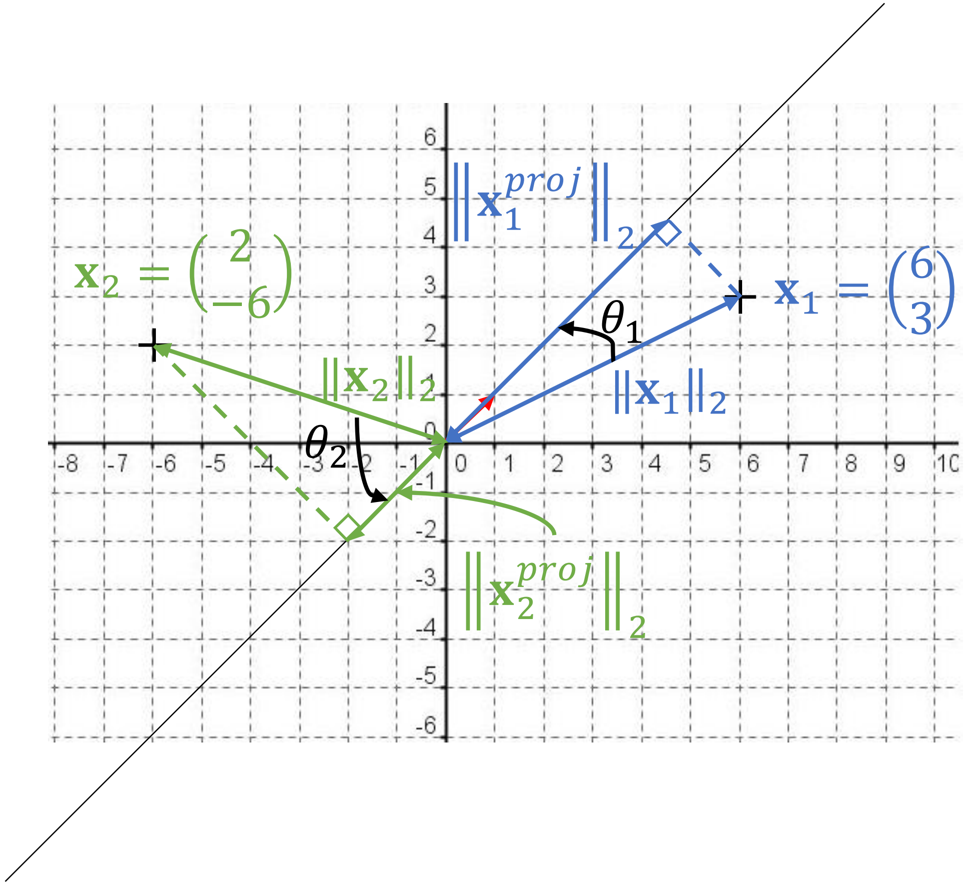
Total Variance – Example in 2D



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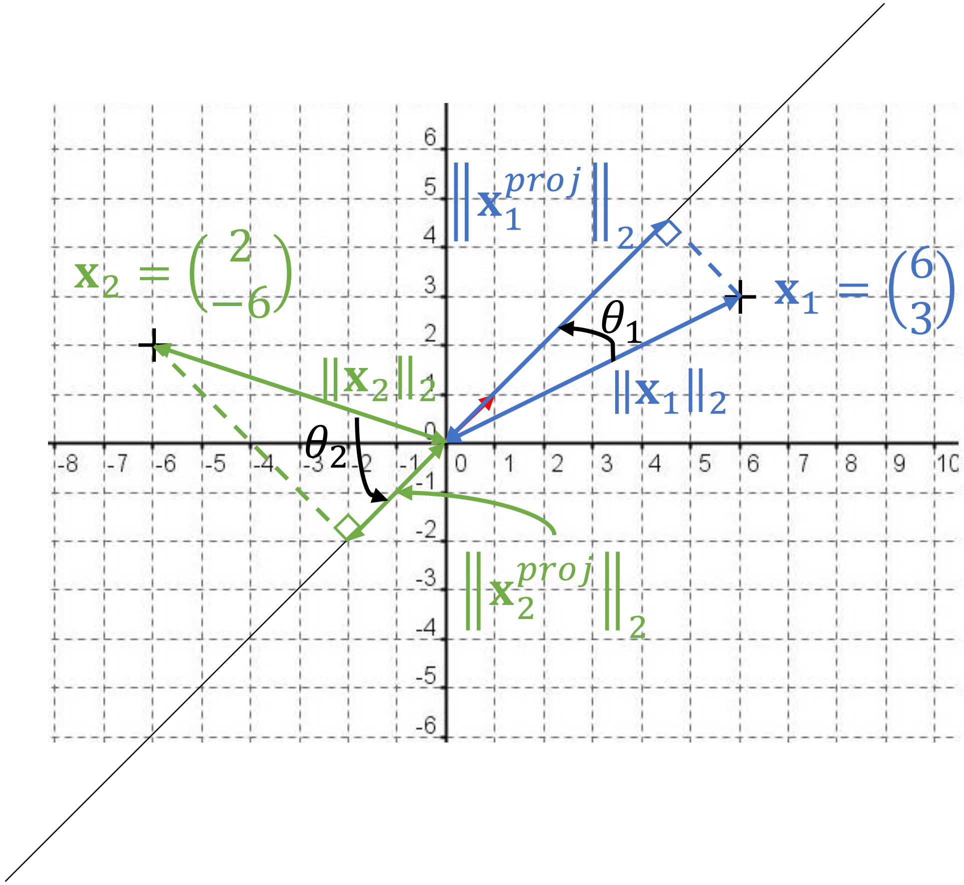
Total Variance – Example in 2D



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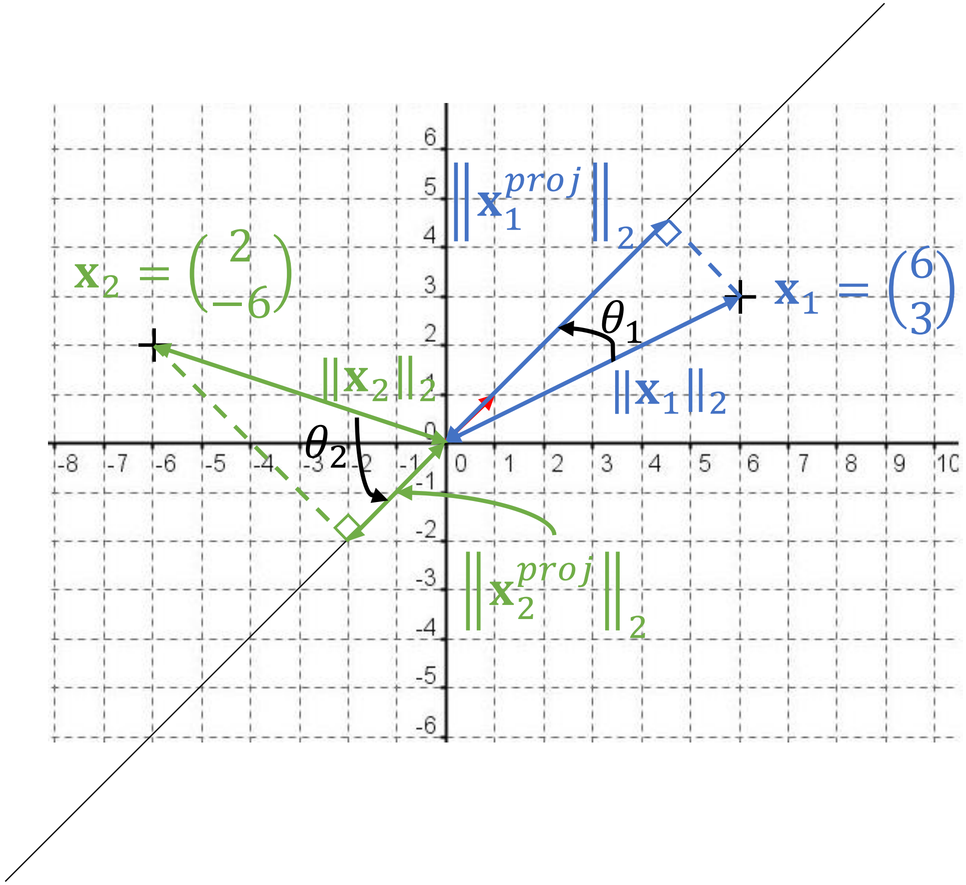

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In the end:

$$\mathrm{TV}^{\mathrm{proj}} = \frac{1}{2}\left((\mathbf{x}_1^\top \mathbf{w})^2 + (\mathbf{x}_2^\top \mathbf{w})^2\right)$$

PCA optimization criterion

$$\mathrm{TV}^{\mathrm{proj}} = \frac{1}{2}\left((\mathbf{x}_1^\top \mathbf{w})^2 + (\mathbf{x}_2^\top \mathbf{w})^2\right)$$

PCA optimization criterion

$$\mathrm{TV}^{\mathrm{proj}} = \frac{1}{2}\left((\mathbf{x}_1^\top \mathbf{w})^2 + (\mathbf{x}_2^\top \mathbf{w})^2\right) = (\mathbf{x}_1^\top \mathbf{w} \quad \mathbf{x}_2^\top \mathbf{w}) \begin{pmatrix} \mathbf{x}_1^\top \mathbf{w} \\ \mathbf{x}_2^\top \mathbf{w} \end{pmatrix}$$

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By the way:

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Hence:

PCA optimization criterion

$$\mathrm{TV}^{\mathrm{proj}} = \frac{1}{2}\left((\mathbf{x}_1^\top \mathbf{w})^2 + (\mathbf{x}_2^\top \mathbf{w})^2\right) = (\mathbf{x}_1^\top \mathbf{w} \quad \mathbf{x}_2^\top \mathbf{w}) \begin{pmatrix} \mathbf{x}_1^\top \mathbf{w} \\ \mathbf{x}_2^\top \mathbf{w} \end{pmatrix}$$

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Hence:

$$\mathrm{TV}^{\mathrm{proj}} = \frac{1}{2}\mathbf{w}^\top \mathbf{X}^\top \mathbf{X}\mathbf{w} = \mathrm{Var}(\mathbf{X}\mathbf{w})$$

PCA optimization criterion

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It is possible to show in the general case that:

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Hence:

$$\mathrm{TV}^{\mathrm{proj}} = \frac{1}{2}\mathbf{w}^\top \mathbf{X}^\top \mathbf{X}\mathbf{w} = \mathrm{Var}(\mathbf{X}\mathbf{w})$$

It is possible to show in the general case that: $\mathrm{TV}^{\mathrm{proj}} = \frac{1}{n}\mathbf{w}^\top \mathbf{X}^\top \mathbf{X}\mathbf{w} = \mathrm{Var}(\mathbf{X}\mathbf{w})$

PCA optimization criterion

$$\mathrm{TV}^{\mathrm{proj}} = \frac{1}{2}\left((\mathbf{x}_1^\top\mathbf{w})^2 + (\mathbf{x}_2^\top\mathbf{w})^2\right) = \begin{pmatrix}\mathbf{x}_1^\top\mathbf{w} & \mathbf{x}_2^\top\mathbf{w}\end{pmatrix}\begin{pmatrix}\mathbf{x}_1^\top\mathbf{w}\\ \mathbf{x}_2^\top\mathbf{w}\end{pmatrix}$$

By the way: $\begin{pmatrix}\mathbf{x}_1^\top\mathbf{w}\\ \mathbf{x}_2^\top\mathbf{w}\end{pmatrix} = \begin{pmatrix}\mathbf{x}_1^\top\\ \mathbf{x}_2^\top\end{pmatrix}\mathbf{w} = \mathbf{X}\mathbf{w}$

Hence:

$$\mathrm{TV}^{\mathrm{proj}} = \frac{1}{2}\mathbf{w}^\top\mathbf{X}^\top\mathbf{X}\mathbf{w} = \mathrm{Var}(\mathbf{X}\mathbf{w})$$

It is possible to show in the general case that: $\mathrm{TV}^{\mathrm{proj}} = \frac{1}{n}\mathbf{w}^\top\mathbf{X}^\top\mathbf{X}\mathbf{w} = \mathrm{Var}(\mathbf{X}\mathbf{w})$

Hence, one possible optimization criterion in order to estimate the first principal direction is:

PCA optimization criterion

$$\mathrm{TV}^{\mathrm{proj}} = \frac{1}{2}\left((\mathbf{x}_1^\top \mathbf{w})^2 + (\mathbf{x}_2^\top \mathbf{w})^2\right) = (\mathbf{x}_1^\top \mathbf{w} \quad \mathbf{x}_2^\top \mathbf{w}) \begin{pmatrix} \mathbf{x}_1^\top \mathbf{w} \\ \mathbf{x}_2^\top \mathbf{w} \end{pmatrix}$$

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Hence:

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It is possible to show in the general case that: $\mathrm{TV}^{\mathrm{proj}} = \frac{1}{n} \mathbf{w}^\top \mathbf{X}^\top \mathbf{X} \mathbf{w} = \mathrm{Var}(\mathbf{X}\mathbf{w})$

Hence, one possible optimization criterion in order to estimate the first principal direction is:

$$\boxed{\max_{\substack{\mathbf{w} \\ \|\mathbf{w}\|_2^2 = 1}} \mathrm{Var}(\mathbf{X}\mathbf{w})}$$

1. Introduction of the case study

2. Unsupervised analysis with one-block:
Principal Component Analysis (PCA)

3. Unsupervised analysis with two-blocks:
Partial Least Squares (PLS) and Canonical Correlation Analysis (CCA)

4. Unsupervised analysis with L-blocks:
Regularized Generalized Canonical Correlation Analysis (RGCCA)

5. Supervised analysis with RGCCA

6. Variable selection in RGCCA:
Sparse Generalized Canonical Correlation Analysis (SGCCA)

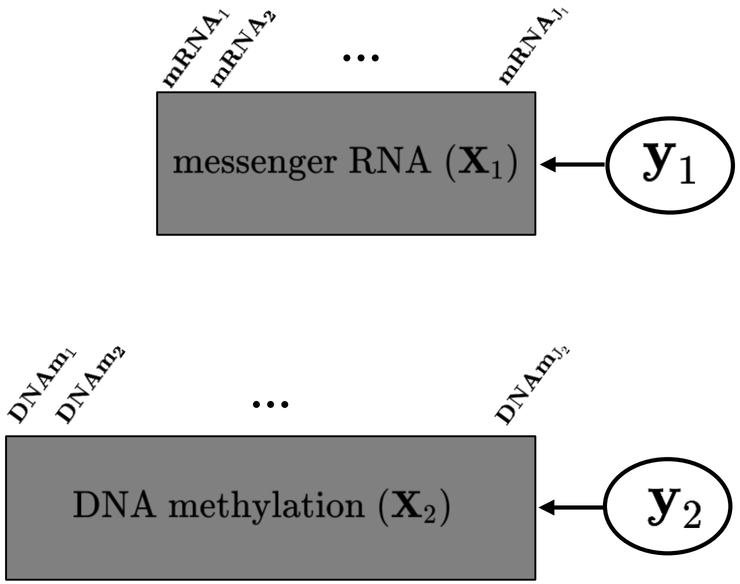
7. The flexible Optimization Framework of RGCCA

→ 7.1 The general principal

→ 7.2 Extension to multi-way analysis

→ 7.3 From Sequential to Global

The philosophy of multiblock component methods



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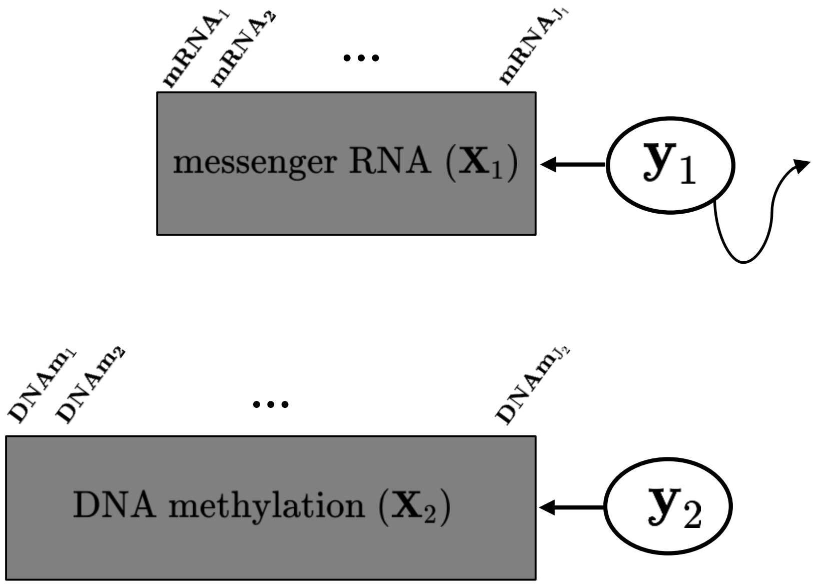

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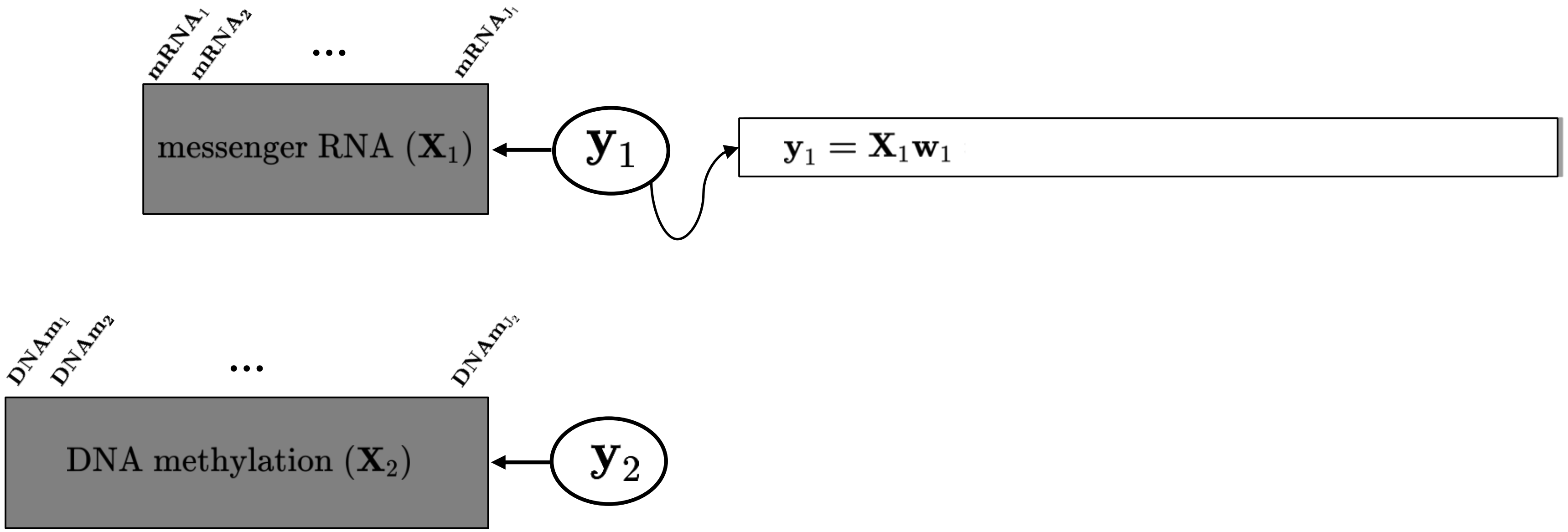

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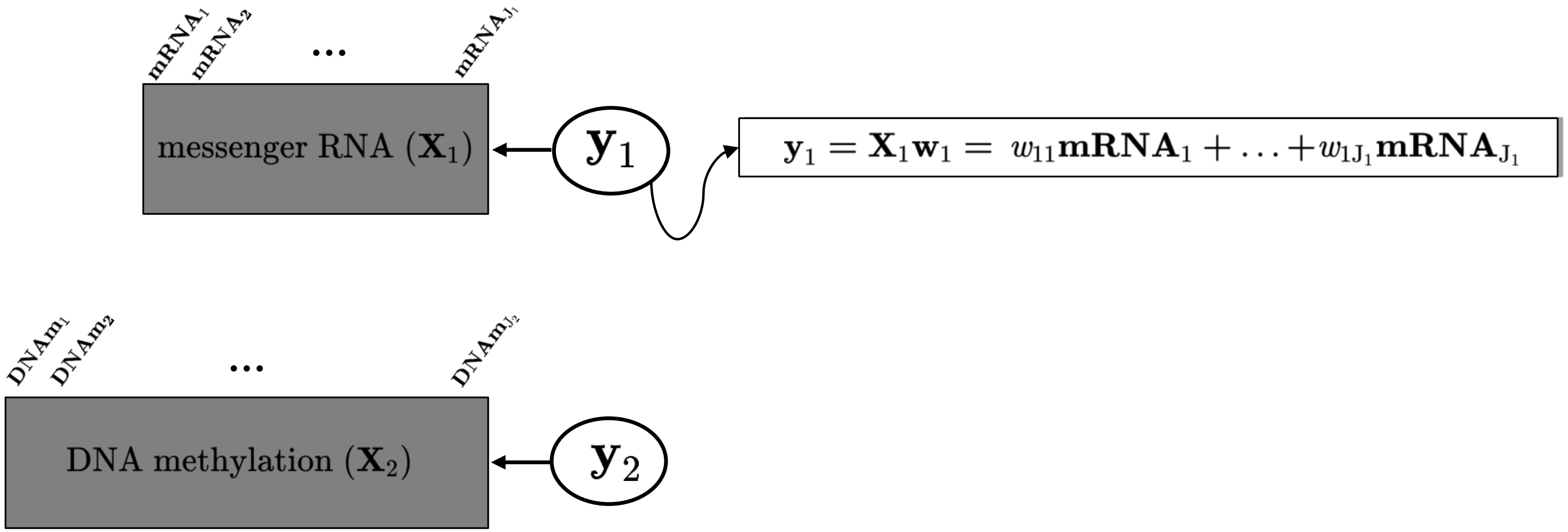

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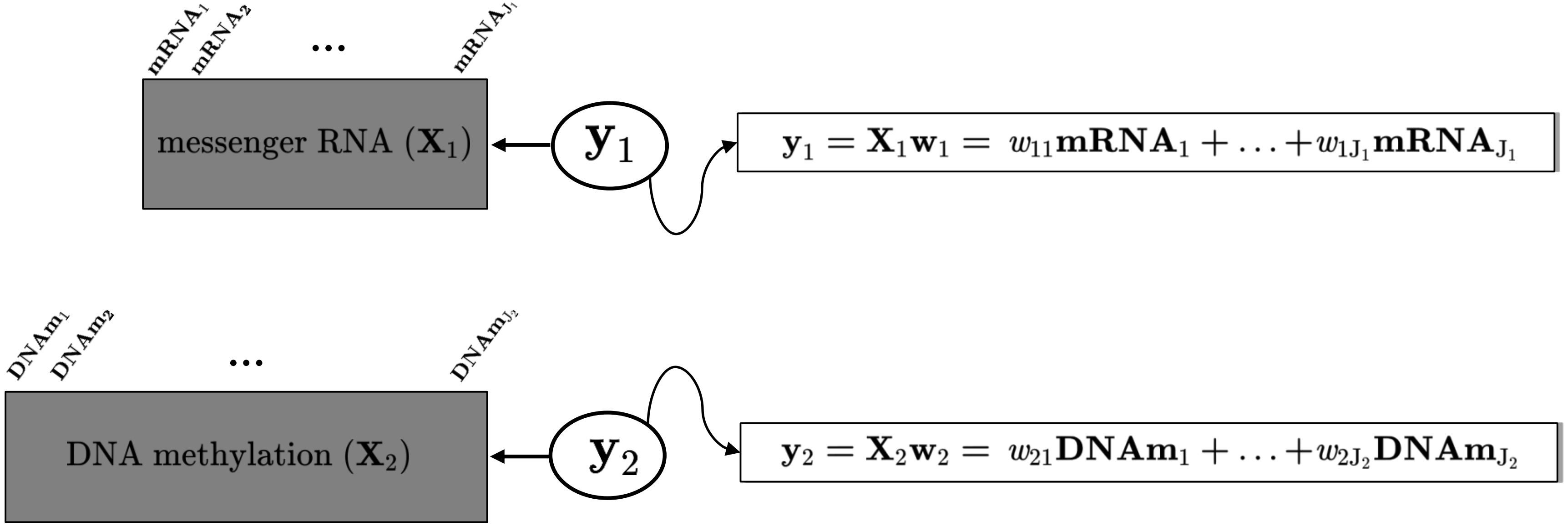

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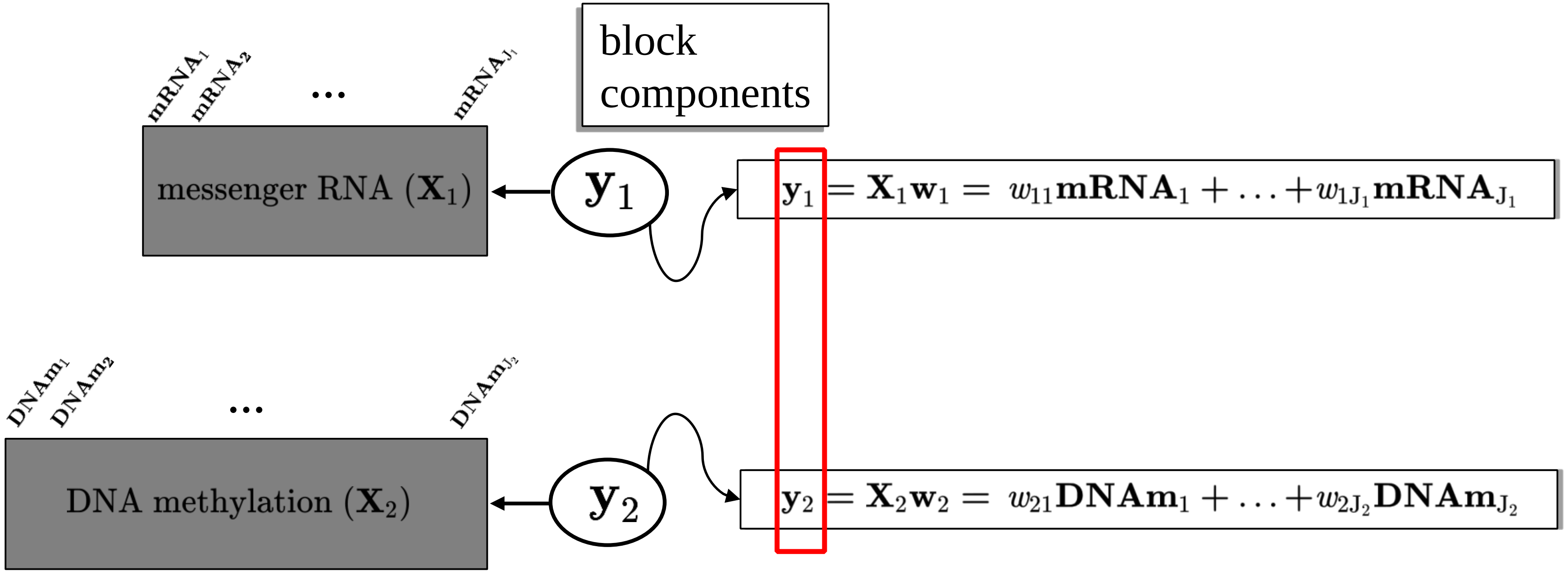

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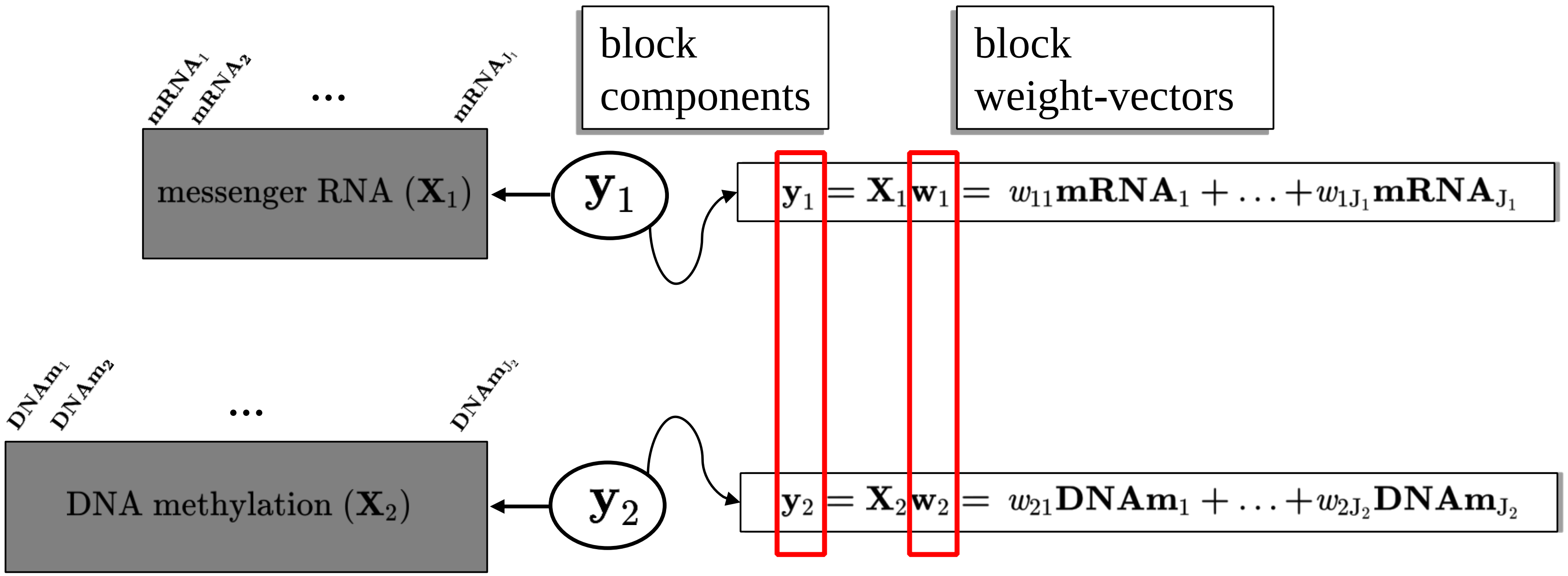

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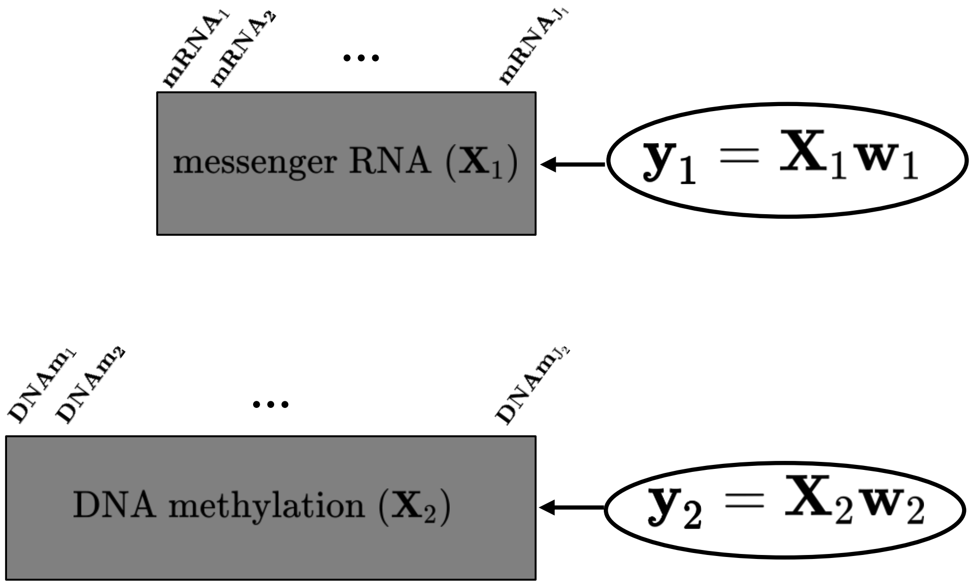
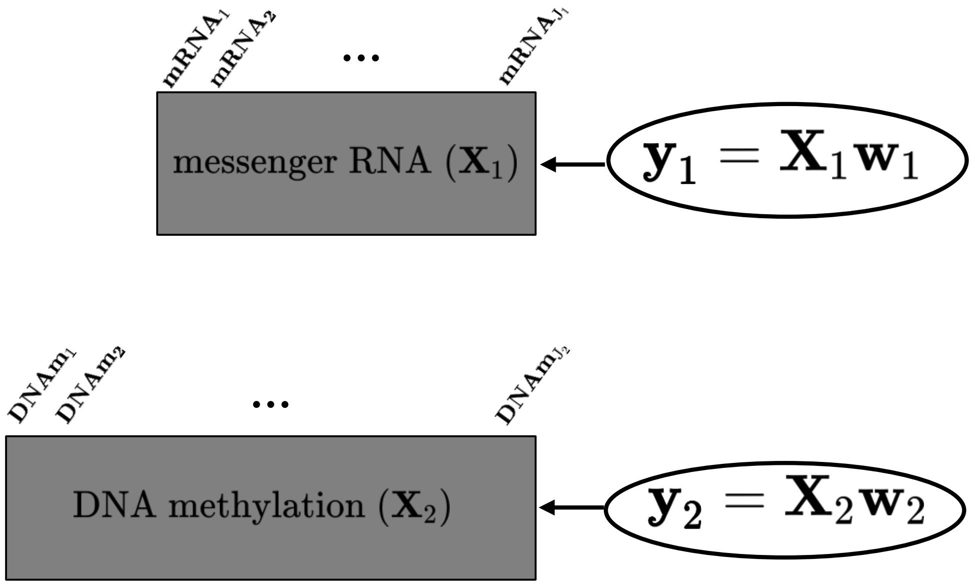


Block components should verified two properties at the same time:

1. Block components well explain their own block.

1. Block components are as correlated as possible for connected blocks.

The philosophy of multiblock component methods



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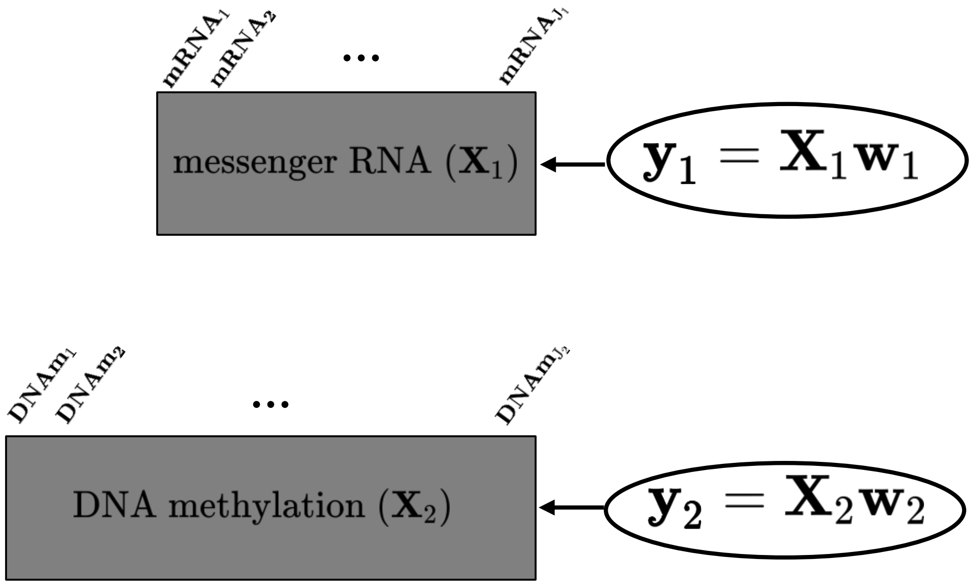


Correlation based methods

Find block-weight vectors $\mathbf{w}_1, \ldots, \mathbf{w}_J$ maximizing a function of $\boldsymbol{\Phi} = \{\mathrm{cor}(\mathbf{X}_j\mathbf{w}_j, \mathbf{X}_k\mathbf{w}_k)\}$.

Covariance based methods

Find block-weight vectors $\mathbf{w}_1, \ldots, \mathbf{w}_J$ maximizing a function of $\boldsymbol{\Psi} = \{\mathrm{cov}(\mathbf{X}_j\mathbf{w}_j, \mathbf{X}_k\mathbf{w}_k)\}$.

Courtesy to Arthur Tenenhaus.

From PCA to PLS/CCA

<u>Principal Component Analysis</u> (PCA)

$$\max_{\substack{\mathbf{w} \\ \|\mathbf{w}\|_2^2=1}} \ \mathrm{Var}(\mathbf{Xw})$$

From PCA to PLS/CCA

How can we "adapt" PCA for two-blocks analysis ?

$$\max_{\substack{\mathbf{w} \\ \|\mathbf{w}\|_2^2=1}} \mathrm{Var}(\mathbf{X}\mathbf{w})$$

From PCA to PLS/CCA

How can we “adapt” PCA for two-blocks analysis ?

$$\max_{\substack{\mathbf{w}_1,\mathbf{w}_2 \\ \|\mathbf{w}_\mathrm{i}\|_2^2 = 1}} \mathrm{Var}(\mathbf{X}_1\mathbf{w}_1)\,\mathrm{Var}(\mathbf{X}_2\mathbf{w}_2)$$

From PCA to PLS/CCA

How can we "adapt" PCA for two-blocks analysis ?

$$\max_{\substack{\mathbf{w}_1,\mathbf{w}_2 \\ \|\mathbf{w}_i\|_2^2 = 1}} \quad \mathrm{Var}(\mathbf{X}_1\mathbf{w}_1) \qquad\qquad \mathrm{Var}(\mathbf{X}_2\mathbf{w}_2)$$

From PCA to PLS/CCA

How can we "adapt" PCA for two-blocks analysis ?

$$\max_{\substack{\mathbf{w}_1,\mathbf{w}_2 \\ \|\mathbf{w}_\mathrm{i}\|_2^2=1}} \ \mathrm{Var}(\mathbf{X}_1\mathbf{w}_1)\,\mathrm{Cor}(\mathbf{X}_1\mathbf{w}_1,\mathbf{X}_2\mathbf{w}_2)\mathrm{Var}(\mathbf{X}_2\mathbf{w}_2)$$

From PCA to PLS/CCA

How can we "adapt" PCA for two-blocks analysis ?

$$\max_{\substack{\mathbf{w}_1,\mathbf{w}_2 \\ \|\mathbf{w}_\mathrm{i}\|_2^2 = 1}} \sqrt{\mathrm{Var}(\mathbf{X}_1\mathbf{w}_1)}\,\mathrm{Cor}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)\sqrt{\mathrm{Var}(\mathbf{X}_2\mathbf{w}_2)}$$

From PCA to PLS/CCA

How can we "adapt" PCA for two-blocks analysis ?

$$\max_{\substack{\mathbf{w}_1,\mathbf{w}_2 \\ \|\mathbf{w}_\mathrm{i}\|_2^2 = 1}} \underbrace{\sqrt{\mathrm{Var}(\mathbf{X}_1\mathbf{w}_1)}\,\mathrm{Cor}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)\sqrt{\mathrm{Var}(\mathbf{X}_2\mathbf{w}_2)}}_{\mathrm{Cov}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)}$$

From PCA to PLS/CCA

How can we "adapt" PCA for two-blocks analysis ?

$$\max_{\substack{\mathbf{w}_1,\mathbf{w}_2 \\ \|\mathbf{w}_\mathrm{i}\|_2^2 = 1}} \mathrm{Cov}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)$$

From PCA to PLS/CCA

<u>How can we "adapt" PCA for two-blocks analysis ?</u>

$$\max_{\substack{\mathbf{w}_1,\mathbf{w}_2 \\ \mathrm{Var}(\mathbf{X}_i\mathbf{w}_i)=1}} \mathrm{Cov}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)$$

From PCA to PLS/CCA

<u>How can we “adapt” PCA for two-blocks analysis ?</u>

$$\max_{\substack{\mathbf{w}_1,\mathbf{w}_2 \\ \mathrm{Var}(\mathbf{X}_i\mathbf{w}_i)=1}} \mathrm{Cov}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2) = \max_{\substack{\mathbf{w}_1,\mathbf{w}_2 \\ \mathrm{Var}(\mathbf{X}_i\mathbf{w}_i)=1}} \mathrm{Cor}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)$$

From PCA to PLS/CCA

From PCA to PLS/CCA

Partial Least Squares (PLS2)

$$\max_{\substack{\mathbf{w}_1,\mathbf{w}_2 \\ \|\mathbf{w}_i\|_2^2=1}} \quad \mathrm{Cov}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)$$

From PCA to PLS/CCA

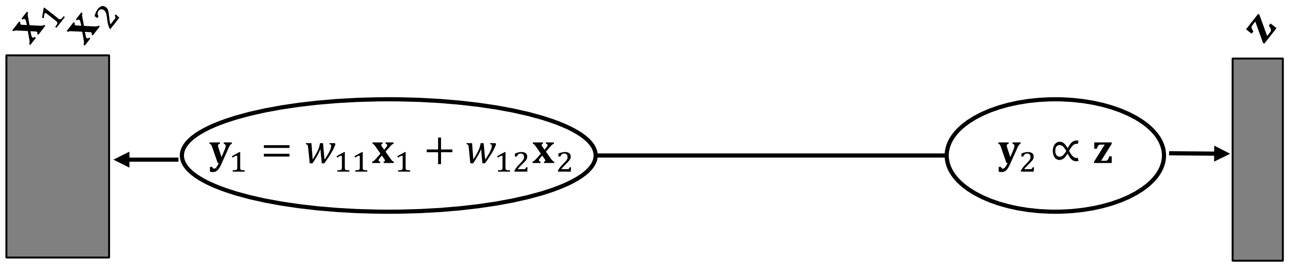
Canonical Correlation Analysis (CCA)

$$\max_{\substack{\mathbf{w}_1,\mathbf{w}_2 \\ \mathrm{Var}(\mathbf{X}_i\mathbf{w}_i)=1}} \mathrm{Cov}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)$$

Partial Least Squares (PLS2)

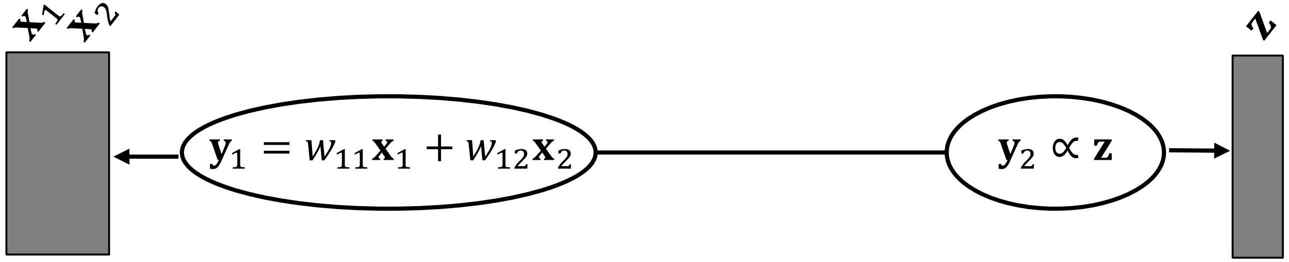
$$\max_{\substack{\mathbf{w}_1,\mathbf{w}_2 \\ \|\mathbf{w}_i\|_2^2=1}} \mathrm{Cov}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)$$

PLS & CCA with a figure



PLS & CCA with a figure

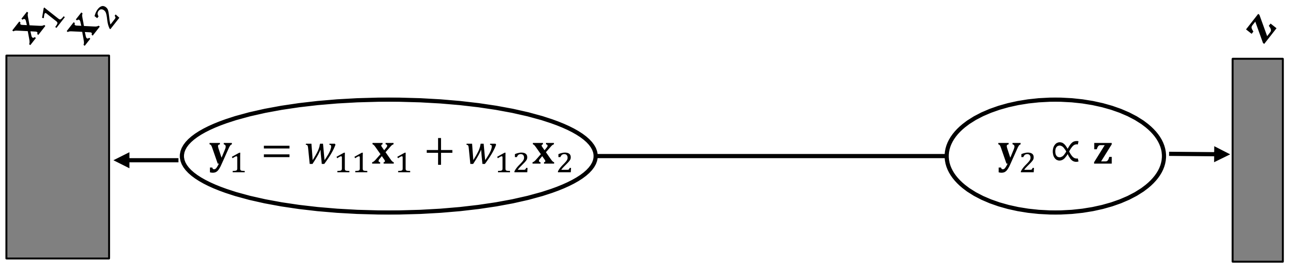
$$[\mathbf{x}_1\ \mathbf{x}_2] \sim \mathcal{N}\left((0,0), \begin{pmatrix} 1 & 0.5 \\ 0.5 & 1 \end{pmatrix}\right)$$



PLS & CCA with a figure

$$[\mathbf{x}_1\ \mathbf{x}_2] \sim \mathcal{N}\left((0,0), \begin{pmatrix} 1 & 0.5 \\ 0.5 & 1 \end{pmatrix}\right)$$

$$(\mathbf{z})_i = \begin{cases} 0 \text{ if } (\mathbf{x}_1)_i < 0 \\ 1 \text{ otherwise} \end{cases}$$



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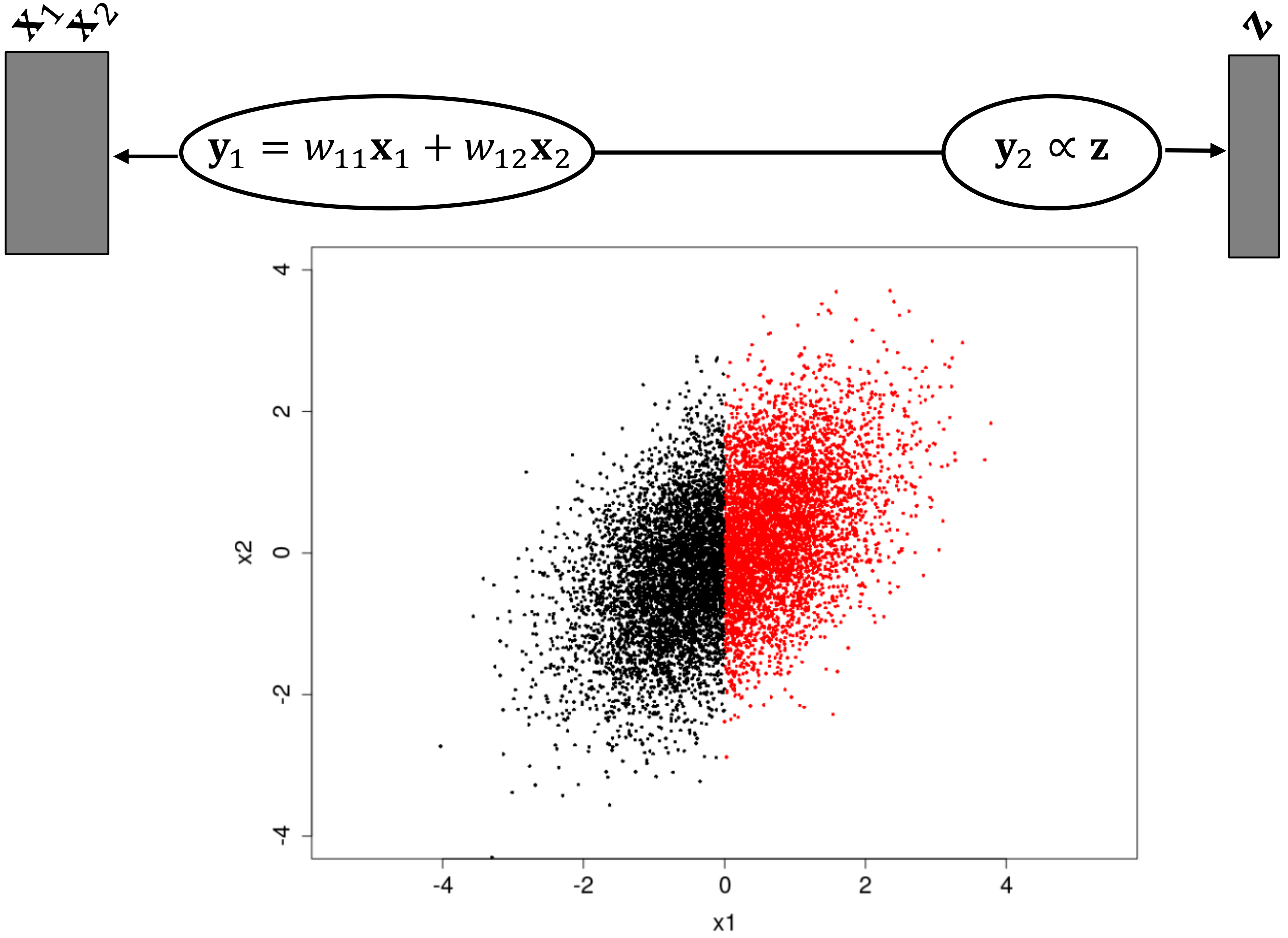

PLS & CCA with a figure

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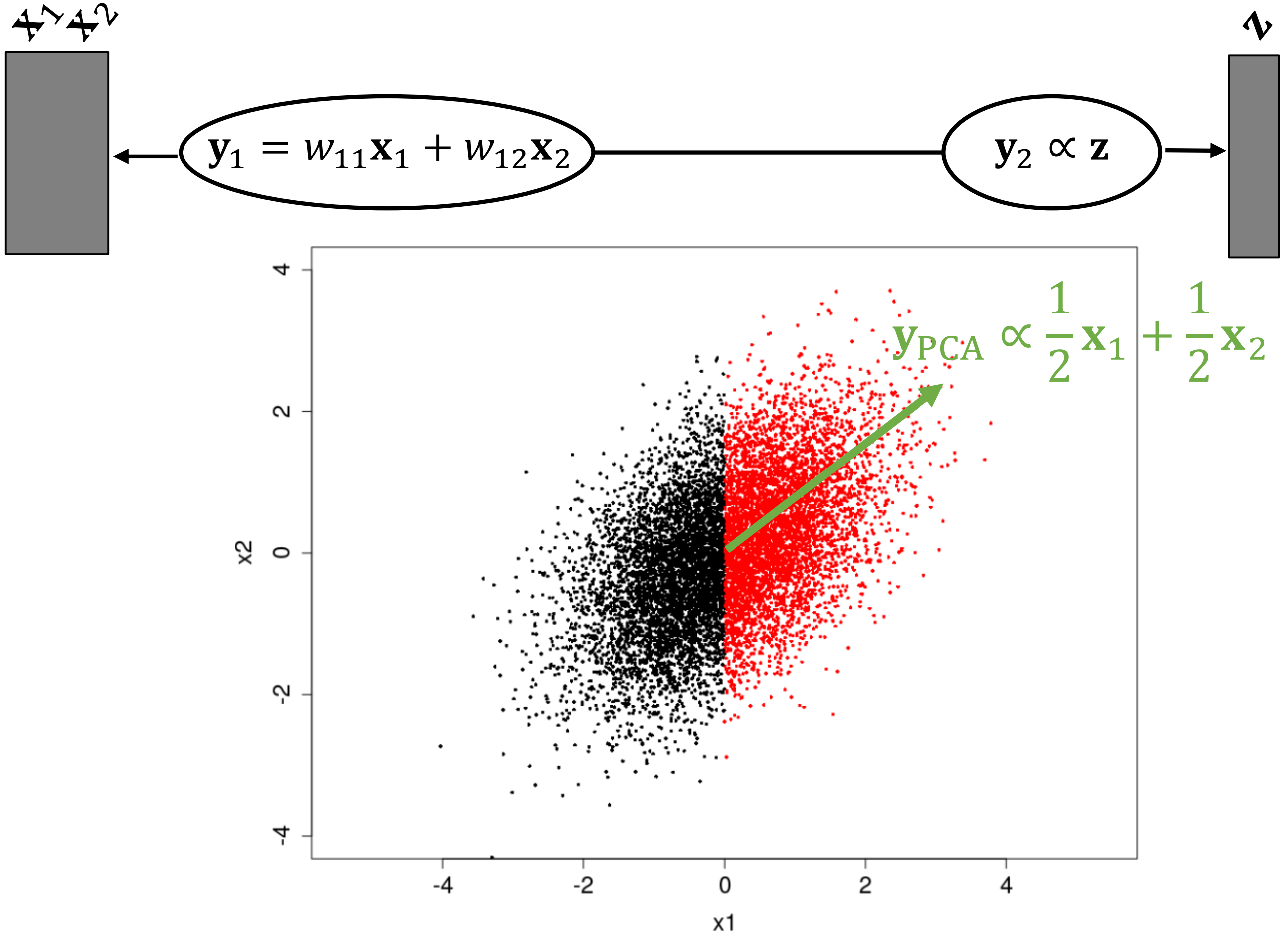

PLS & CCA with a figure

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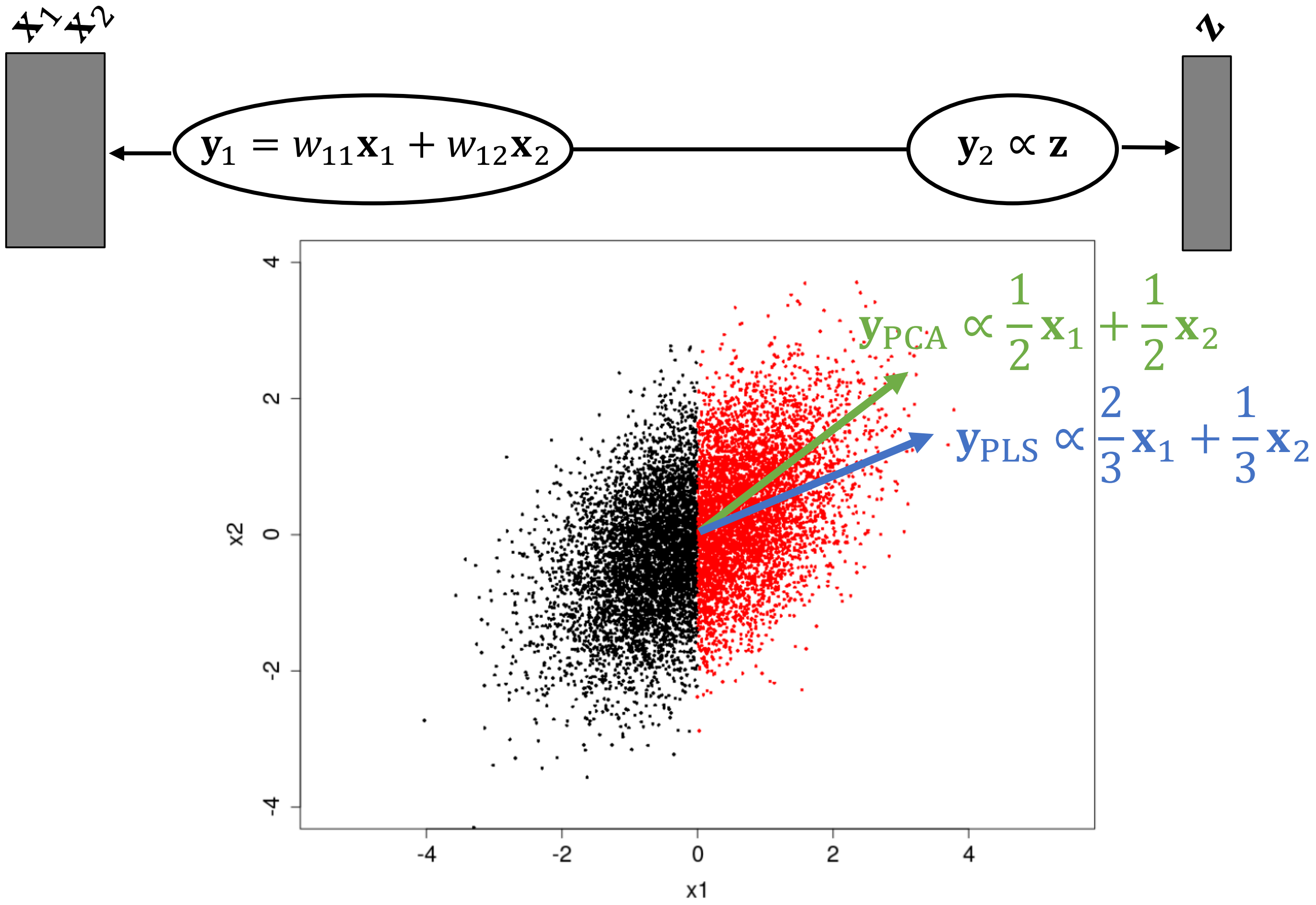

PLS & CCA with a figure

$$[\mathbf{x}_1\ \mathbf{x}_2] \sim \mathcal{N}\left((0,0), \begin{pmatrix} 1 & 0.5 \\ 0.5 & 1 \end{pmatrix}\right)$$

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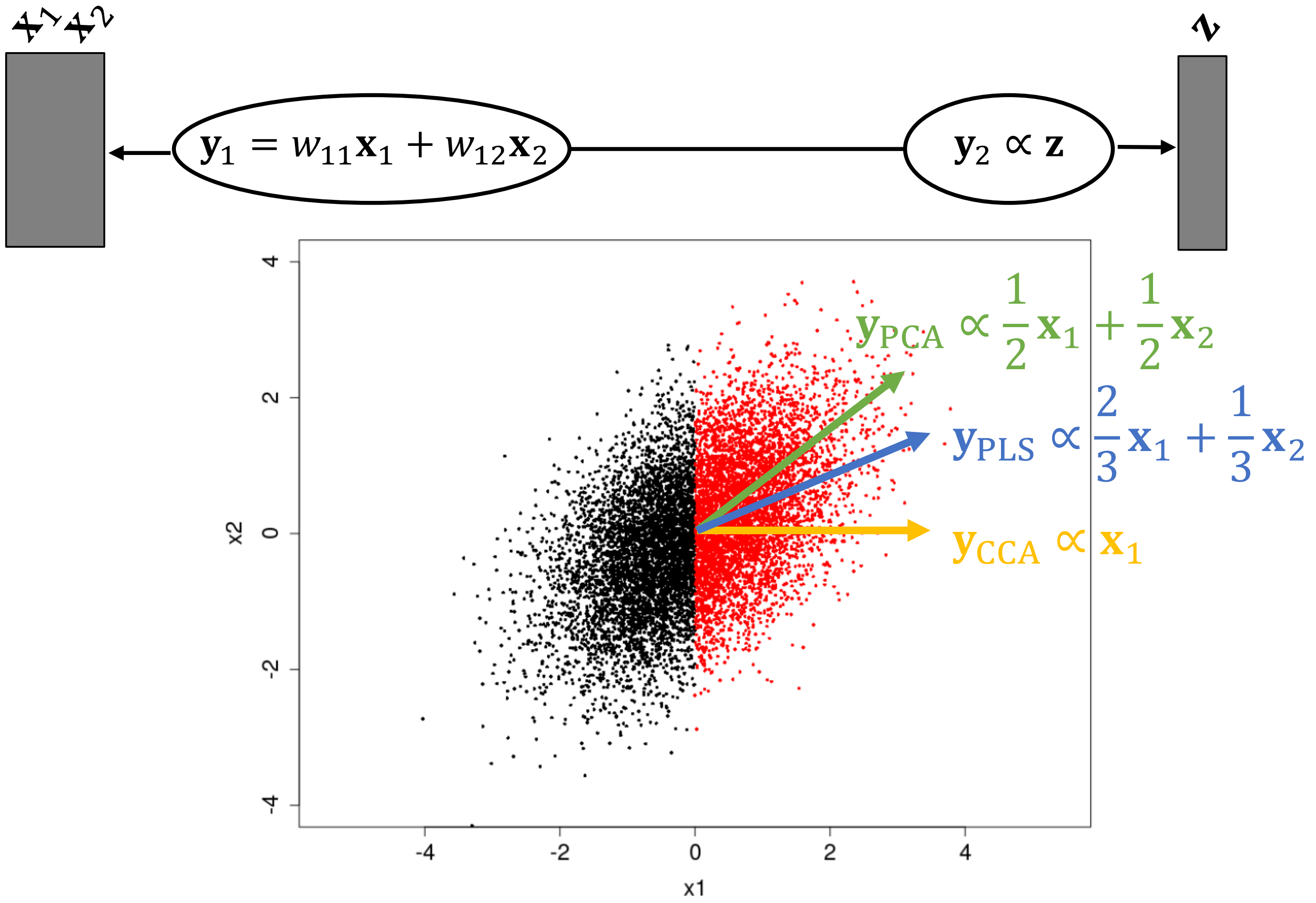


Two-blocks special cases: PLS & CCA

Canonical Correlation Analysis (CCA)

$$\max_{\substack{\mathbf{w}_1,\mathbf{w}_2 \\ \mathrm{Var}(\mathbf{X}_i\mathbf{w}_i)=1}} \mathrm{Cov}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)$$

Partial Least Squares (PLS2)

$$\max_{\substack{\mathbf{w}_1,\mathbf{w}_2 \\ \|\mathbf{w}_i\|_2^2=1}} \mathrm{Cov}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)$$

Two-blocks special cases: PLS & CCA ... and Regularized-CCA

Canonical Correlation Analysis (CCA)

$$\max_{\substack{\mathbf{w}_1,\mathbf{w}_2 \\ \mathrm{Var}(\mathbf{X}_i\mathbf{w}_i)=1}} \mathrm{Cov}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)$$

Partial Least Squares (PLS2)

$$\max_{\substack{\mathbf{w}_1,\mathbf{w}_2 \\ \|\mathbf{w}_i\|_2^2=1}} \mathrm{Cov}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)$$

Regularized-CCA

$$\max_{\mathbf{w}_1,\mathbf{w}_2} \mathrm{Cov}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)$$

$$\mathrm{s.t.}\ (1-\tau_i)\mathrm{Var}(\mathbf{X}_i\mathbf{w}_i) + \tau_i\|\mathbf{w}_i\|_2^2 = 1.$$

Two-blocks special cases: PLS & CCA … and Regularized-CCA

Canonical Correlation Analysis (CCA)

$$\max_{\substack{\mathbf{w}_1,\mathbf{w}_2 \\ \mathrm{Var}(\mathbf{X}_i\mathbf{w}_i)=1}} \mathrm{Cov}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)$$

Partial Least Squares (PLS2)

$$\max_{\substack{\mathbf{w}_1,\mathbf{w}_2 \\ \|\mathbf{w}_i\|_2^2=1}} \mathrm{Cov}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)$$

Regularized-CCA

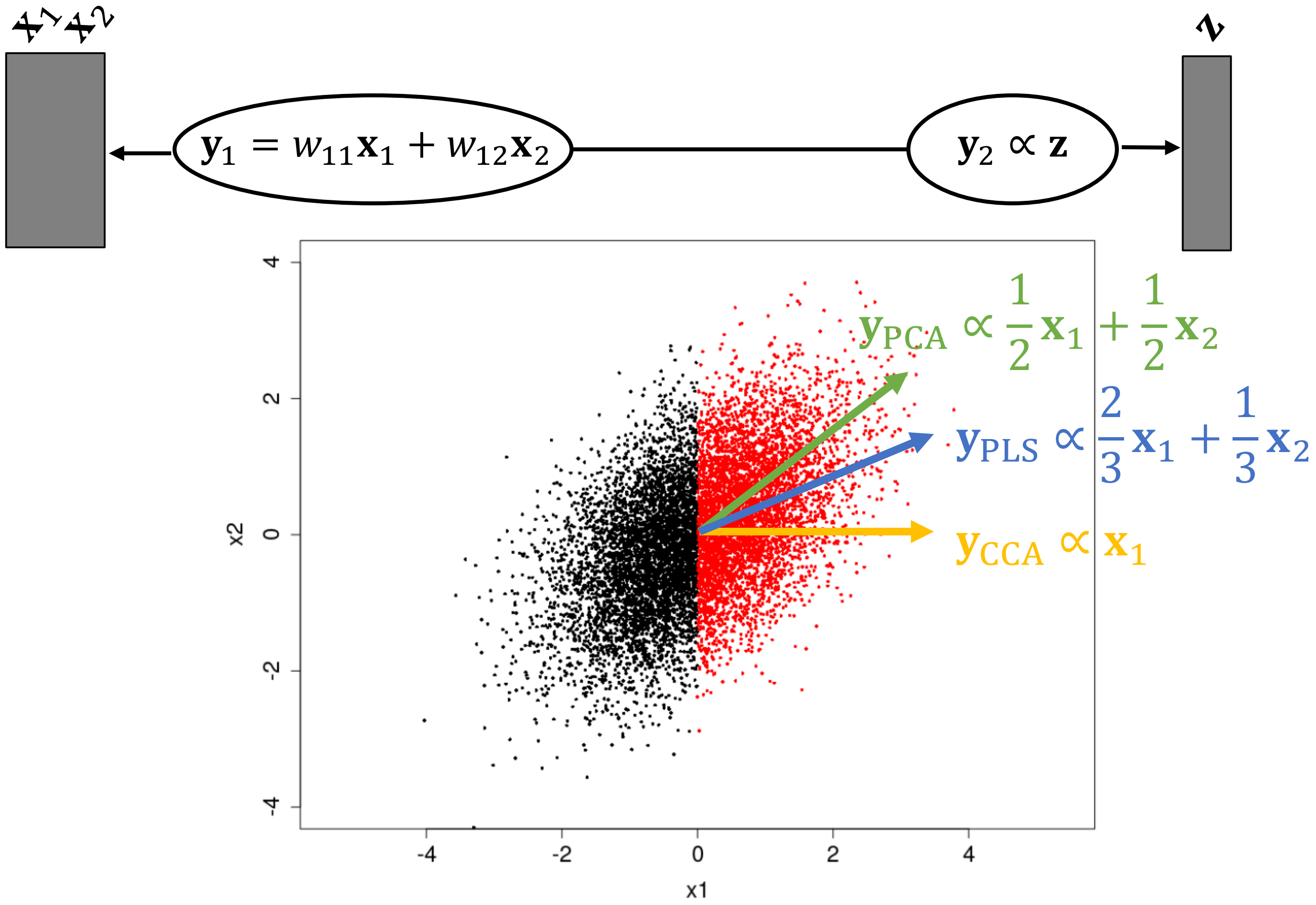
$$\max_{\mathbf{w}_1,\mathbf{w}_2} \mathrm{Cov}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)$$

$$\text{s.t. } (1-\tau_i)\mathrm{Var}(\mathbf{X}_i\mathbf{w}_i) + \tau_i\|\mathbf{w}_i\|_2^2 = 1.$$

PLS & CCA with a figure

$$[\mathbf{x}_1\ \mathbf{x}_2] \sim \mathcal{N}\left((0,0), \begin{pmatrix} 1 & 0.5 \\ 0.5 & 1 \end{pmatrix}\right)$$

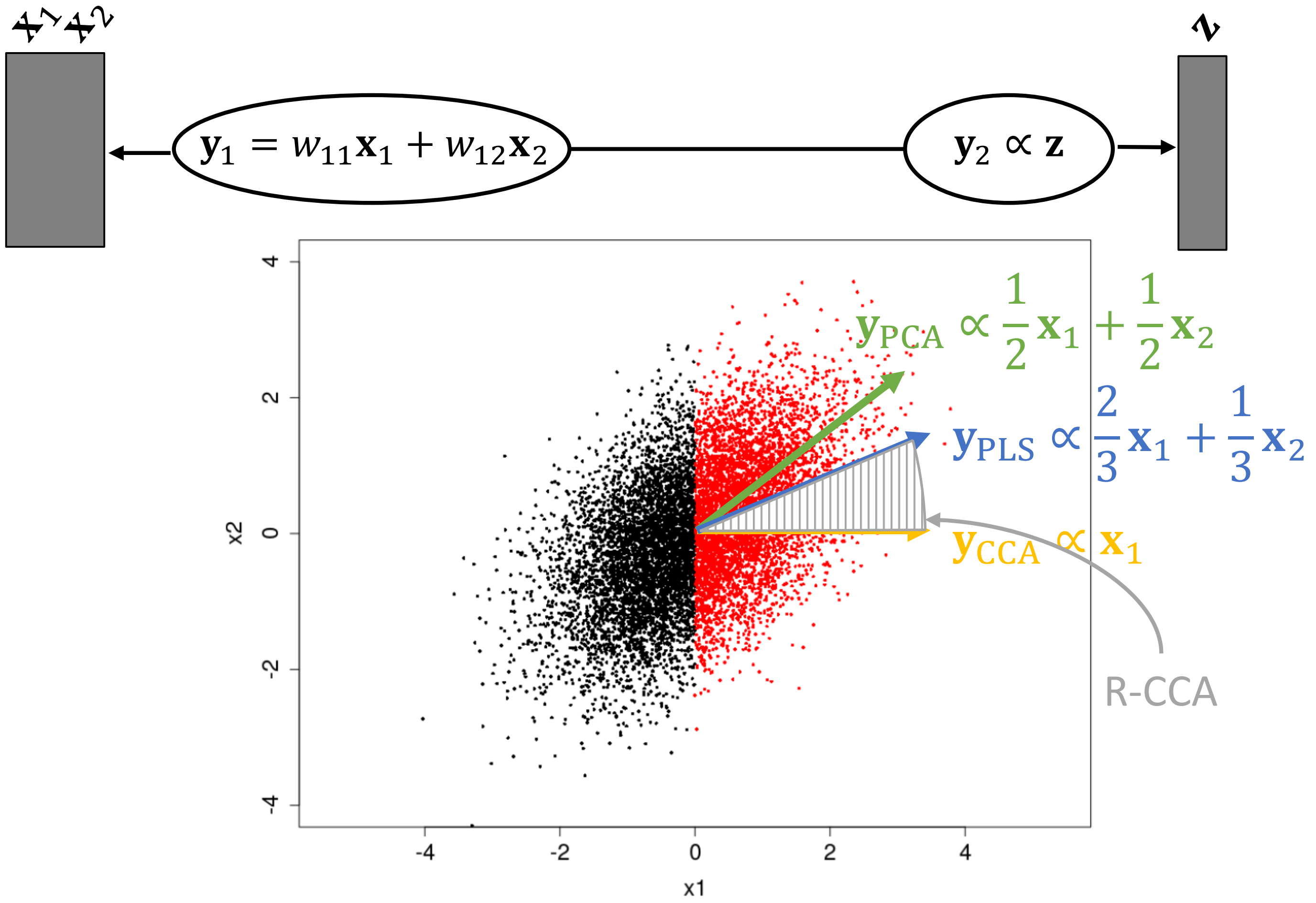
$$(\mathbf{z})_i = \begin{cases} 0 \text{ if } (\mathbf{x}_1)_i < 0 \\ 1 \text{ otherwise} \end{cases}$$



PLS & CCA with a figure

$$[\mathbf{x}_1\ \mathbf{x}_2] \sim \mathcal{N}\left((0,0), \begin{pmatrix} 1 & 0.5 \\ 0.5 & 1 \end{pmatrix}\right)$$

$$(\mathbf{z})_i = \begin{cases} 0 \text{ if } (\mathbf{x}_1)_i < 0 \\ 1 \text{ otherwise} \end{cases}$$



1. Introduction of the case study

2. Unsupervised analysis with one-block:
Principal Component Analysis (PCA)

3. Unsupervised analysis with two-blocks:
Partial Least Squares (PLS) and Canonical Correlation Analysis (CCA)

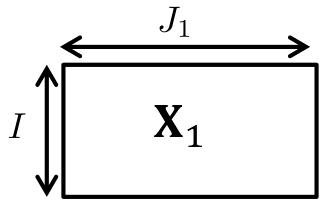
4. Unsupervised analysis with L-blocks:
Regularized Generalized Canonical Correlation Analysis (RGCCA)

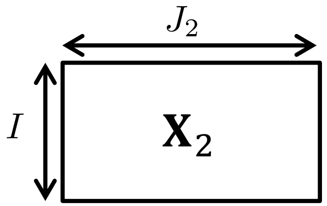
5. Supervised analysis with RGCCA

6. Variable selection in RGCCA:
Sparse Generalized Canonical Correlation Analysis (SGCCA)

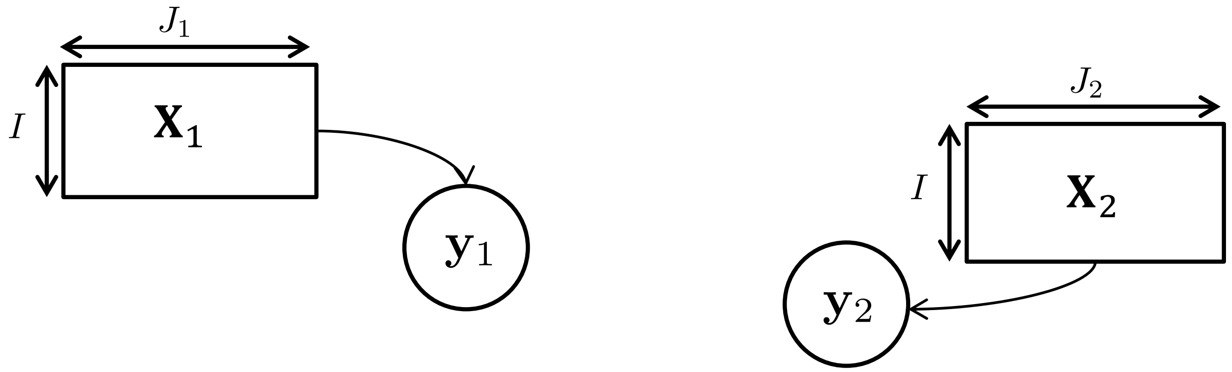
7. The flexible Optimization Framework of RGCCA
- → 7.1 The general principal
- → 7.2 Extension to multi-way analysis
- → 7.3 From Sequential to Global

Regularized Generalized Canonical Correlation Analysis (RGCCA)

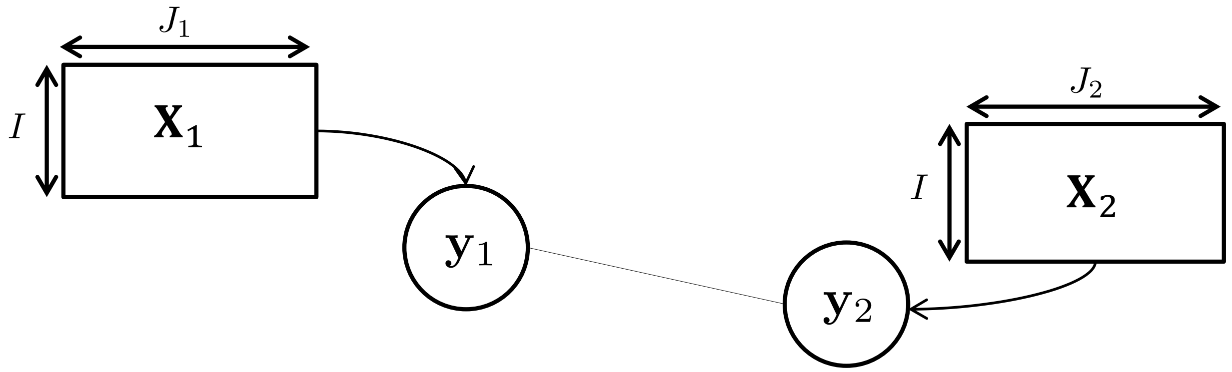




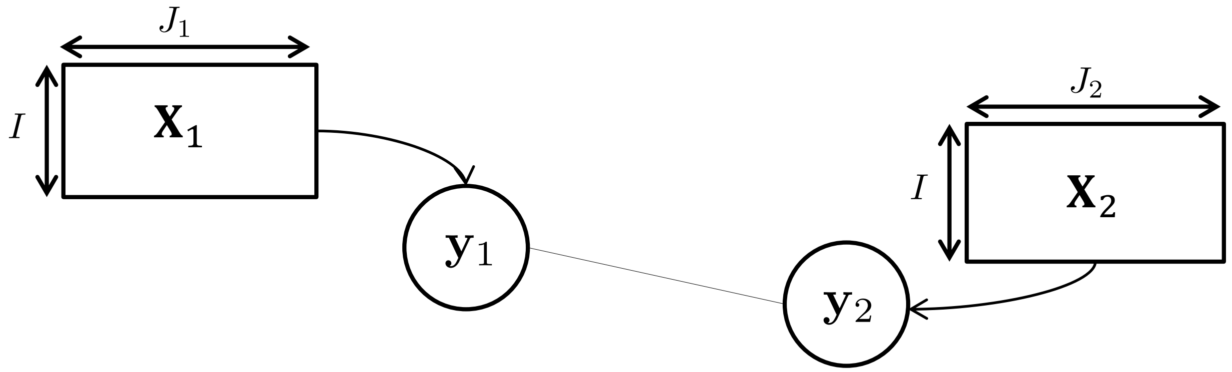
Regularized Generalized Canonical Correlation Analysis (RGCCA)



Regularized Generalized Canonical Correlation Analysis (RGCCA)

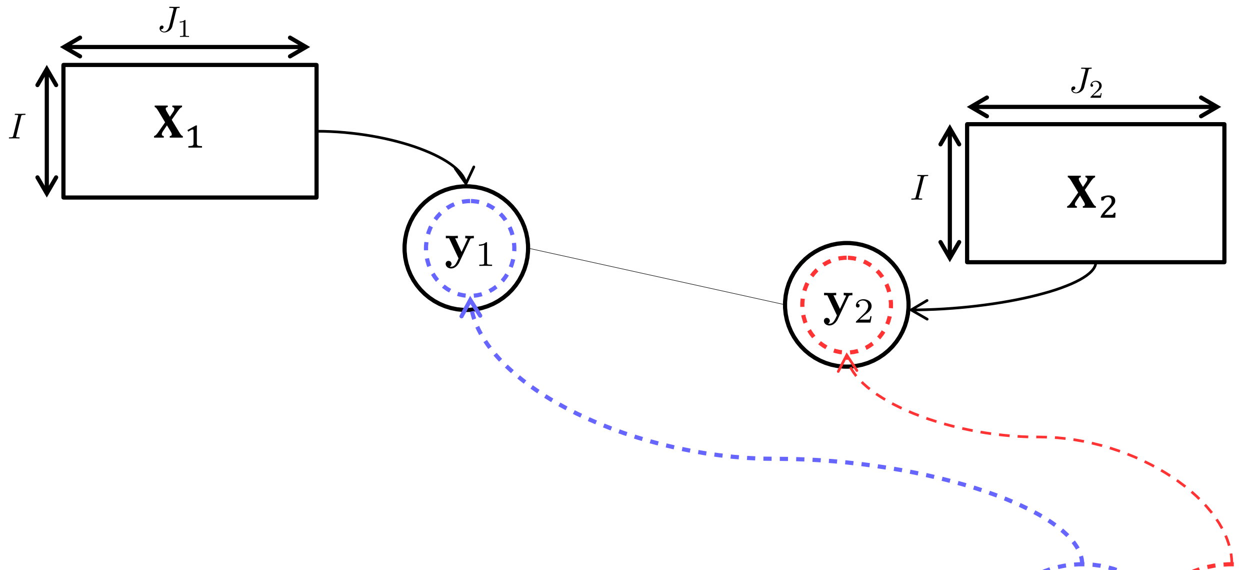


Regularized Generalized Canonical Correlation Analysis (RGCCA)



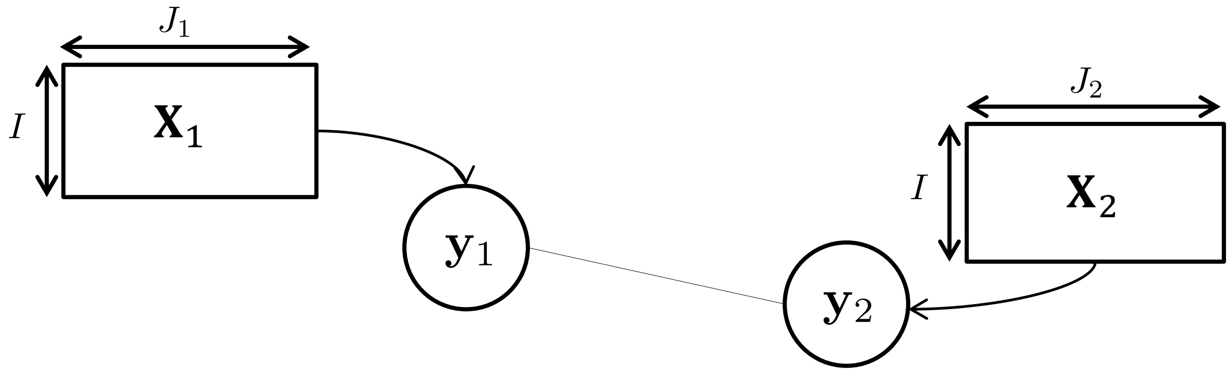
$$\max_{\mathbf{w}_1,\mathbf{w}_2} \mathrm{Cov}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)$$

Regularized Generalized Canonical Correlation Analysis (RGCCA)



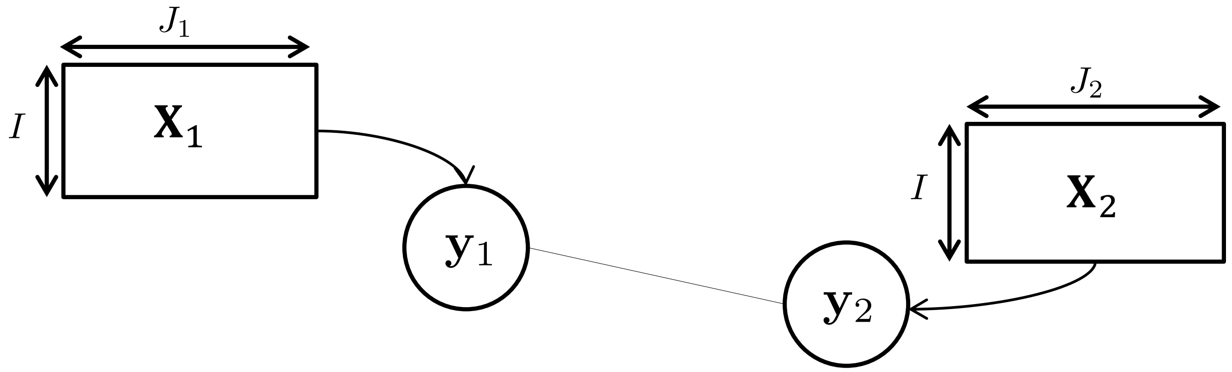
$$\max_{\mathbf{w}_1,\mathbf{w}_2} \text{Cov}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)$$

Regularized Generalized Canonical Correlation Analysis (RGCCA)



$$\max_{\mathbf{w}_1, \mathbf{w}_2} \mathrm{Cov}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)$$

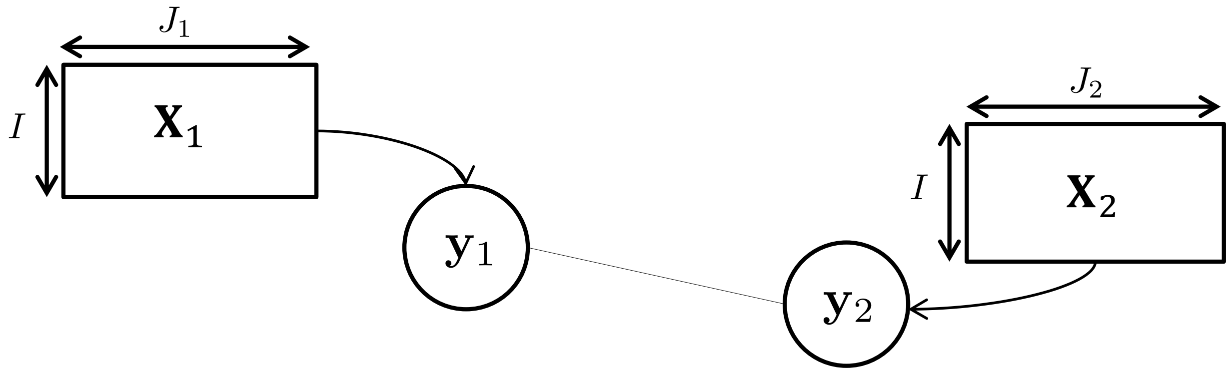
Regularized Generalized Canonical Correlation Analysis (RGCCA)



$$\max_{\mathbf{w}_1,\mathbf{w}_2} \mathrm{Cov}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)$$

$$\text{s.t. } \mathbf{w}_l^\top \mathbf{X}_l^\top \mathbf{X}_l \mathbf{w}_l = I, \qquad l = 1, 2.$$

Regularized Generalized Canonical Correlation Analysis (RGCCA)

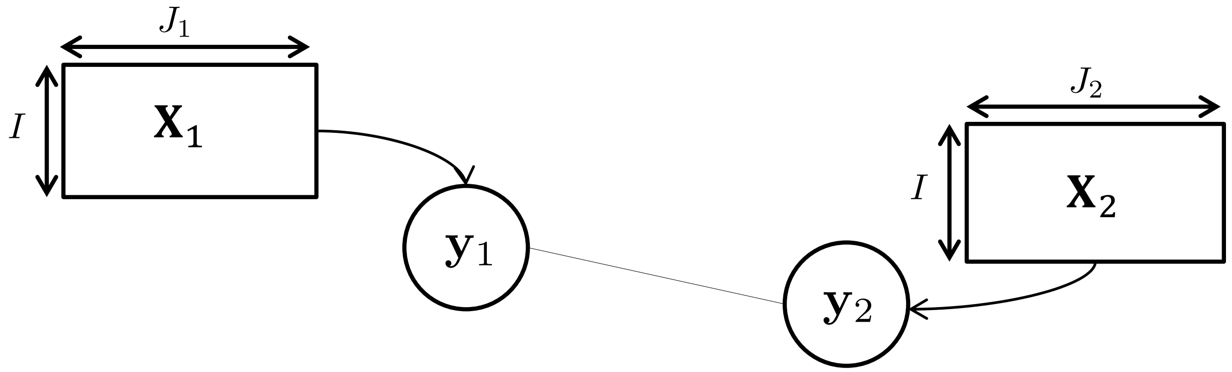


$$\max_{\mathbf{w}_1,\mathbf{w}_2} \mathrm{Cov}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)$$

$$\text{s.t. } \mathbf{w}_l^\top \mathbf{X}_l^\top \mathbf{X}_l \mathbf{w}_l = I, \qquad l = 1, 2.$$

➡ Canonical Correlation Analysis

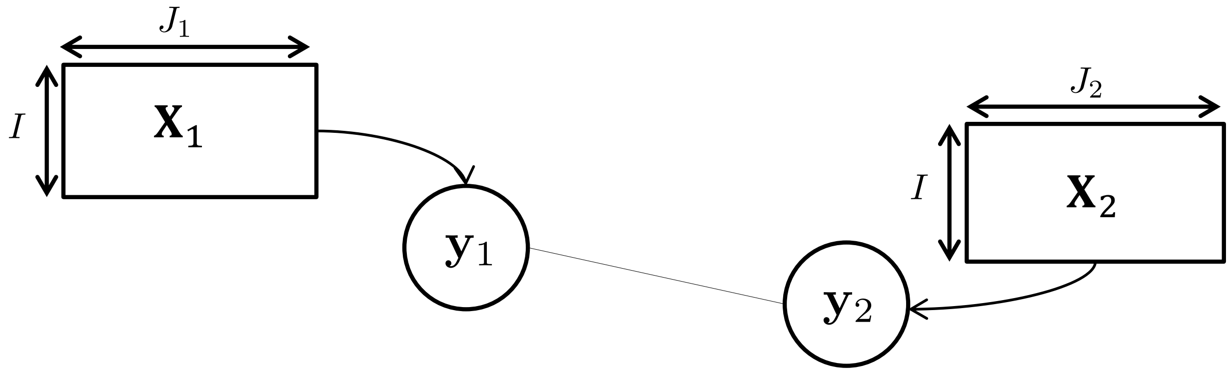
Regularized Generalized Canonical Correlation Analysis (RGCCA)



$$\max_{\mathbf{w}_1,\mathbf{w}_2} \mathrm{Cov}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)$$

$$\text{s.t. } \mathbf{w}_l^\top \mathbf{X}_l^\top \mathbf{X}_l \mathbf{w}_l = I, \qquad l = 1, 2.$$

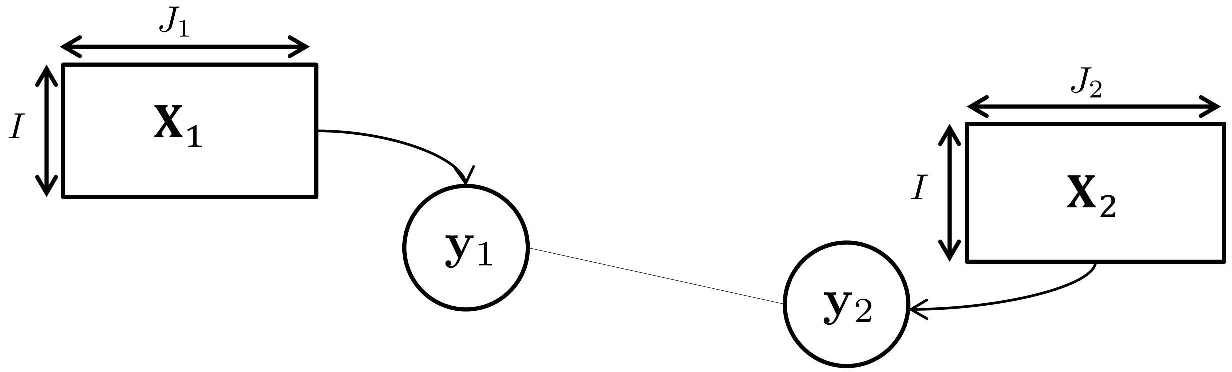
Regularized Generalized Canonical Correlation Analysis (RGCCA)



$$\max_{\mathbf{w}_1,\mathbf{w}_2} \mathrm{Cov}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)$$

$$\text{s.t. } \|\mathbf{w}_l\|_2^2 = 1, \qquad l = 1, 2.$$

Regularized Generalized Canonical Correlation Analysis (RGCCA)

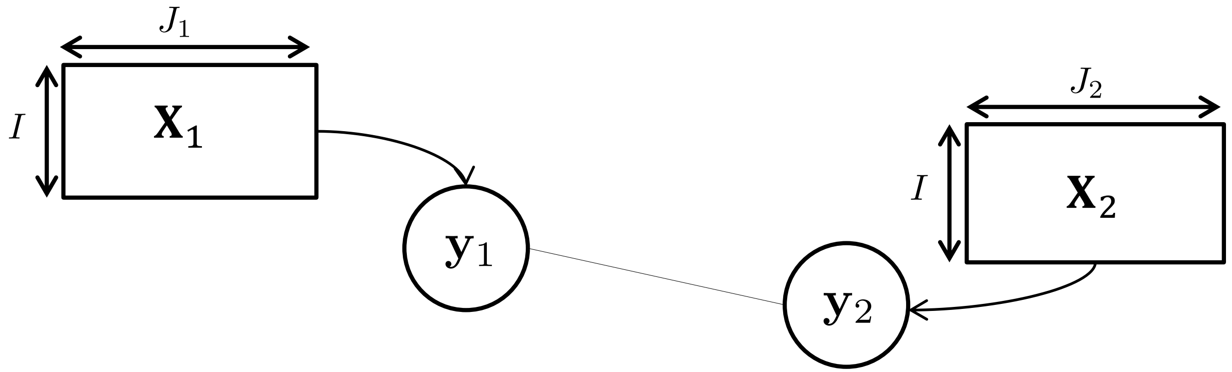


$$\max_{\mathbf{w}_1, \mathbf{w}_2} \mathrm{Cov}(\mathbf{X}_1 \mathbf{w}_1, \mathbf{X}_2 \mathbf{w}_2)$$

$$\mathrm{s.t.} \ \|\mathbf{w}_l\|_2^2 = 1, \qquad l = 1, 2.$$

Partial Least Squares 2

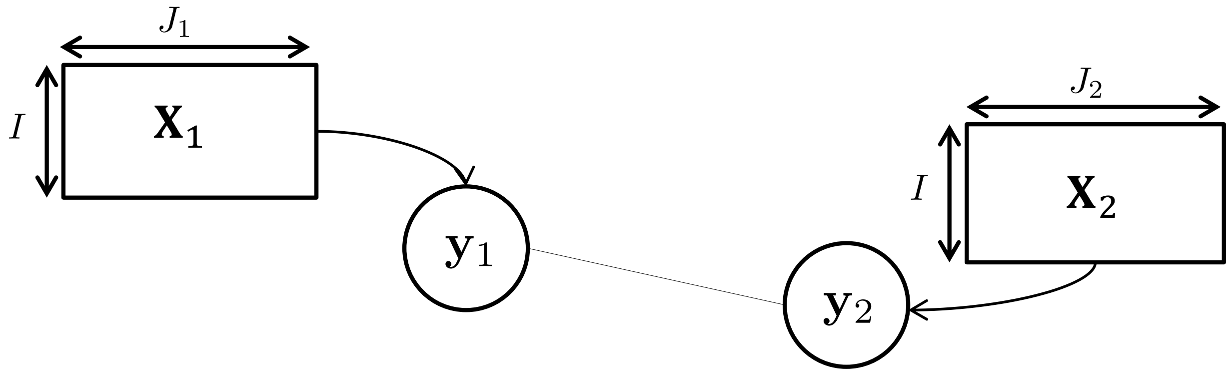
Regularized Generalized Canonical Correlation Analysis (RGCCA)



$$\max_{\mathbf{w}_1, \mathbf{w}_2} \mathrm{Cov}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)$$

$$\text{s.t. } \|\mathbf{w}_l\|_2^2 = 1, \qquad l = 1, 2.$$

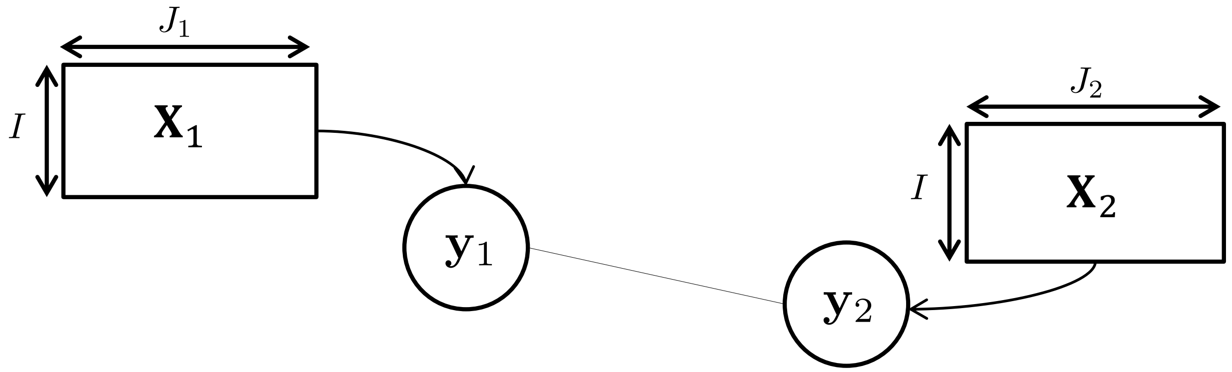
Regularized Generalized Canonical Correlation Analysis (RGCCA)



$$\max_{\mathbf{w}_1,\mathbf{w}_2} \mathrm{Cov}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)$$

$$\text{s.t.}\ \mathbf{w}_l^\top \mathbf{M}_l \mathbf{w}_l = 1, \qquad l = 1, 2.$$

Regularized Generalized Canonical Correlation Analysis (RGCCA)

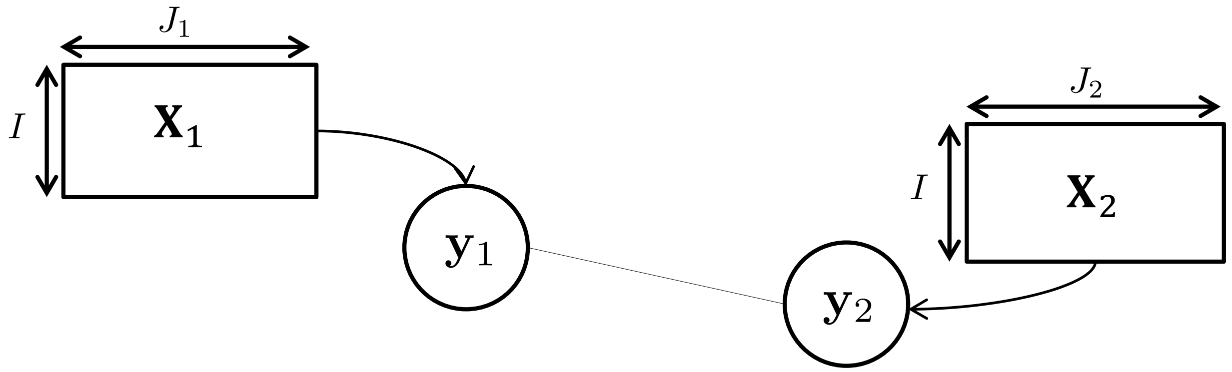


$$\max_{\mathbf{w}_1, \mathbf{w}_2} \mathrm{Cov}(\mathbf{X}_1 \mathbf{w}_1, \mathbf{X}_2 \mathbf{w}_2)$$

$$\mathrm{s.t.}\ \mathbf{w}_l^\top \mathbf{M}_l \mathbf{w}_l = 1, \qquad l = 1, 2.$$

where $\mathbf{M}_l$ is any $J_l \times J_l$ positive definite matrix

Regularized Generalized Canonical Correlation Analysis (RGCCA)



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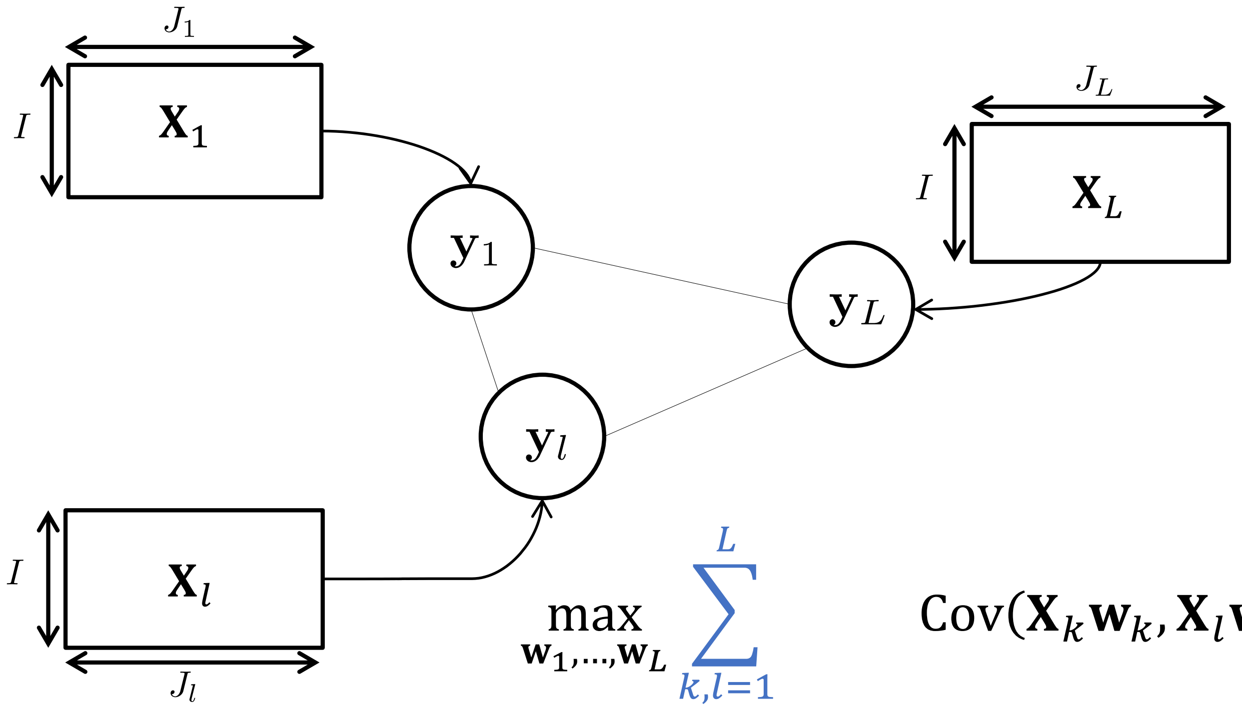
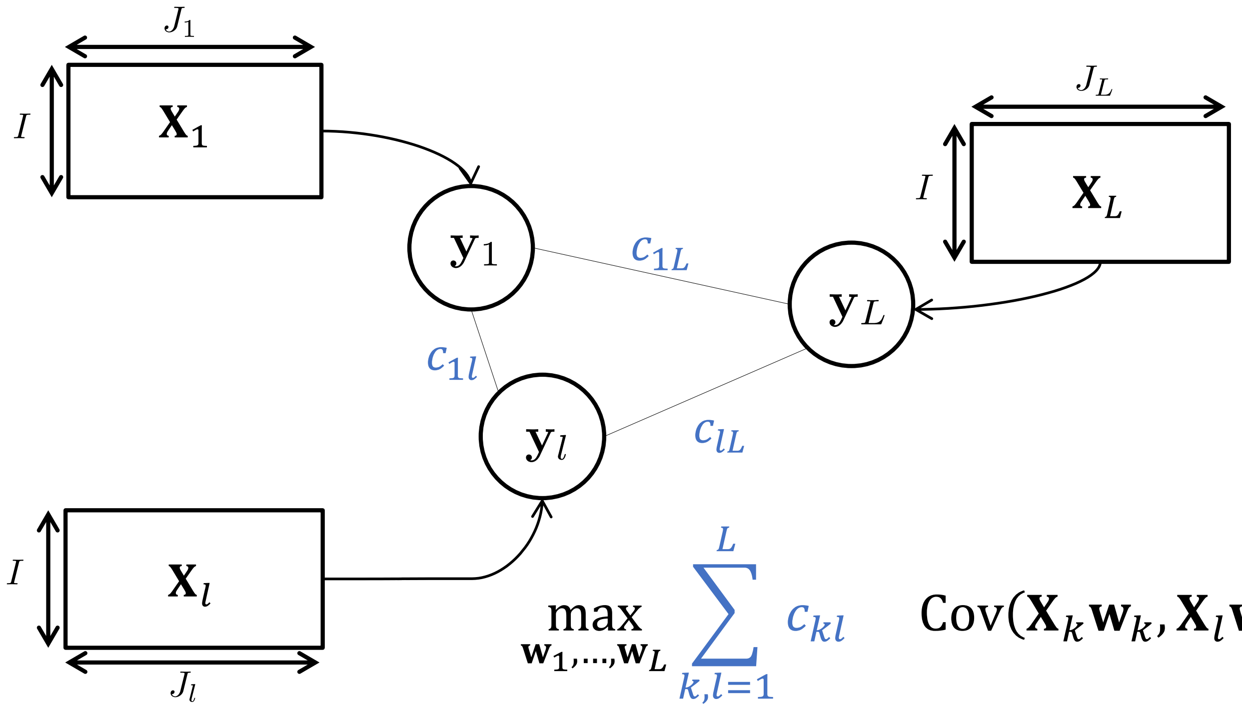


$$\max_{\mathbf{w}_1,\ldots,\mathbf{w}_L} \sum_{k,l=1}^{L} \mathrm{Cov}(\mathbf{X}_k\mathbf{w}_k, \mathbf{X}_l\mathbf{w}_l)$$

$$\text{s.t. } \mathbf{w}_l^\top \mathbf{M}_l \mathbf{w}_l = 1,\ \ l = 1, \ldots, L.$$

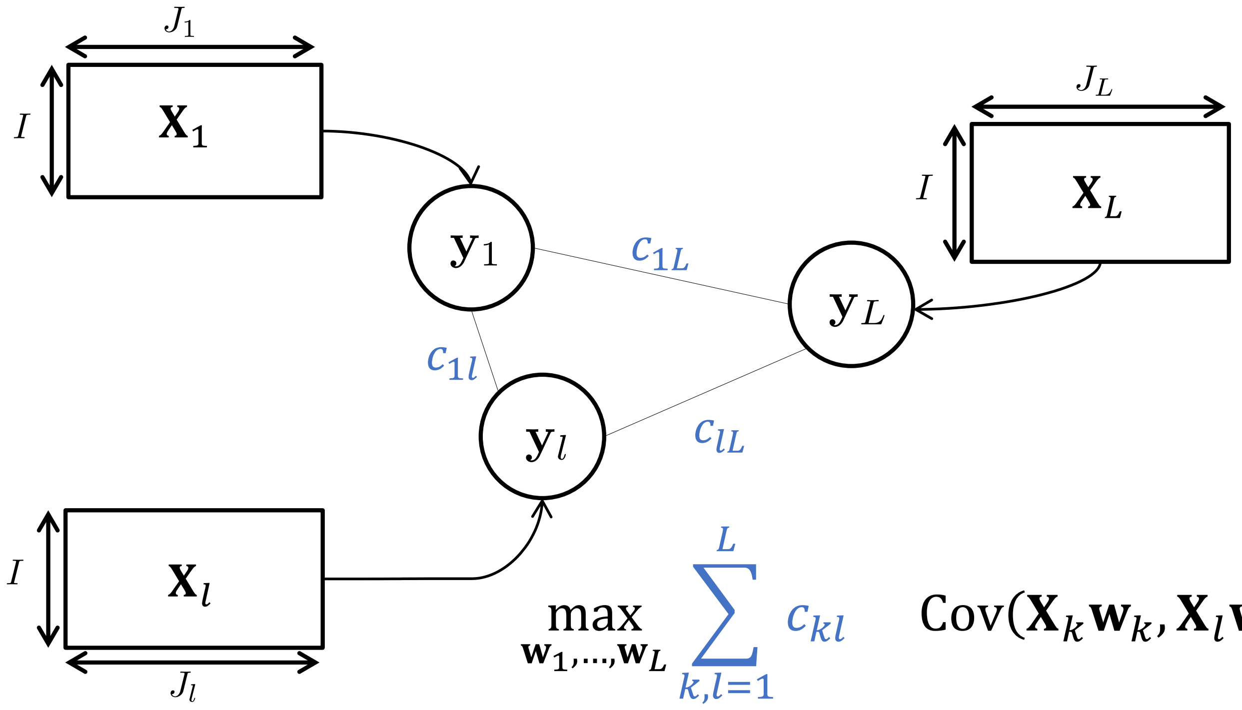
Regularized Generalized Canonical Correlation Analysis (RGCCA)



$$\max_{\mathbf{w}_1,\dots,\mathbf{w}_L} \sum_{k,l=1}^{L} c_{kl} \quad \mathrm{Cov}(\mathbf{X}_k\mathbf{w}_k, \mathbf{X}_l\mathbf{w}_l)$$

$$\text{s.t. } \mathbf{w}_l^\top \mathbf{M}_l \mathbf{w}_l = 1, \; l = 1, \dots, L.$$

Regularized Generalized Canonical Correlation Analysis (RGCCA)

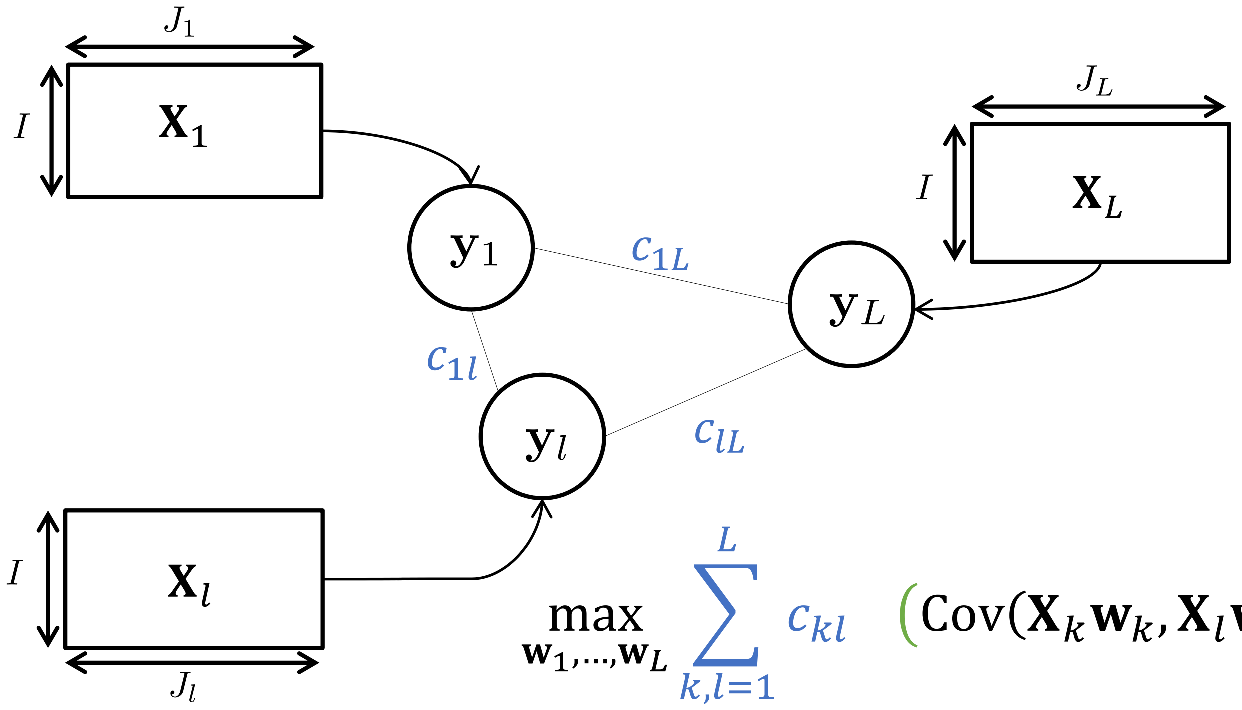


$$\max_{\mathbf{w}_1,\ldots,\mathbf{w}_L} \sum_{k,l=1}^{L} c_{kl} \quad \mathrm{Cov}(\mathbf{X}_k\mathbf{w}_k, \mathbf{X}_l\mathbf{w}_l)$$

$$\text{s.t. } \mathbf{w}_l^\top \mathbf{M}_l \mathbf{w}_l = 1, \ l = 1, \ldots, L.$$

$\Rightarrow$ if all blocks are connected and $\mathbf{M}_l = \mathbf{I}_l$ $\Rightarrow$ SUMCOV-2

Regularized Generalized Canonical Correlation Analysis (RGCCA)

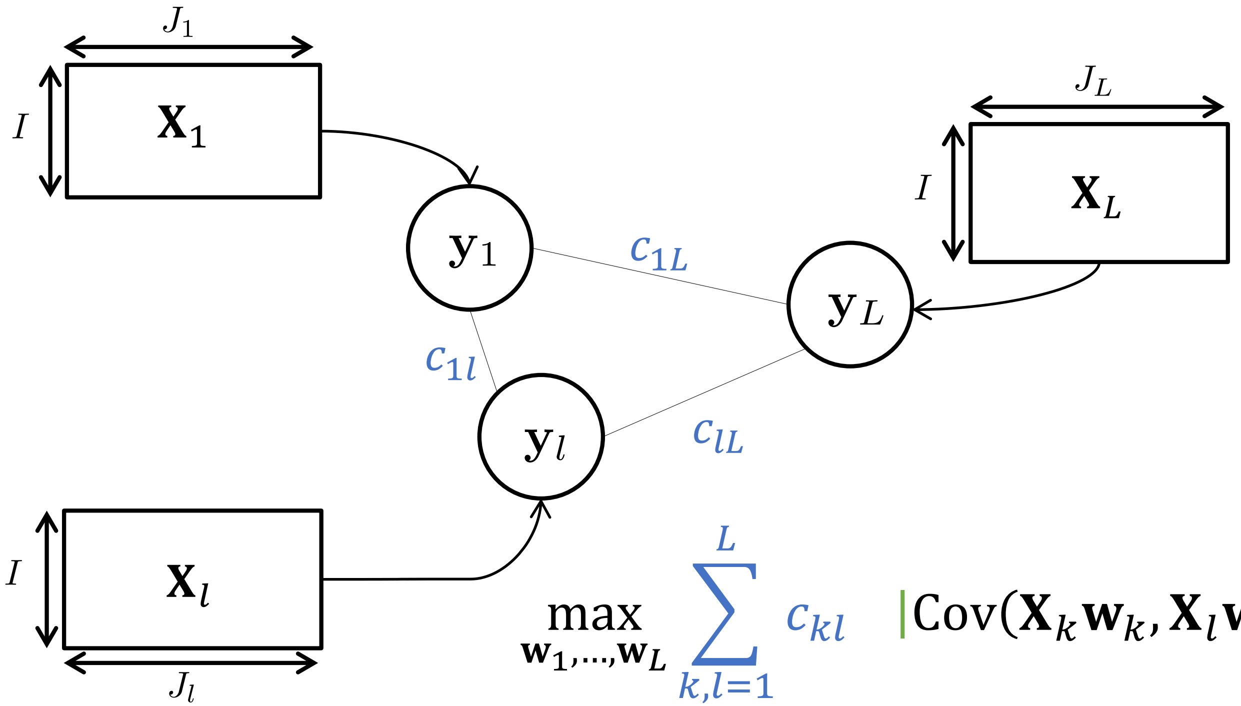


$$\max_{\mathbf{w}_1,\dots,\mathbf{w}_L} \sum_{k,l=1}^{L} c_{kl} \left(\mathrm{Cov}(\mathbf{X}_k\mathbf{w}_k, \mathbf{X}_l\mathbf{w}_l)\right)^2$$

$$\text{s.t. } \mathbf{w}_l^\top \mathbf{M}_l \mathbf{w}_l = 1,\ l = 1, \dots, L.$$

if all blocks are connected and $\mathbf{M}_l = \mathbf{I}_l$ SSQCOV-2

Regularized Generalized Canonical Correlation Analysis (RGCCA)

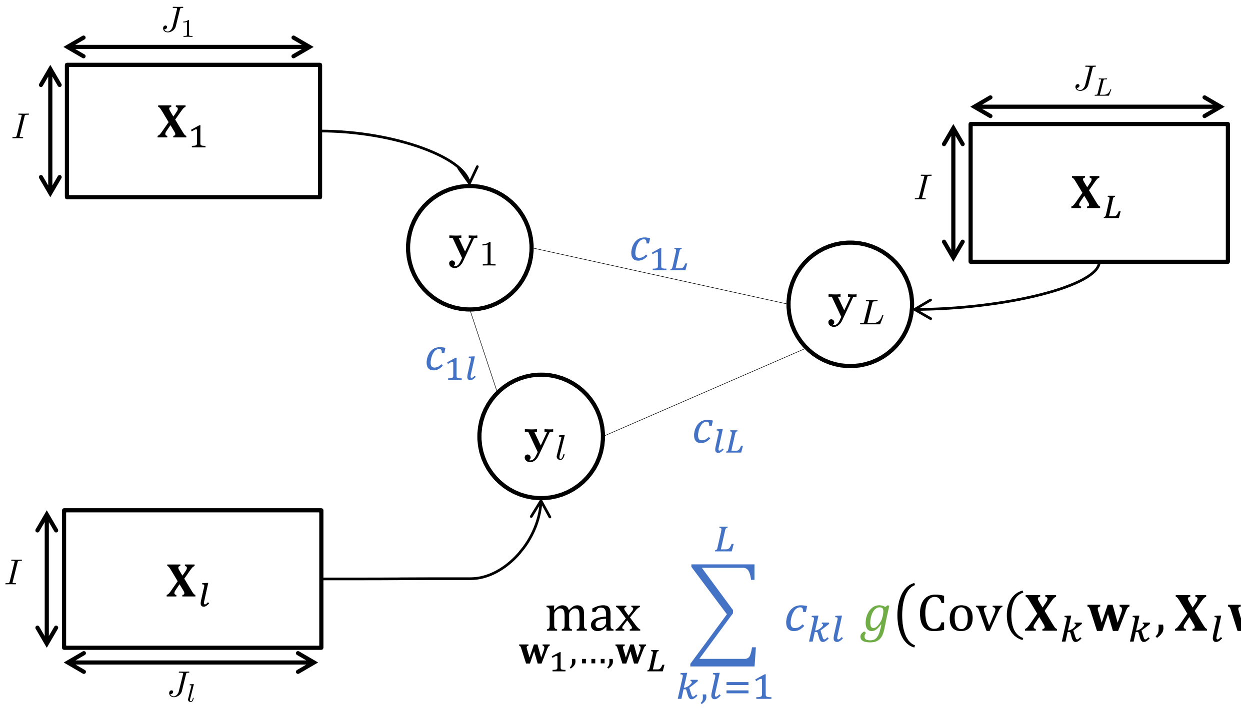


$$\max_{\mathbf{w}_1,\ldots,\mathbf{w}_L} \sum_{k,l=1}^{L} c_{kl} \left|\mathrm{Cov}(\mathbf{X}_k\mathbf{w}_k, \mathbf{X}_l\mathbf{w}_l)\right|$$

$$\text{s.t. } \mathbf{w}_l^\top \mathbf{M}_l \mathbf{w}_l = 1,\ l = 1, \ldots, L.$$

➡ if all blocks are connected and $\mathbf{M}_l = \mathbf{I}_l$ ➡ SABSCOV-2

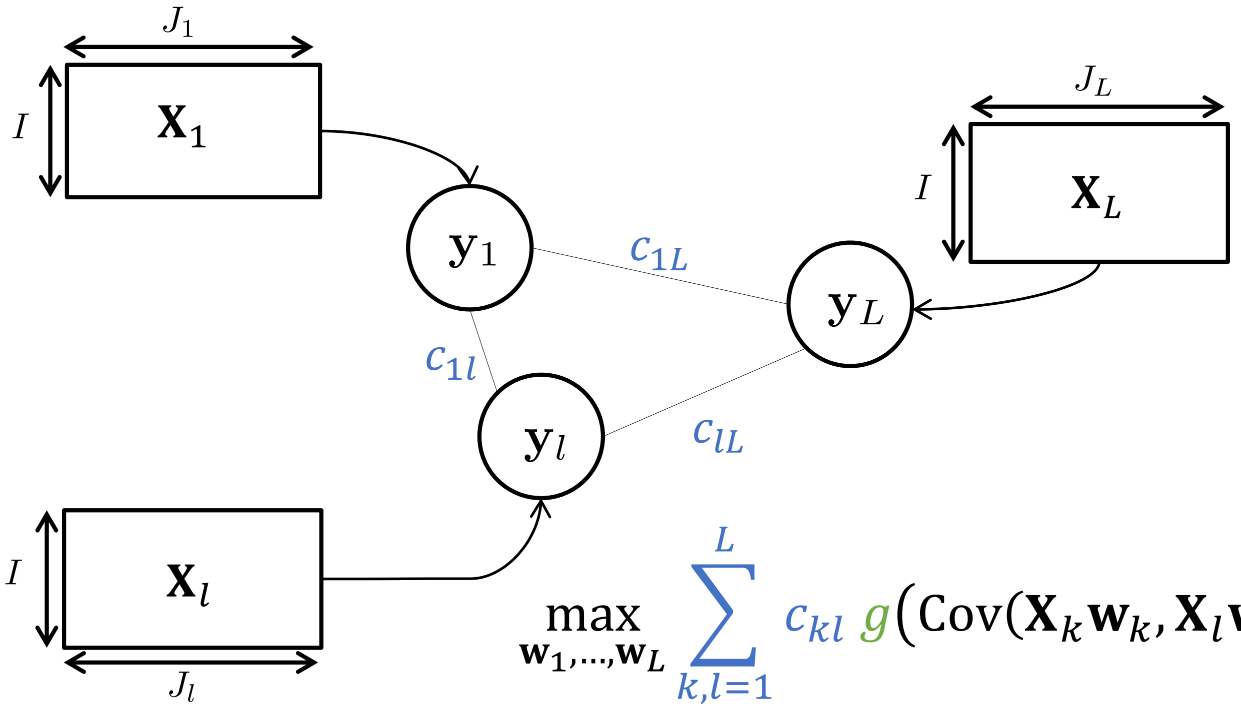
Regularized Generalized Canonical Correlation Analysis (RGCCA)



$$\max_{\mathbf{w}_1,\dots,\mathbf{w}_L} \sum_{k,l=1}^{L} c_{kl}\, g\big(\mathrm{Cov}(\mathbf{X}_k\mathbf{w}_k, \mathbf{X}_l\mathbf{w}_l)\big)$$

$$\text{s.t. } \mathbf{w}_l^\top \mathbf{M}_l \mathbf{w}_l = 1,\ \ l = 1, \dots, L.$$

Regularized Generalized Canonical Correlation Analysis (RGCCA)



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➡ with g a continuous, convex and derivable function.

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$$\max_{\mathbf{w}_1,\ldots,\mathbf{w}_L} \sum_{k,l=1}^{L} c_{kl}\, g\big(\mathrm{Cov}(\mathbf{X}_k\mathbf{w}_k, \mathbf{X}_l\mathbf{w}_l)\big)$$

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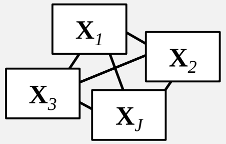
Overview of the Multi-Block litterature

ALL BLOCKS ARE INTERCONNECTED	
SUMCOR (Horst, 1961)	$\max_{\mathbf{w}_j} \sum_{j,k} \mathrm{cor}(\mathbf{X}_j\mathbf{w}_j, \mathbf{X}_k\mathbf{w}_k)$
SSQCOR (Kettenring, 1961)	$\max_{\mathbf{w}_j} \sum_{j,k} \mathrm{cor}^2(\mathbf{X}_j\mathbf{w}_j, \mathbf{X}_k\mathbf{w}_k)$
SABSCOR (Wold, 1982)	$\max_{\mathbf{w}_j} \sum_{j,k} \lvert\mathrm{cor}(\mathbf{X}_j\mathbf{w}_j, \mathbf{X}_k\mathbf{w}_k)\rvert$

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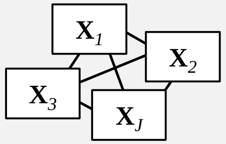

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SUMCOV (Van de Geer, 1984)	$\max_{\lVert\mathbf{w}_j\rVert=1} \sum_{j,k} \mathrm{cov}(\mathbf{X}_j\mathbf{w}_j, \mathbf{X}_k\mathbf{w}_k)$
SSQCOV (Hanafi & Kiers, 2006)	$\max_{\lVert\mathbf{w}_j\rVert=1} \sum_{j,k} \mathrm{cov}^2(\mathbf{X}_j\mathbf{w}_j, \mathbf{X}_k\mathbf{w}_k)$
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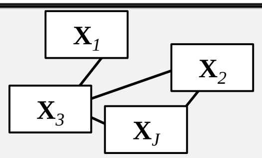

BLOCKS ARE PARTIALLY CONNECTED $c_{jk} = 1$ if $\mathbf{X}_j \leftrightarrow \mathbf{X}_k$, 0 otherwise	
SUMCOR	$\max_{\mathbf{w}_j} \sum_{j,k} c_{jk} \operatorname{cor}(\mathbf{X}_j\mathbf{w}_j, \mathbf{X}_k\mathbf{w}_k)$
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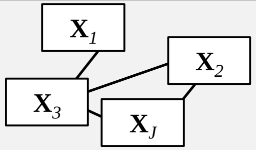
BLOCKS ARE PARTIALLY CONNECTED $c_{jk} = 1$ if $\mathbf{X}_j \leftrightarrow \mathbf{X}_k$, 0 otherwise	
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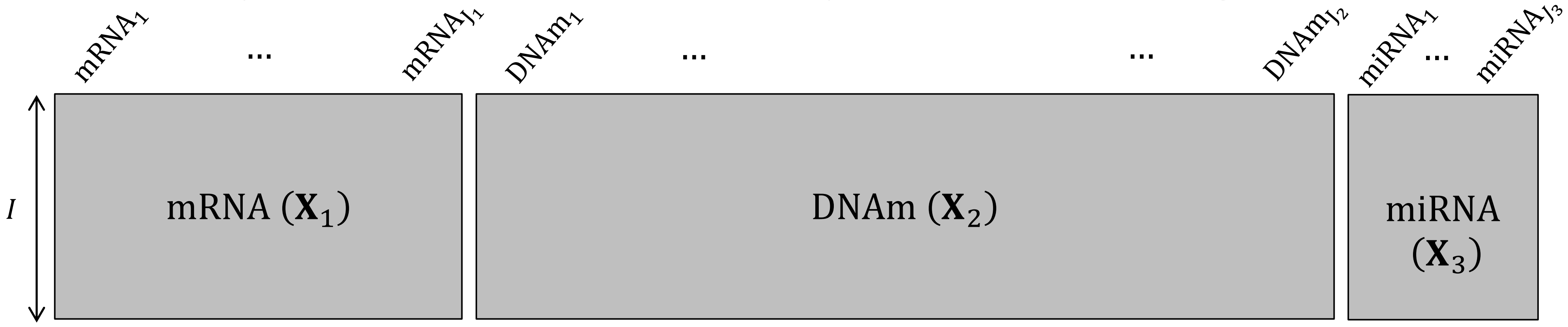
Tune parameters in an unsupervised setting



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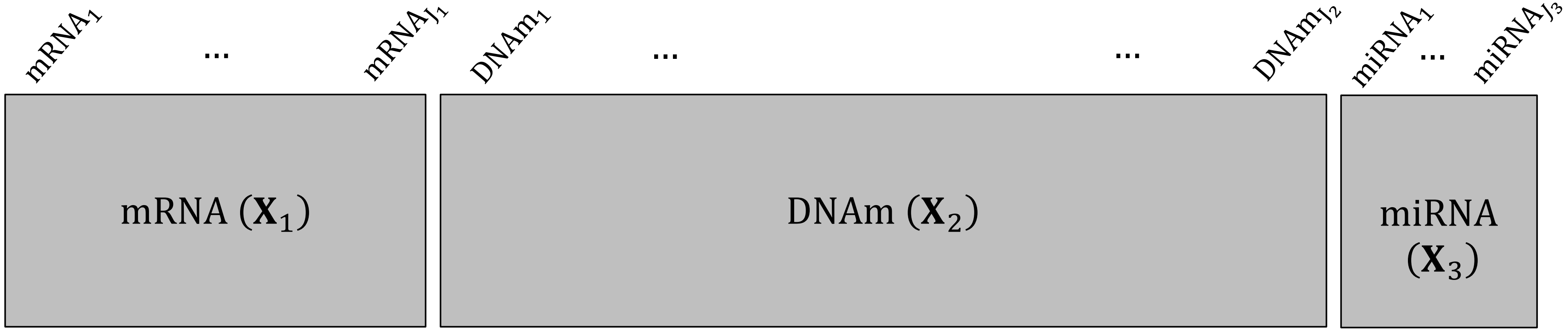

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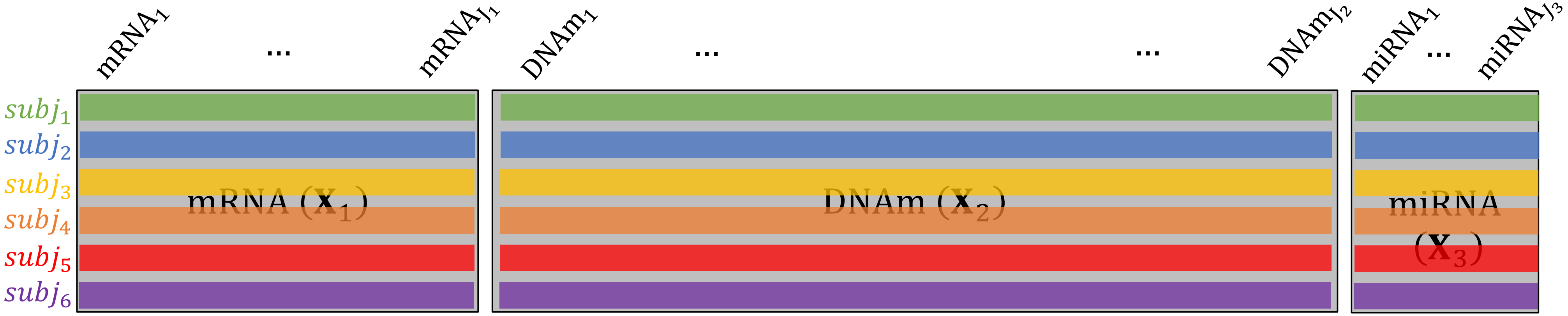

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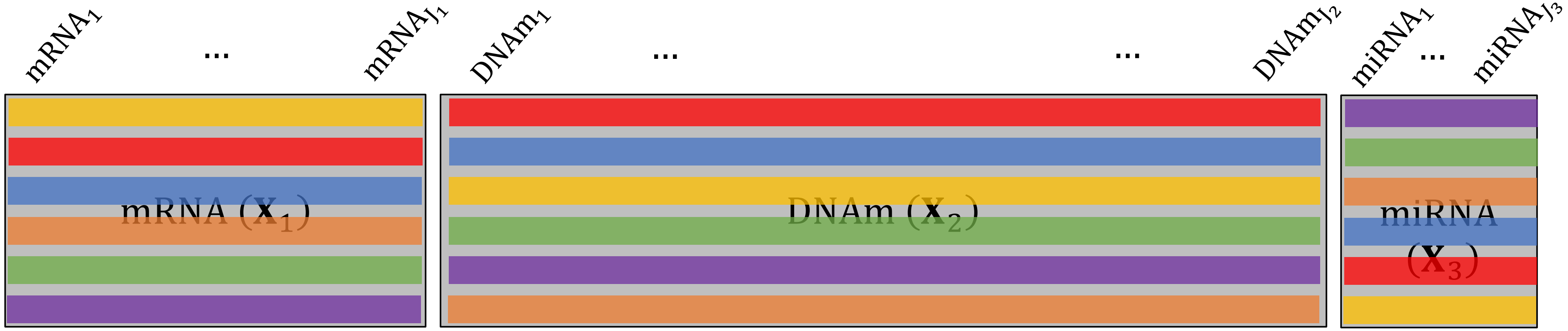
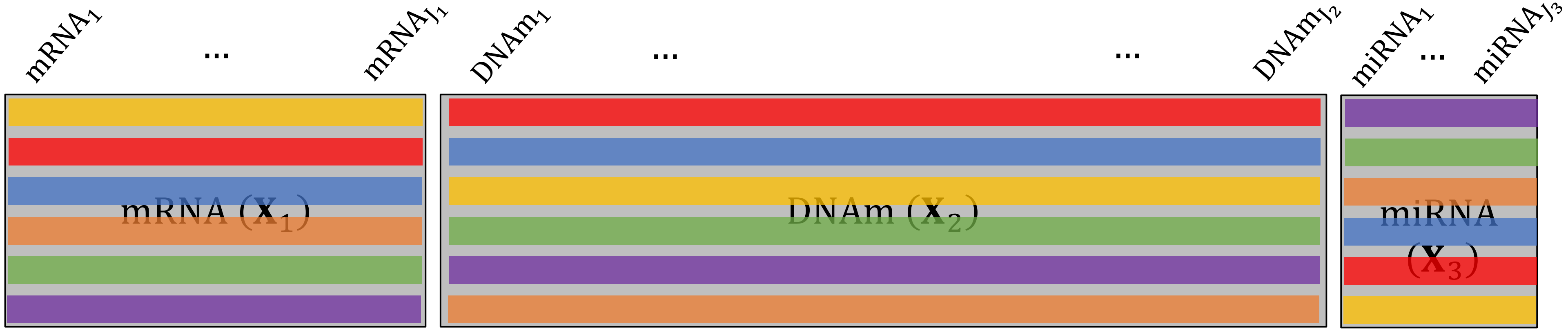


Permutation n°1

Tune parameters in an unsupervised setting



Permutation n°1

Parameter set n°1

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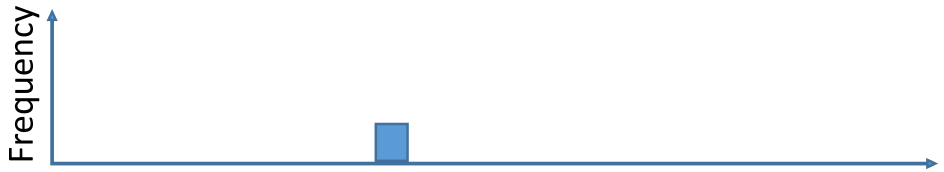

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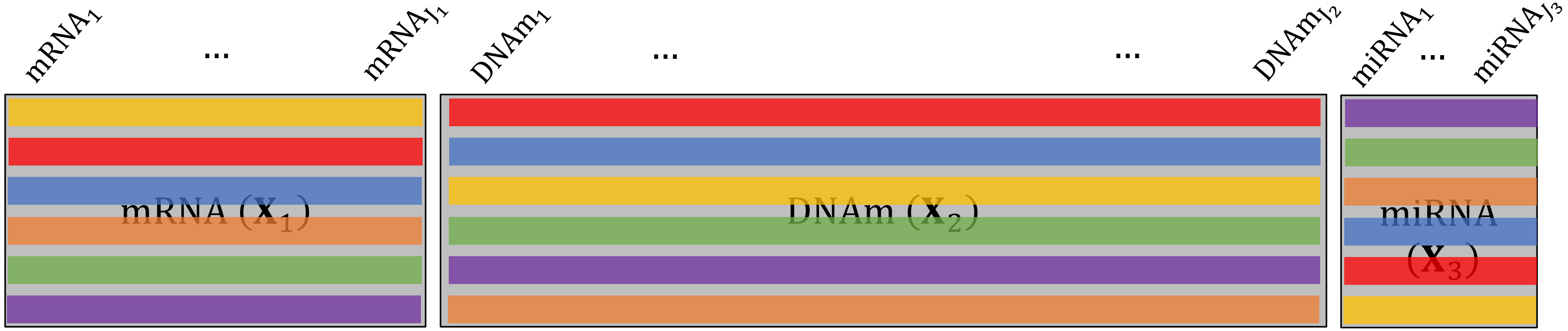

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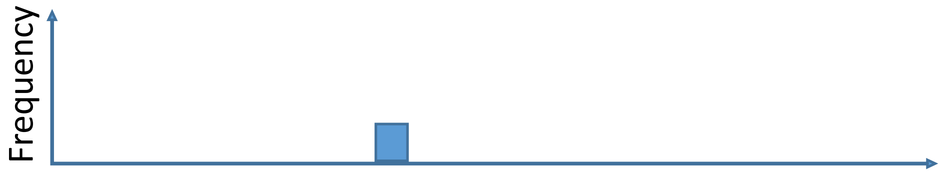

⋮

Parameter set n°K

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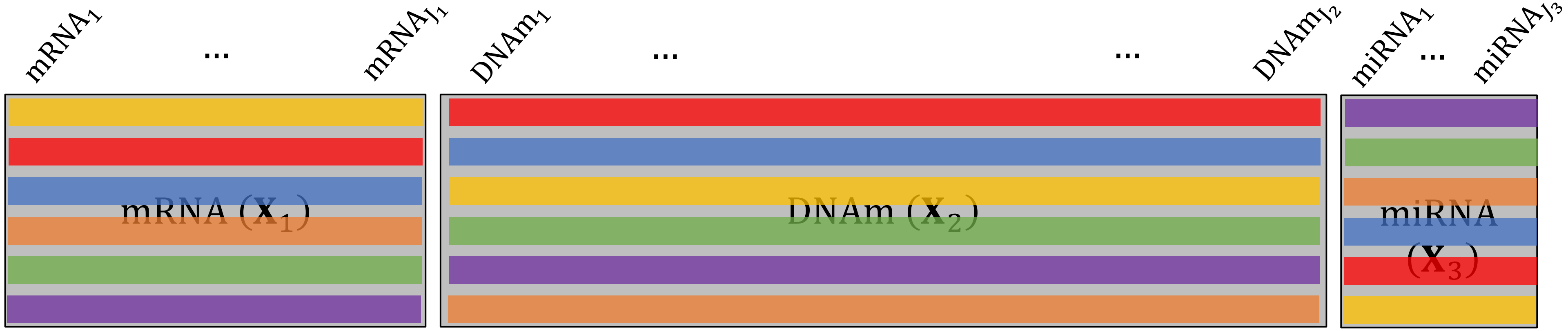

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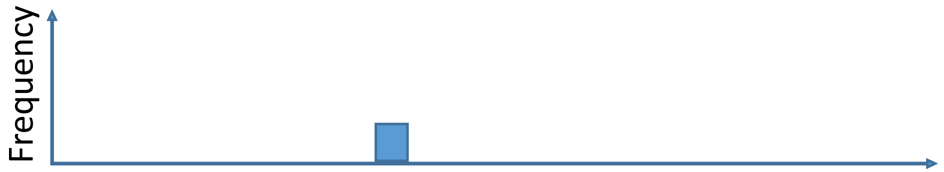

⋮ ⋮

Parameter set n°K

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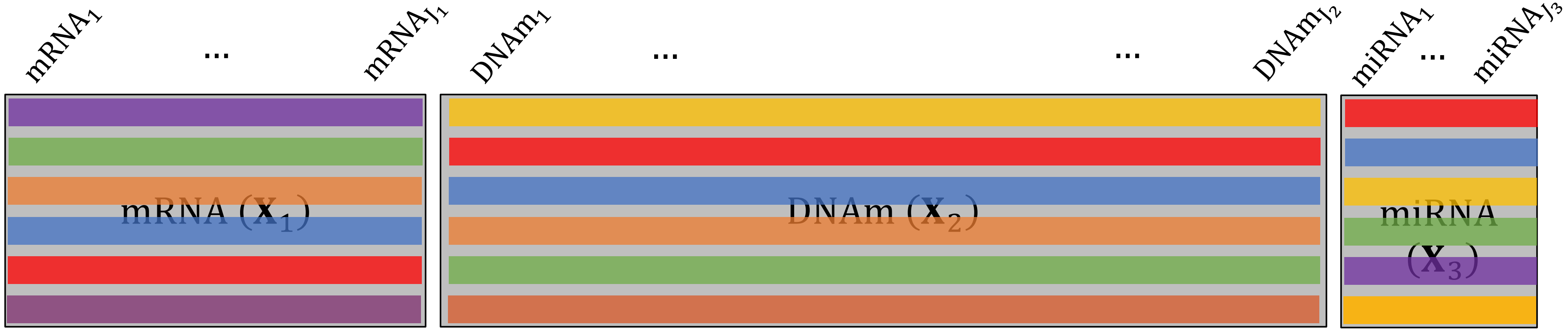
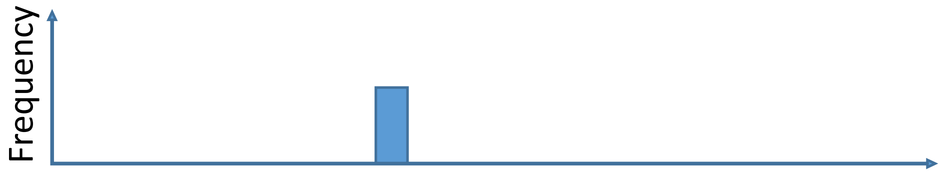


Permutation n°2

Parameter set n°1



⋮ ⋮

Parameter set n°K

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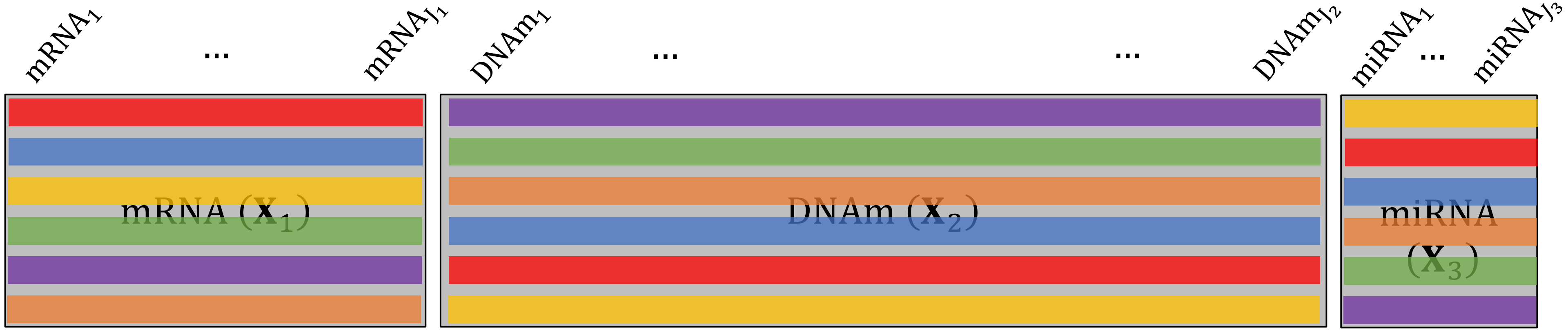
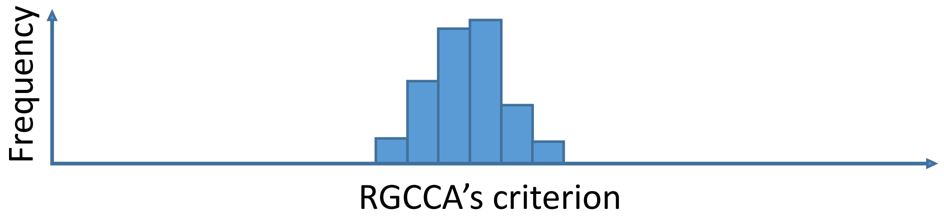


Permutation n°N

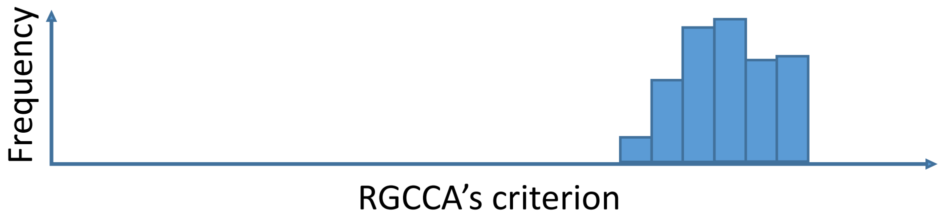
Parameter set n°1



⋮

⋮

Parameter set n°K



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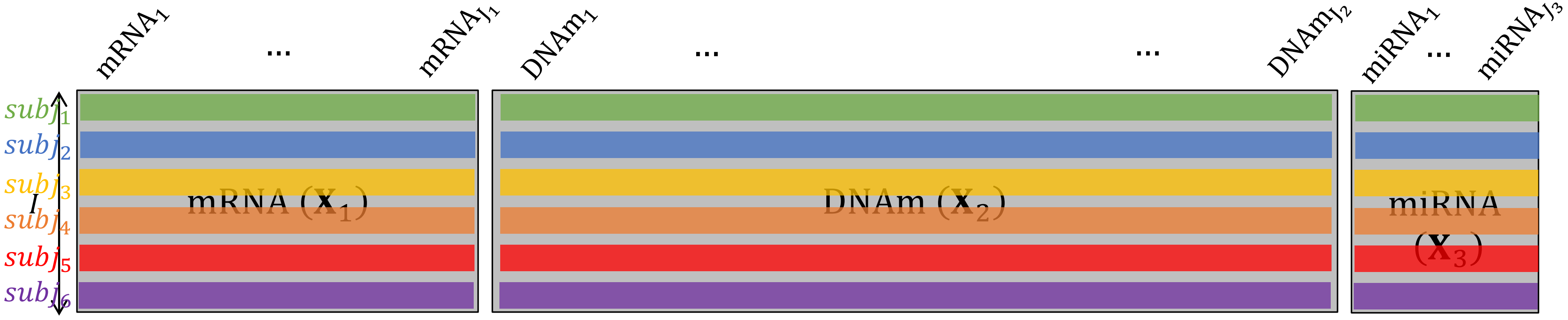
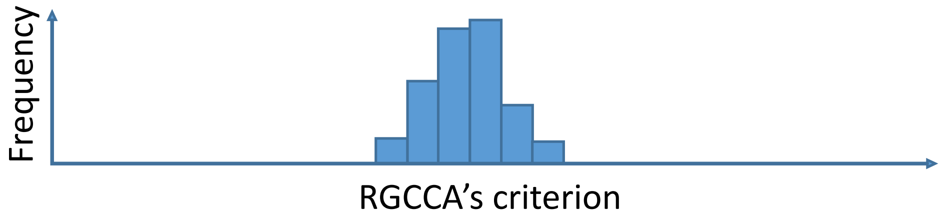


No Permutation

Parameter set n°1



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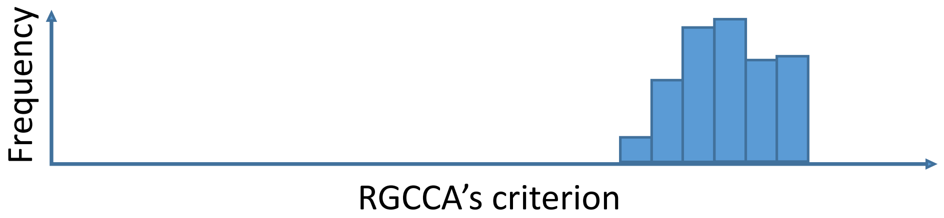

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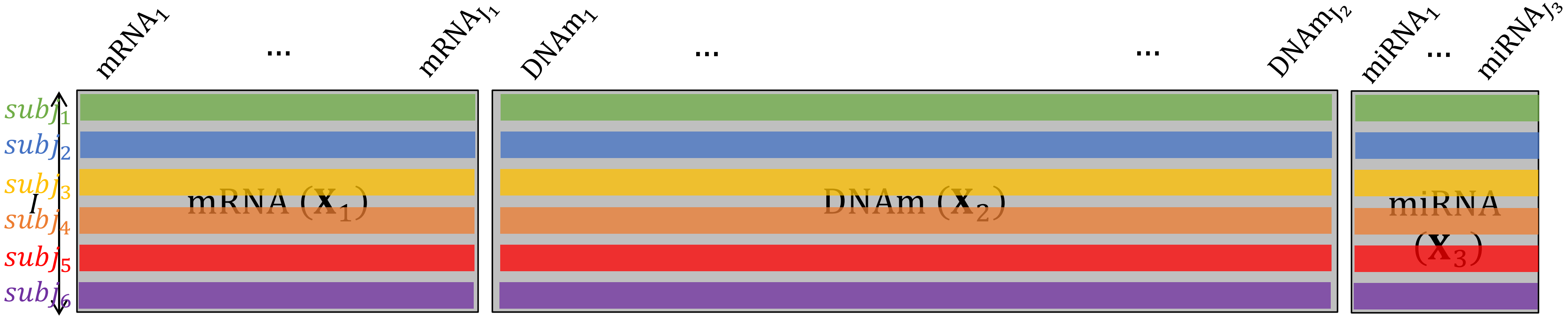

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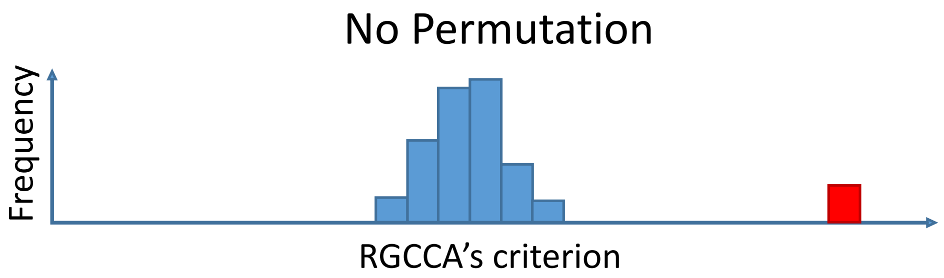

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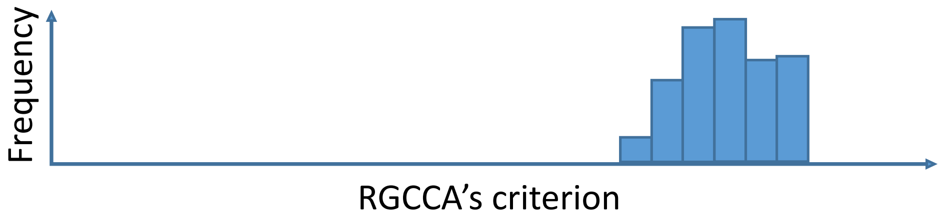

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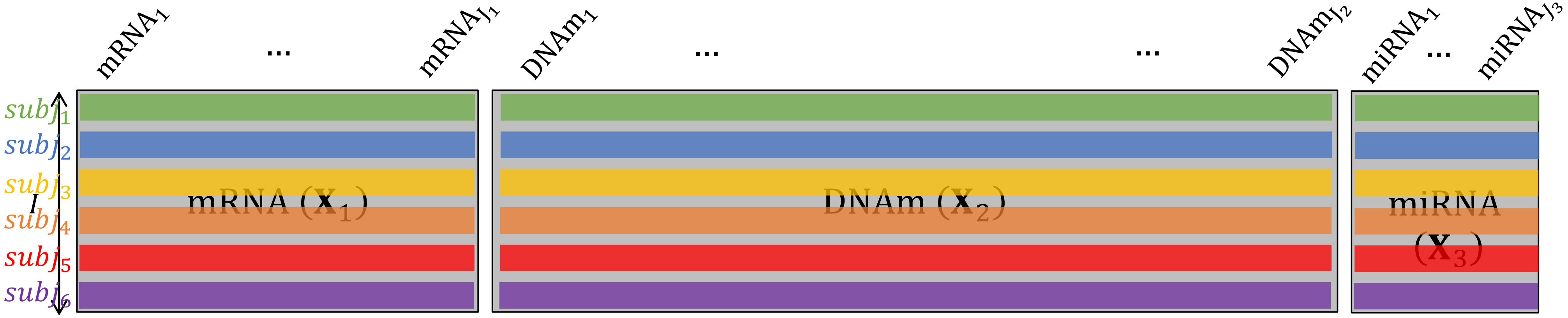

No Permutation

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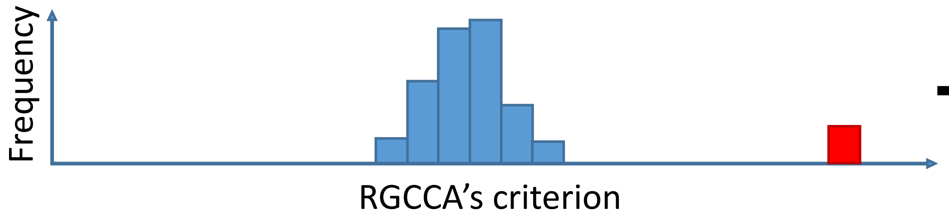
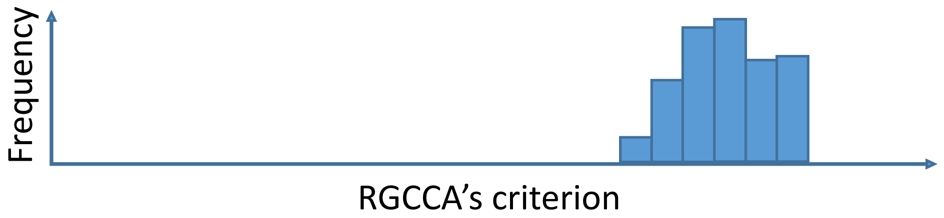


➔ The set of parameters is likely to be selected.

⋮ ⋮

Parameter set n°K



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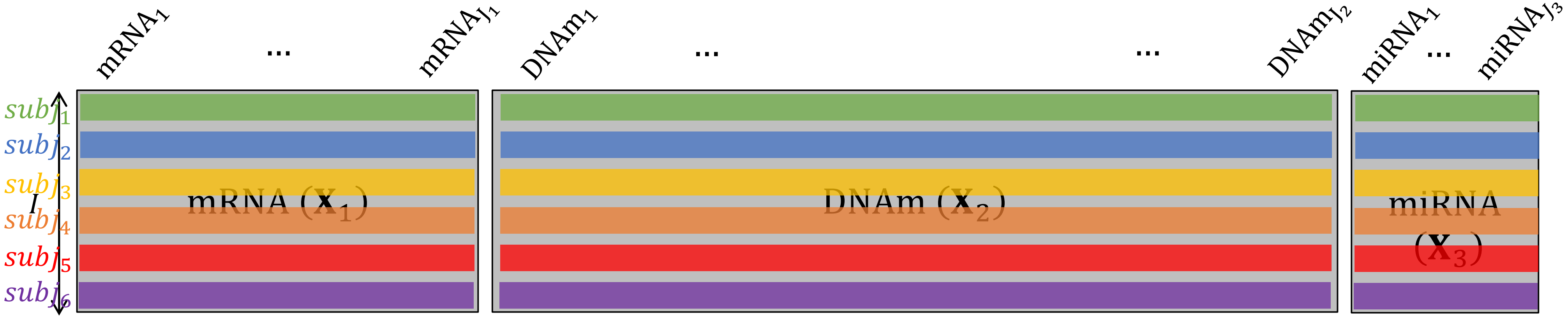
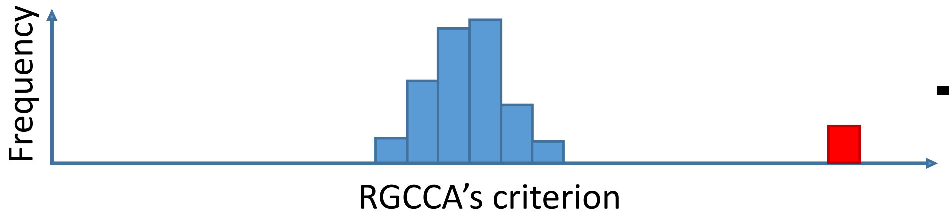


No Permutation

Parameter set n°1



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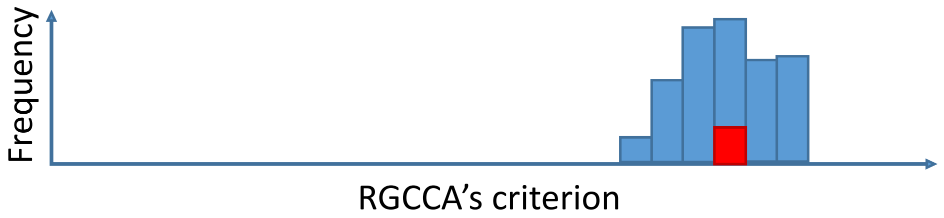

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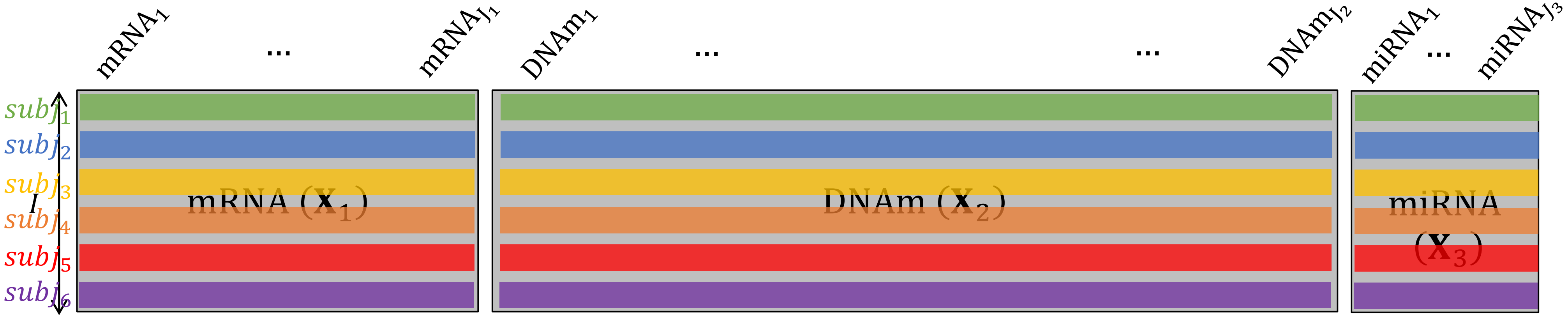

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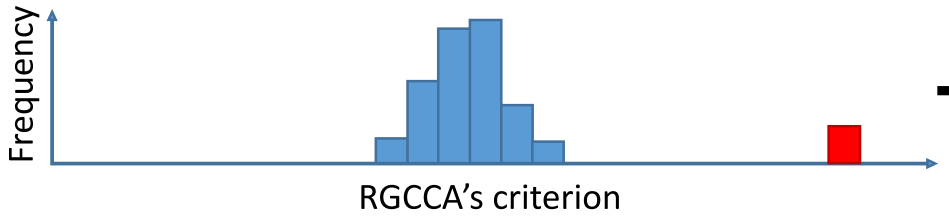

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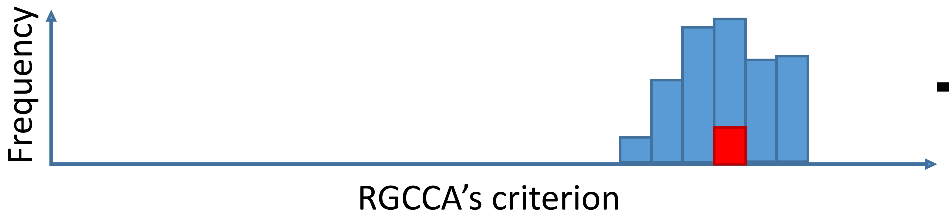

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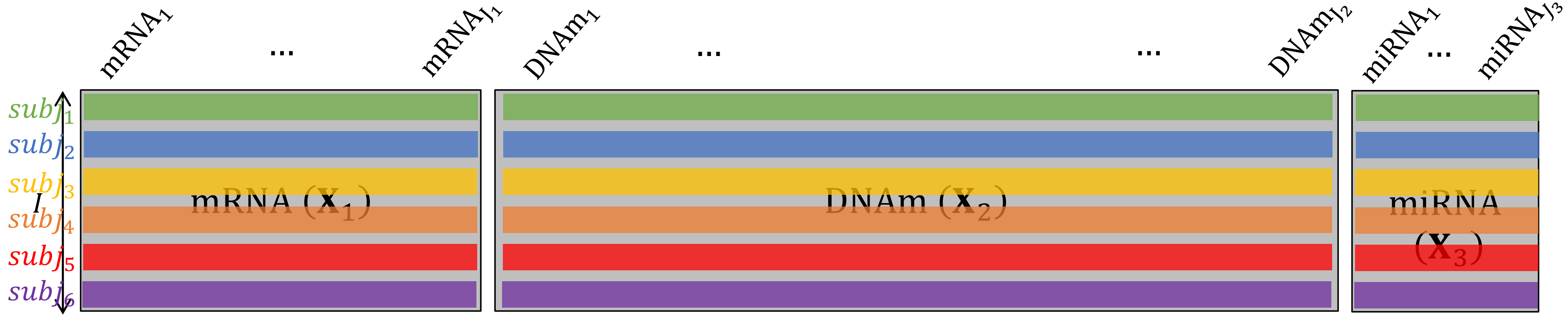

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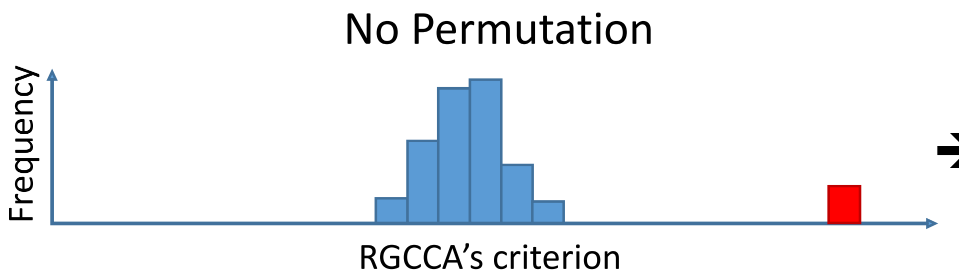

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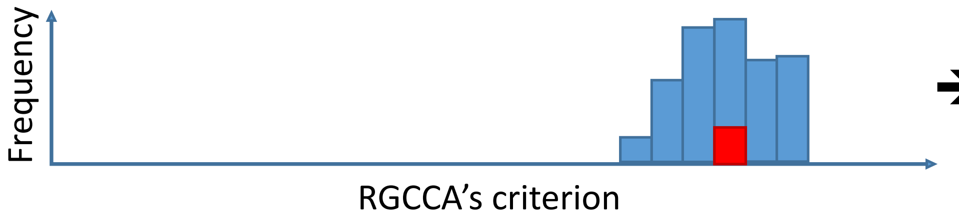
⋮

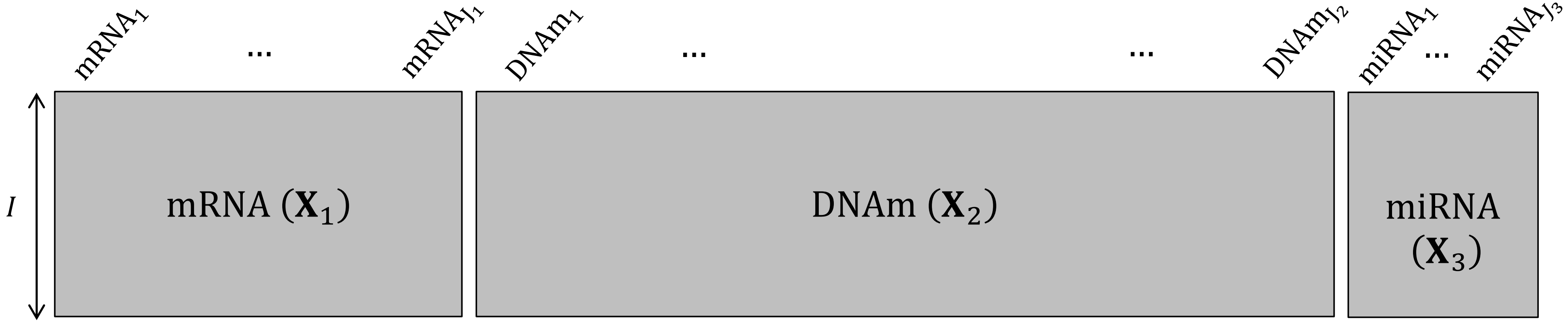
RGCCA choose the best set of parameters as the one with the highest value of $Z_k = \frac{(crit_{unperm} - \mu_{crit}^{perm})}{\sigma_{crit}^{perm}}$

Parameter set n°K



➔ The set of parameters is unlikely to be selected.

Evaluate the robustness of the model by bootstrapping.



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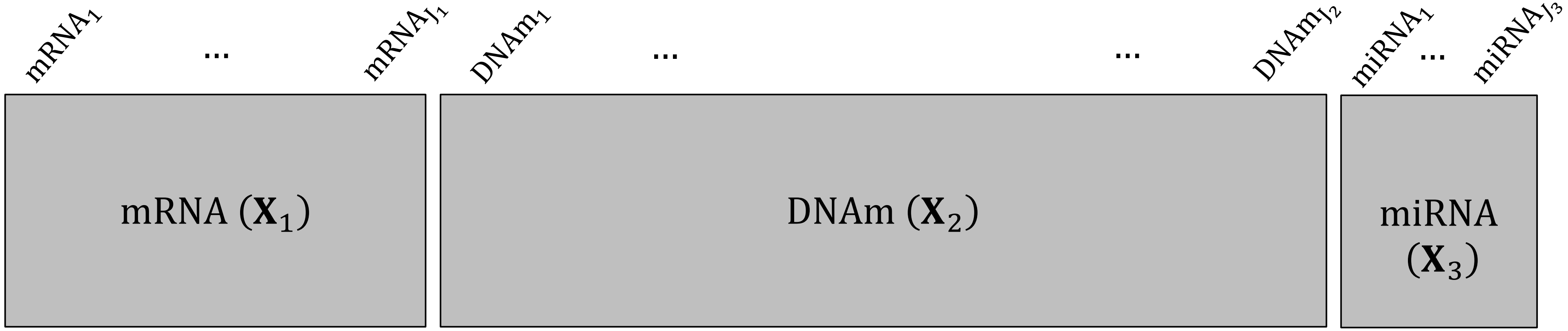

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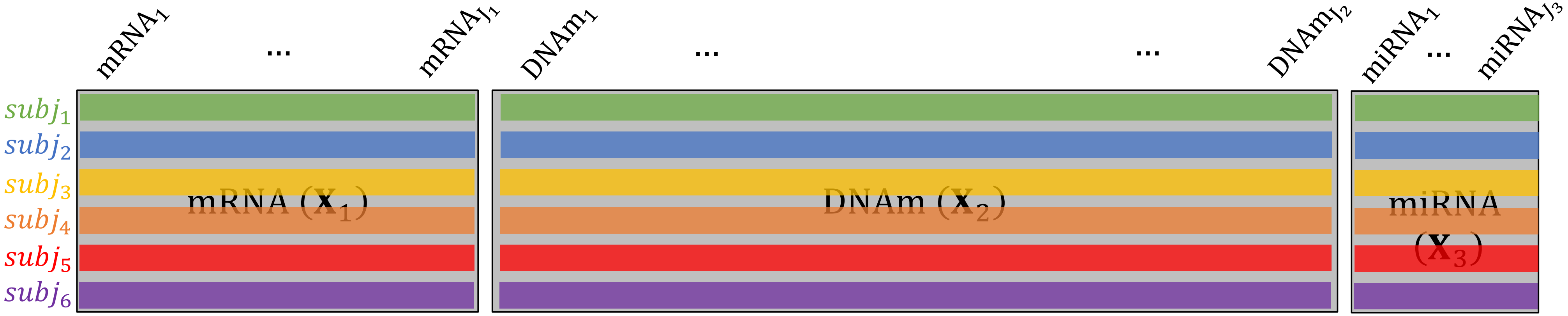

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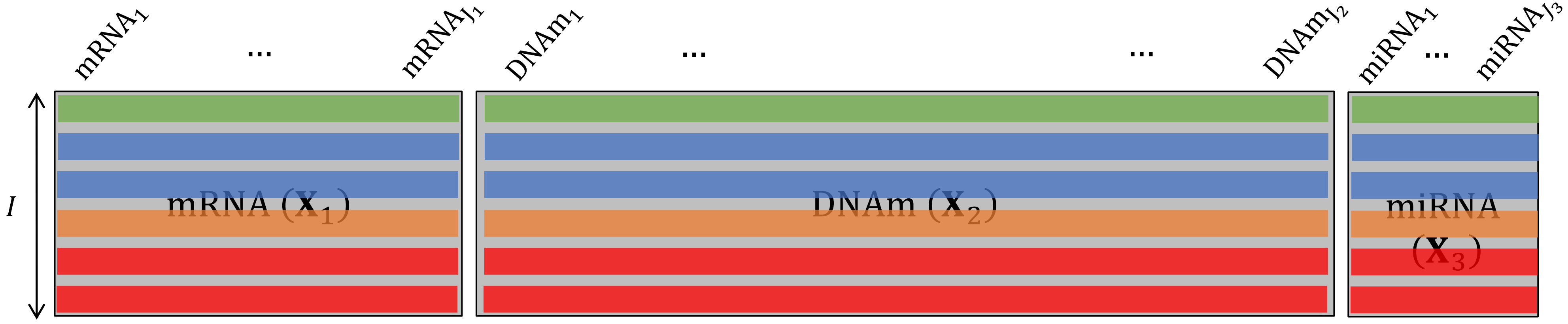

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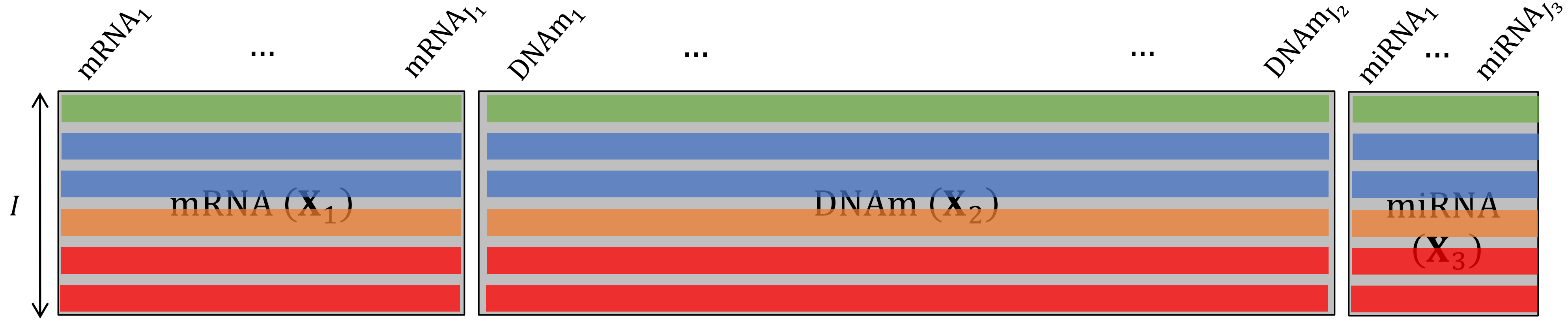
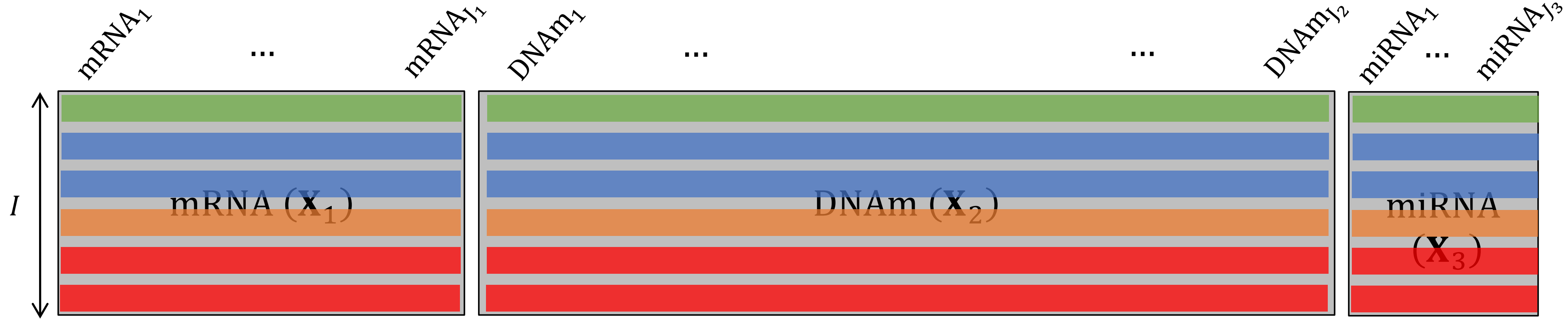


Bootstrap sample n°1

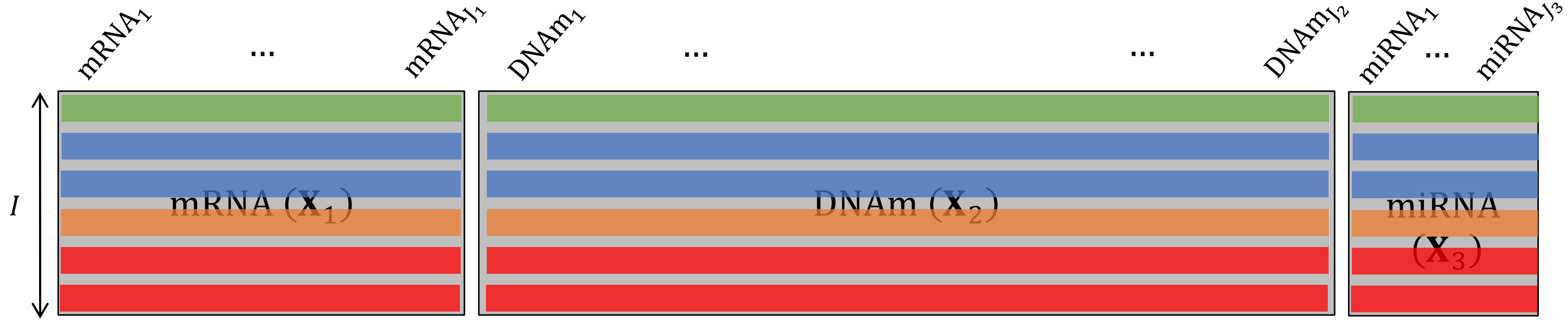
Evaluate the robustness of the model by bootstrapping.



Bootstrap sample n°1

Weight for mRNA_1

Evaluate the robustness of the model by bootstrapping.



Bootstrap sample n°1

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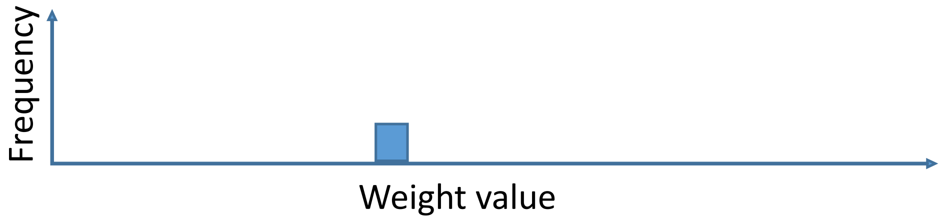

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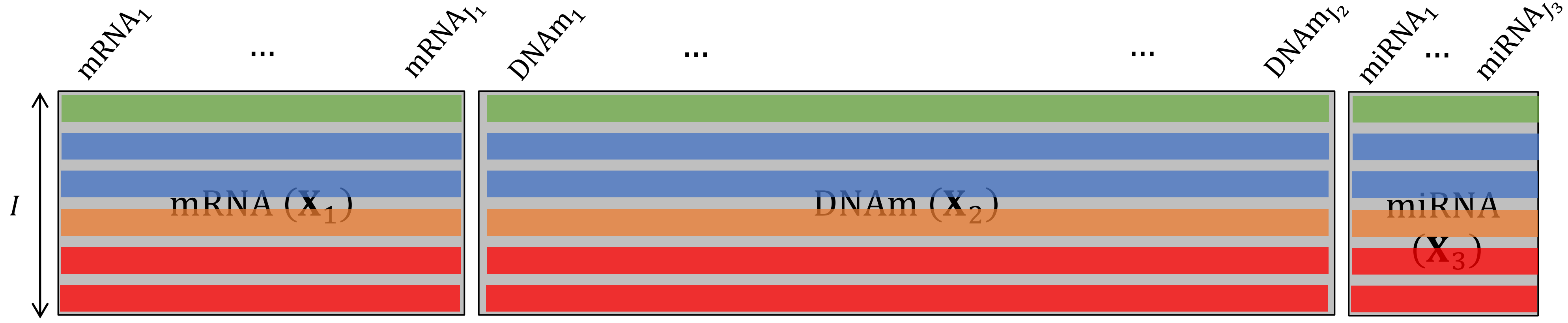

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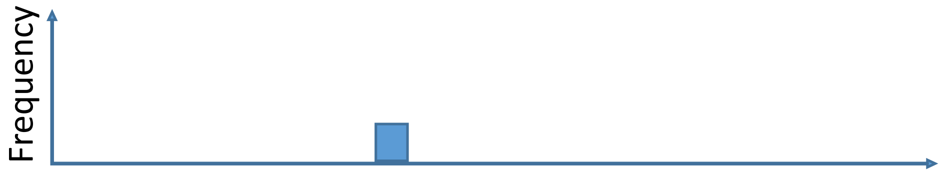
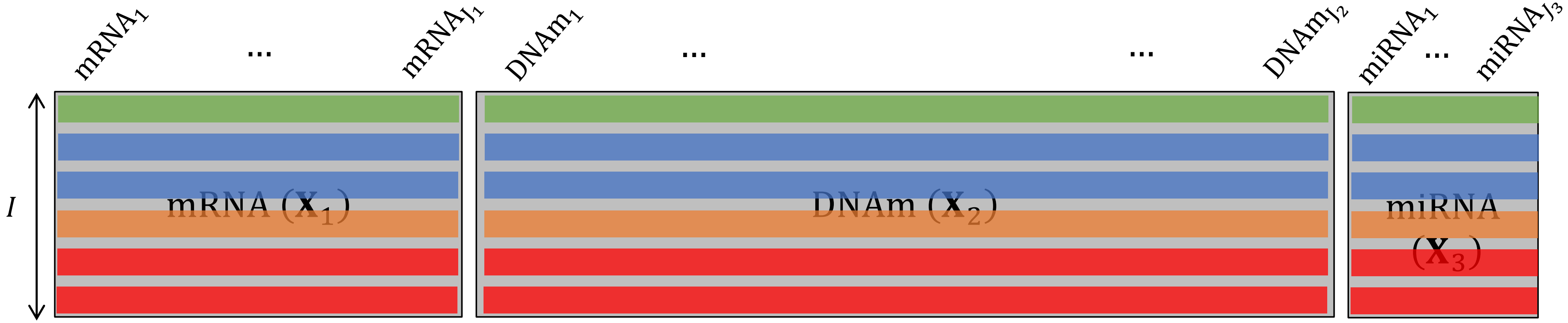


Weight for mRNA_1

⋮

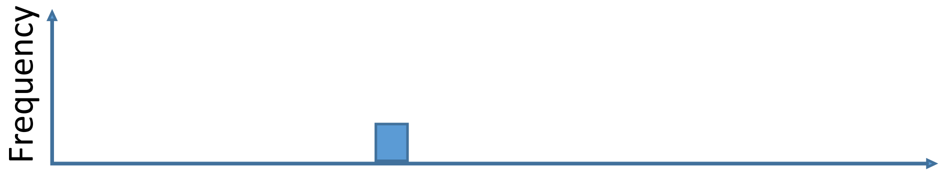
Weight for miRNA_{J_3}

Evaluate the robustness of the model by bootstrapping.



Bootstrap sample n°1

Weight for mRNA_1



⋮ ⋮

Weight for miRNA_{J_3}

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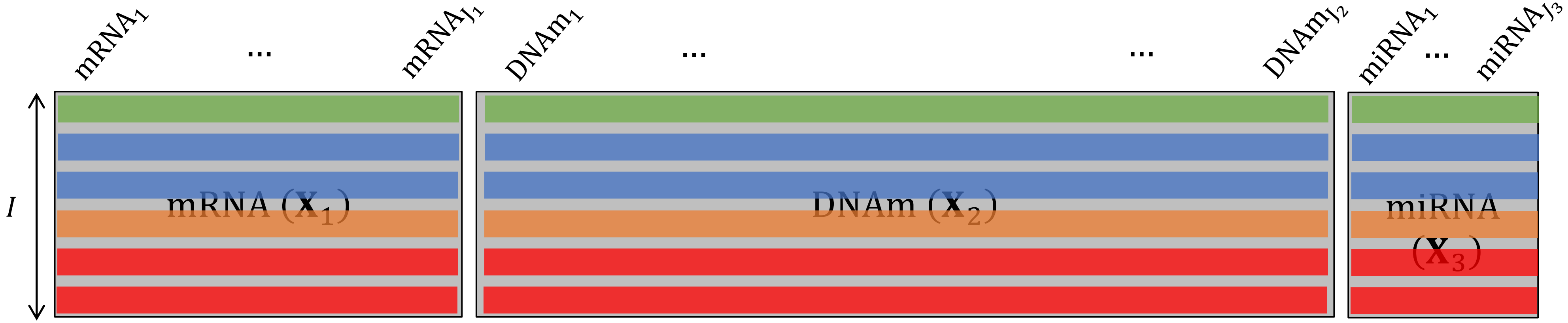
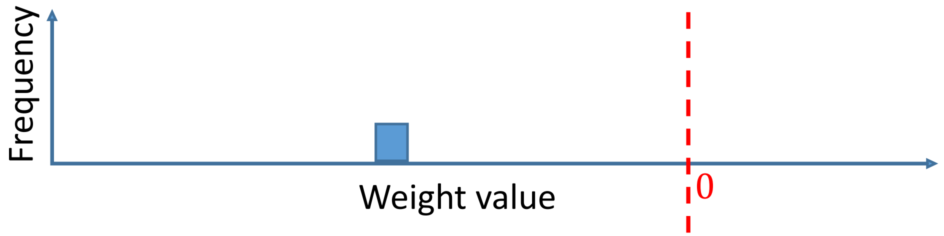


Bootstrap sample n°1

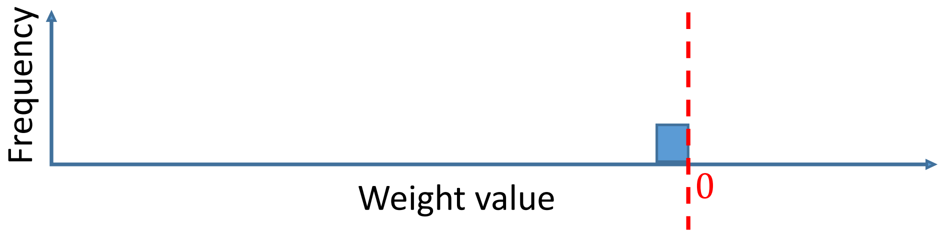
Weight for $mRNA_1$



⋮

⋮

Weight for $miRNA_{J_3}$



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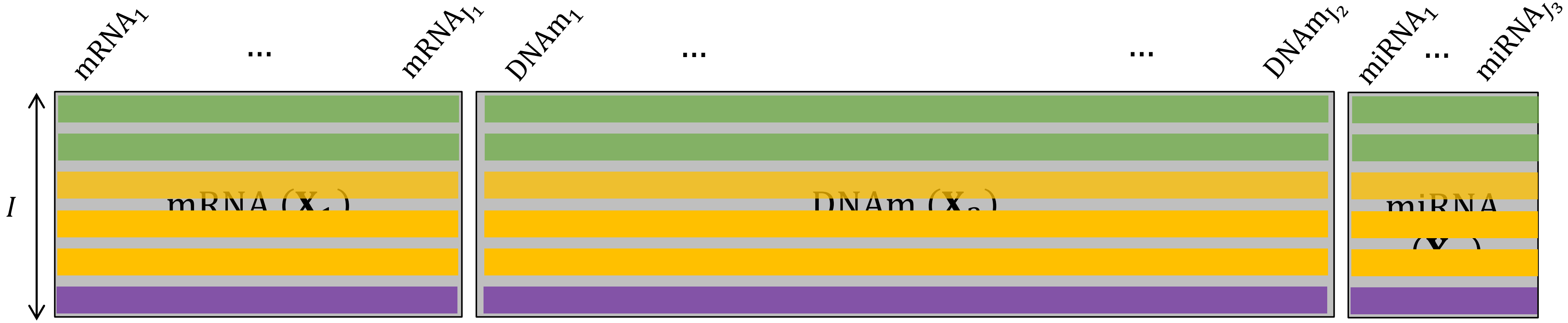
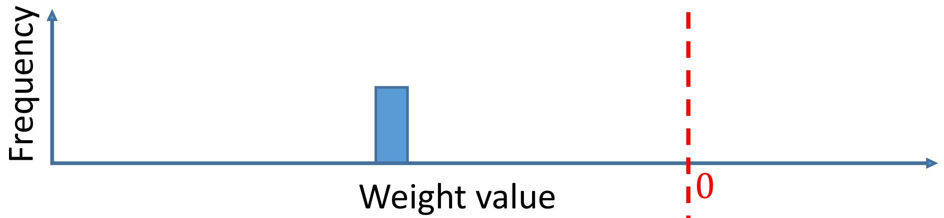


Bootstrap sample n°2

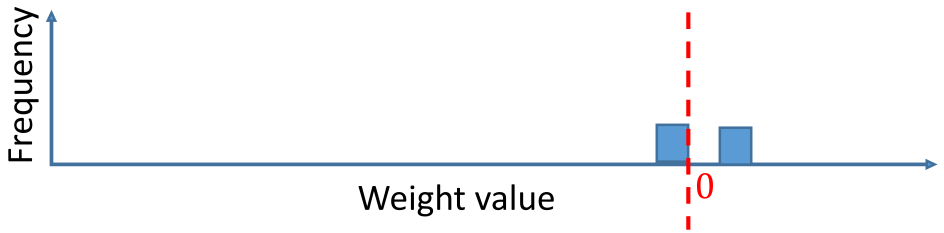
Weight for mRNA_1



⋮

⋮

Weight for miRNA_{J_3}



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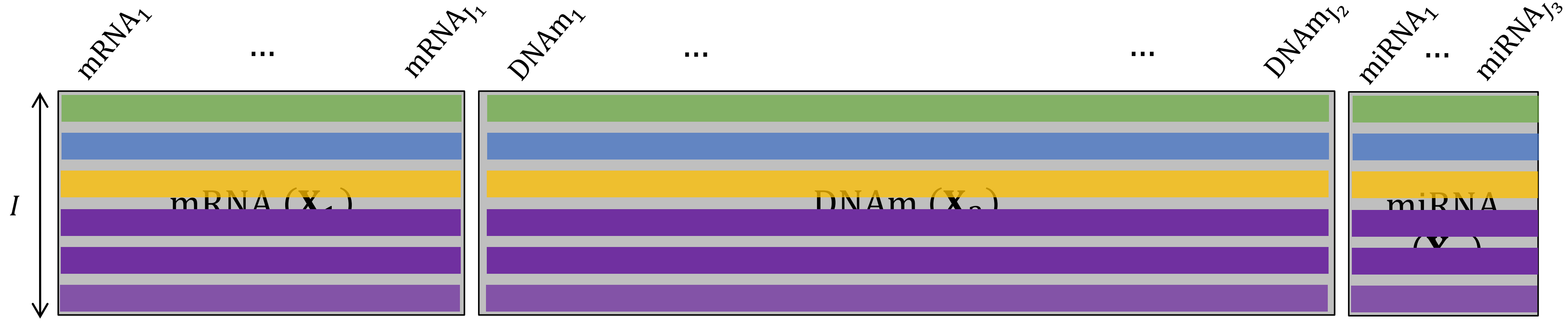

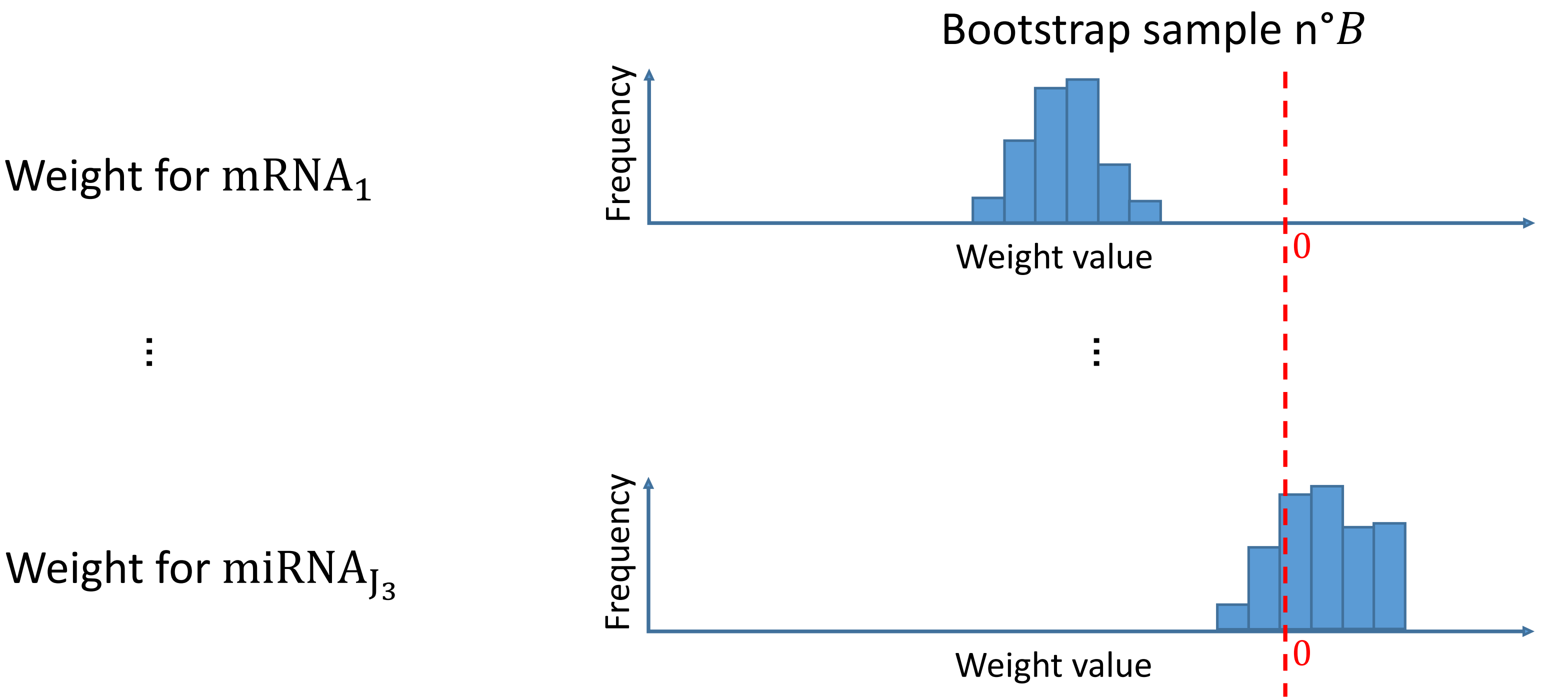

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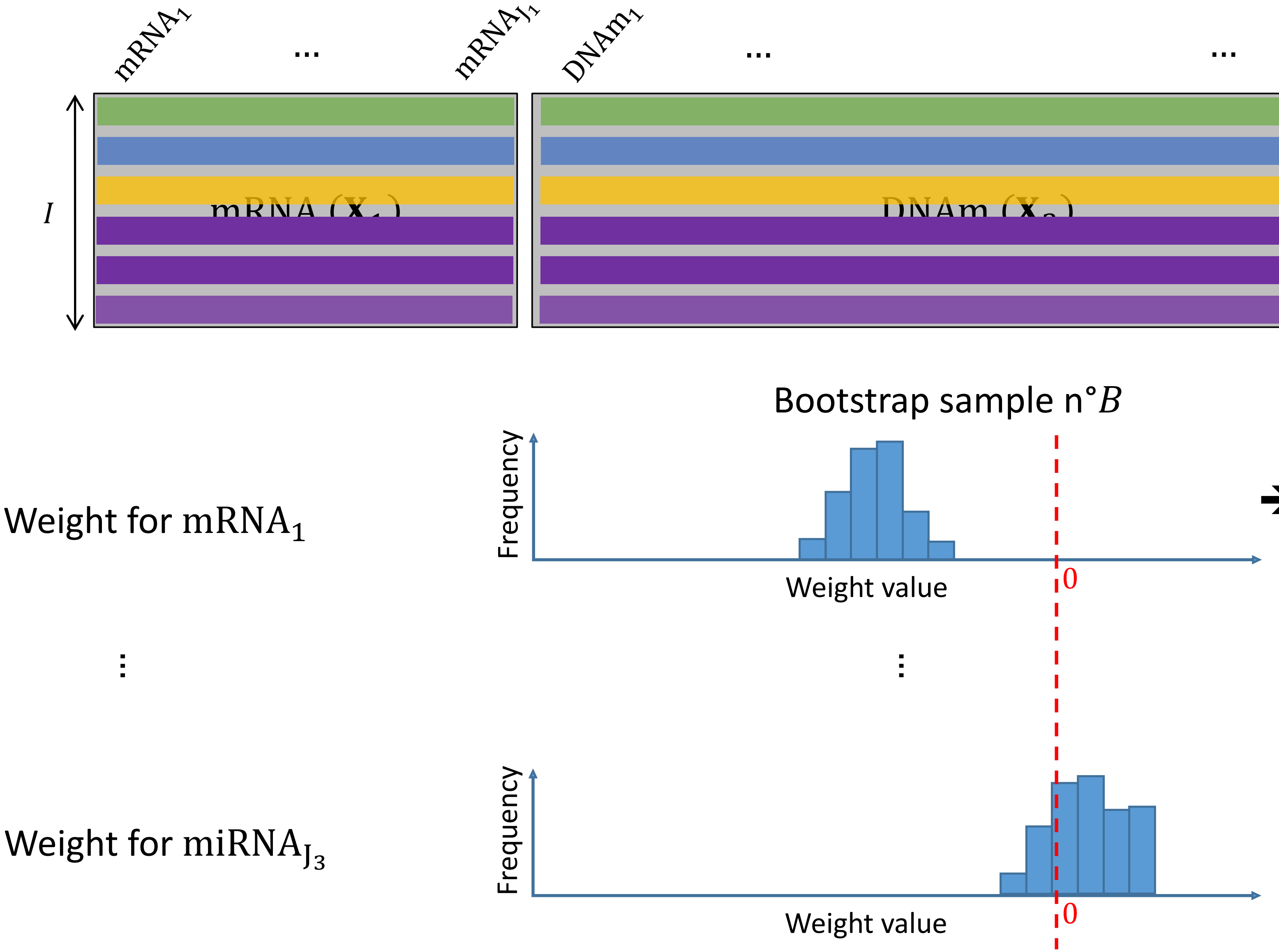

➔ The weight is likely to be considered as significantly different from 0.

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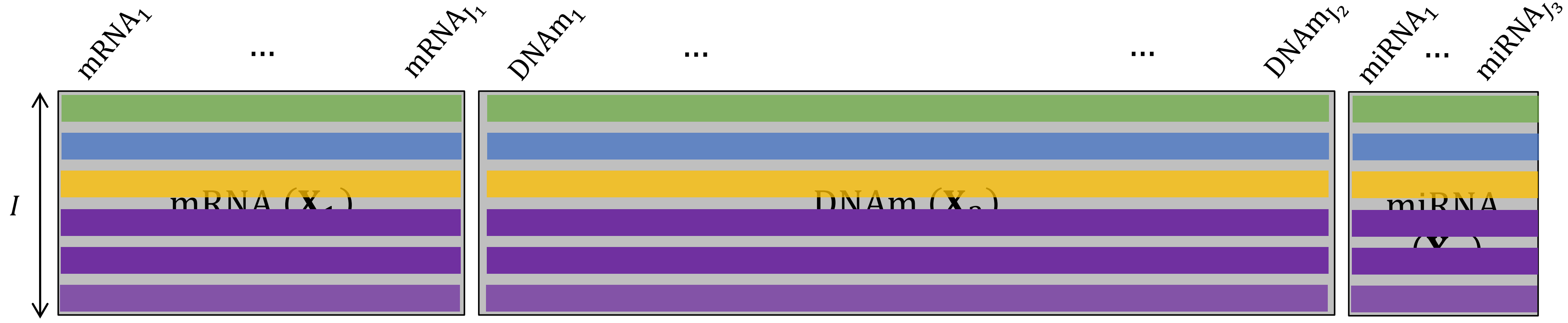
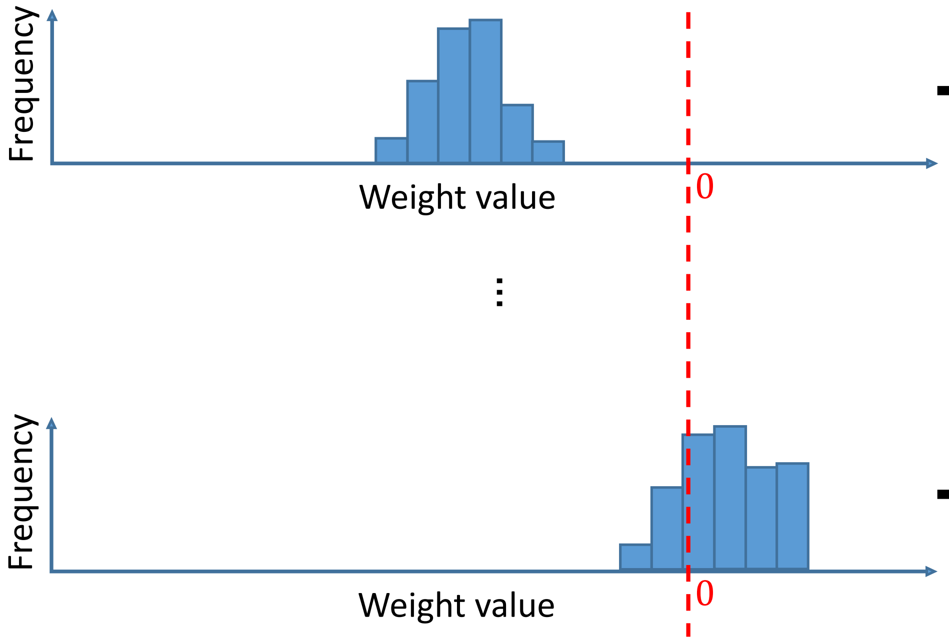


Bootstrap sample n°B

Weight for mRNA$_1$

⋮

Weight for miRNA$_{J_3}$



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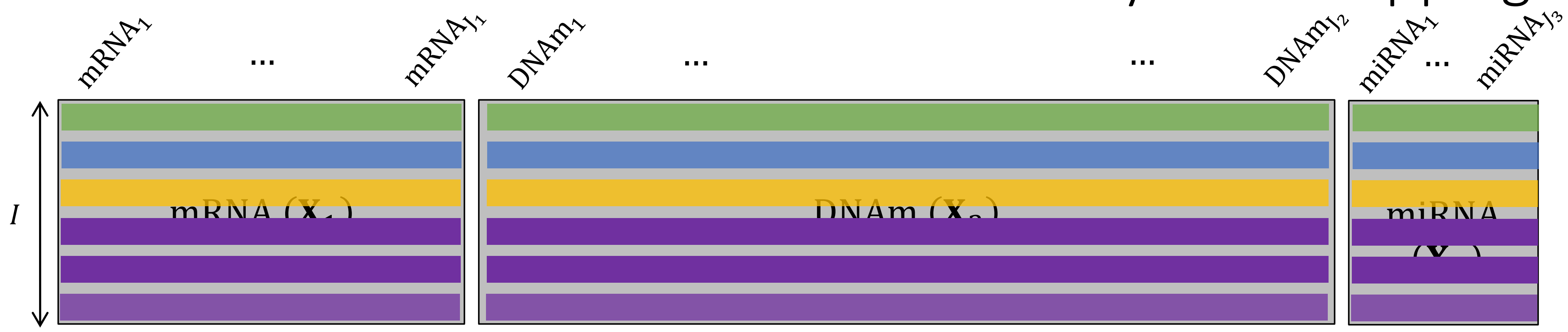
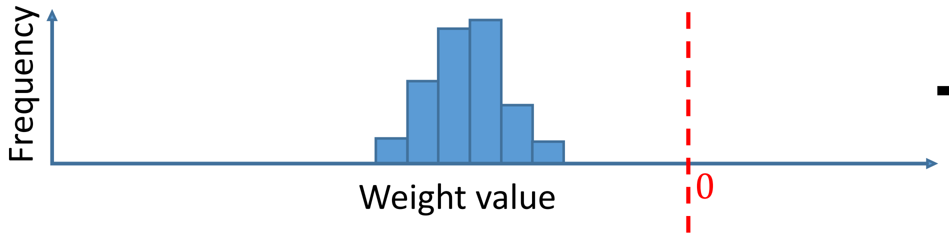


Bootstrap sample n°B

Weight for mRNA_1



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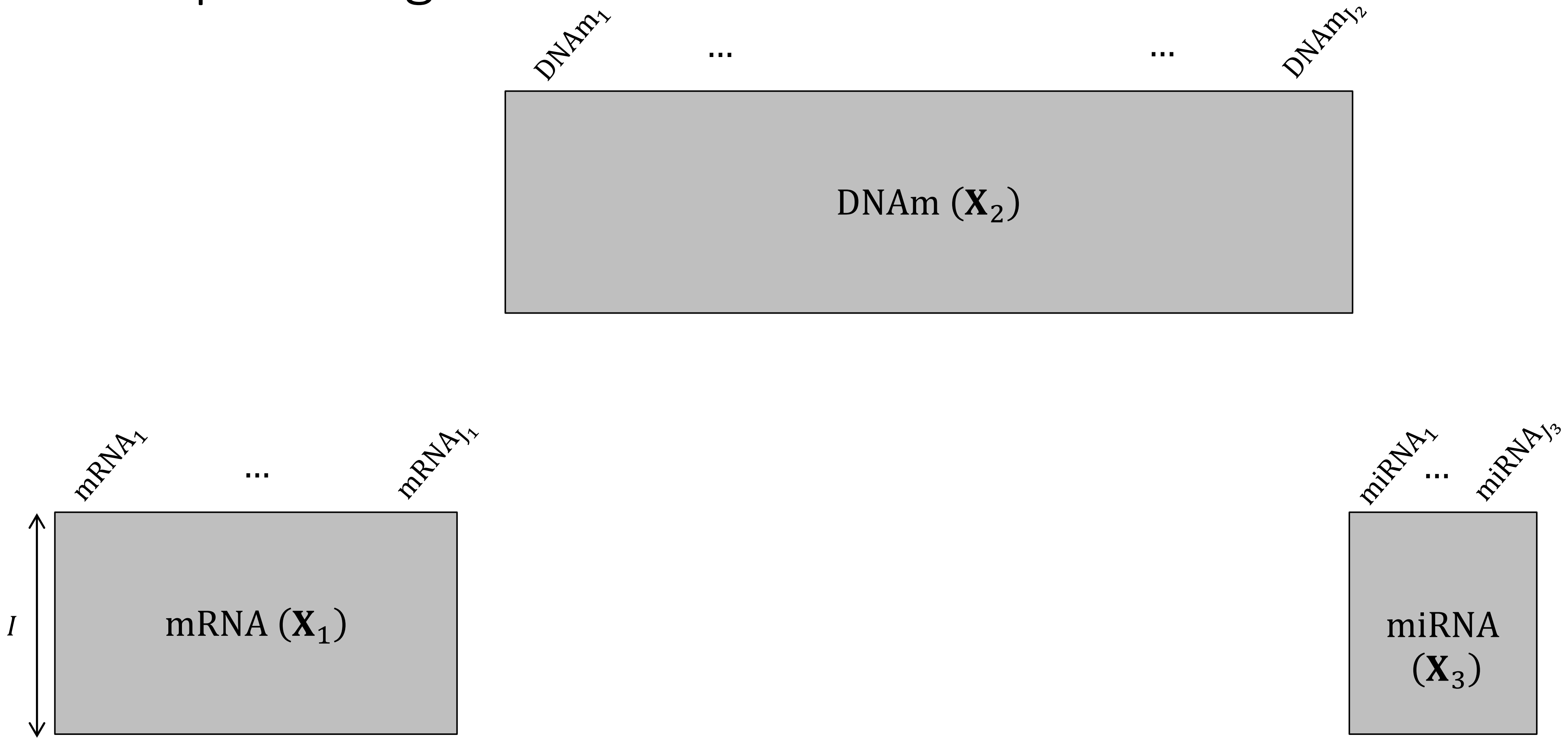
⋮

Out of these distributions, RGCCA non-parametrically estimates confidence intervals $([q_{0.025}, q_{0.975}])$ and p-values $\left(min(Nb_{\geq 0}, Nb_{\leq 0})/max(Nb_{\geq 0}, Nb_{\leq 0})\right)$.

Weight for miRNA_{J_3}

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

Supervising with RGCCA



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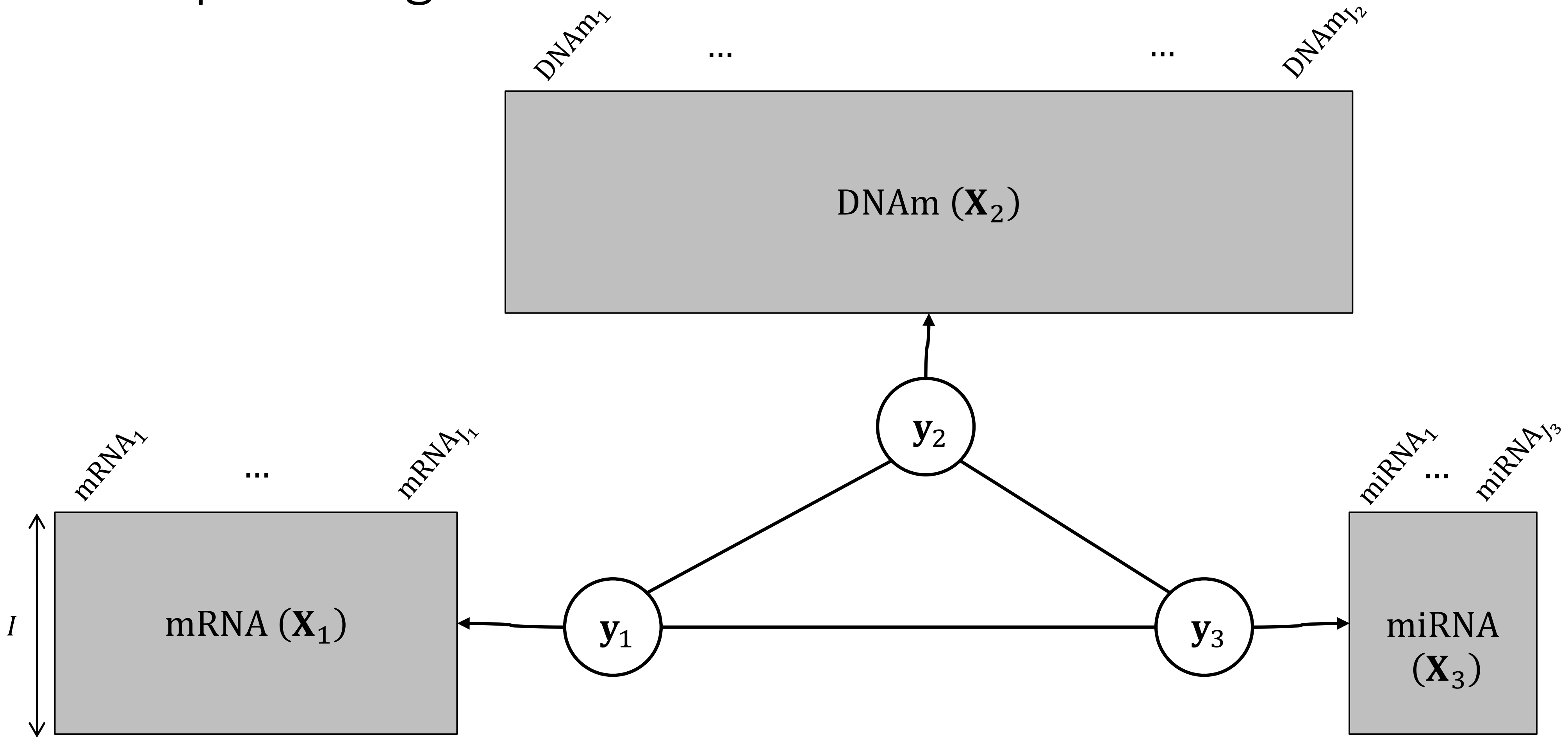

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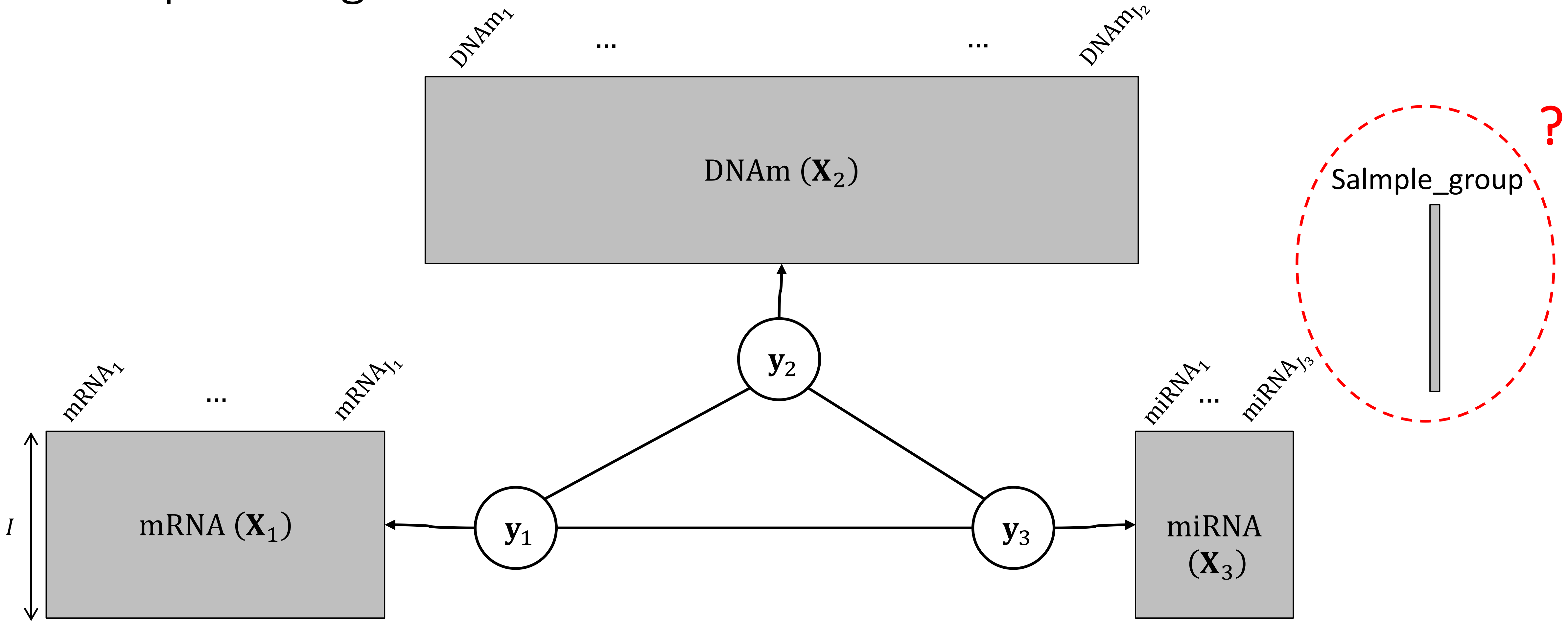

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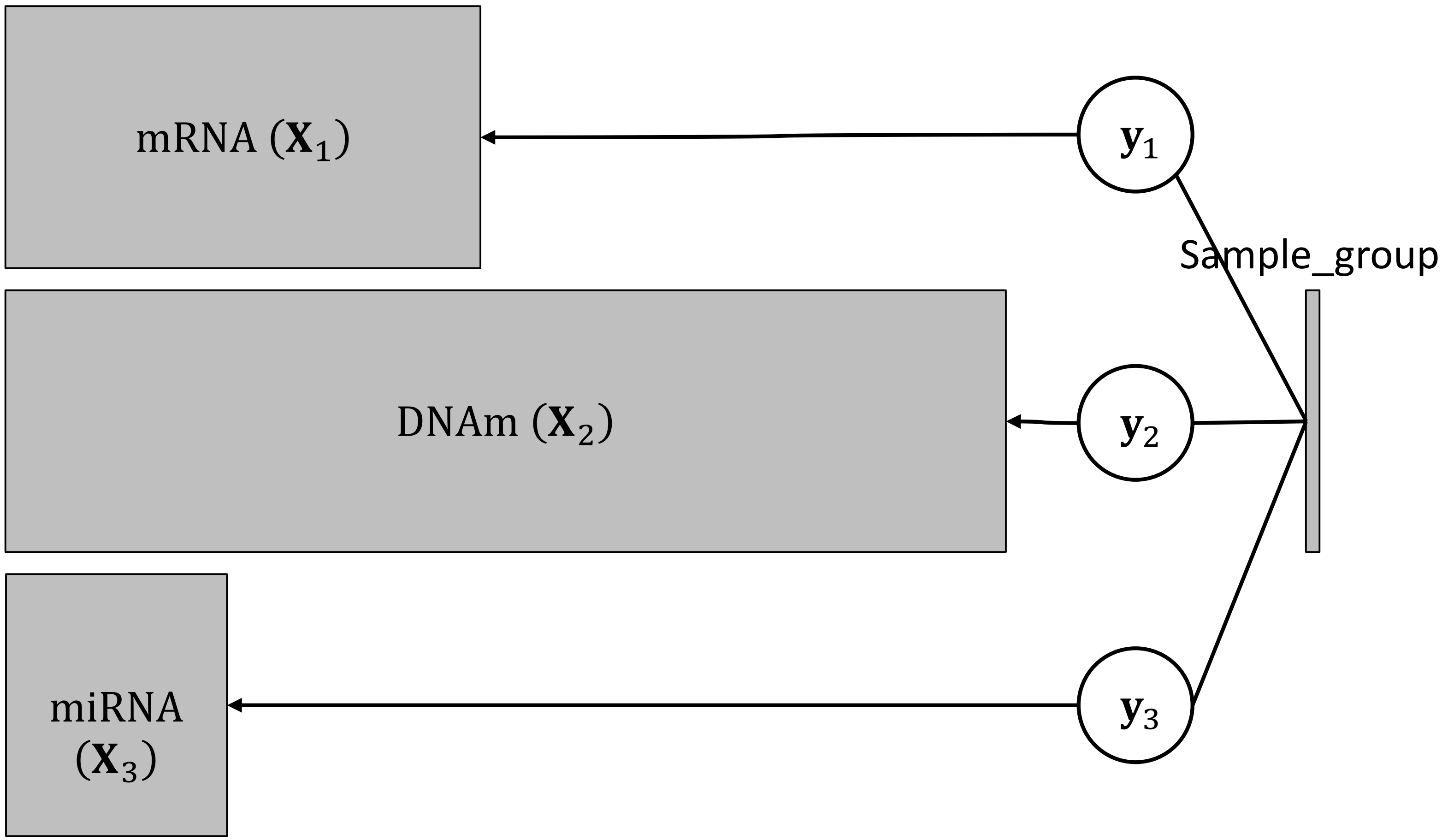

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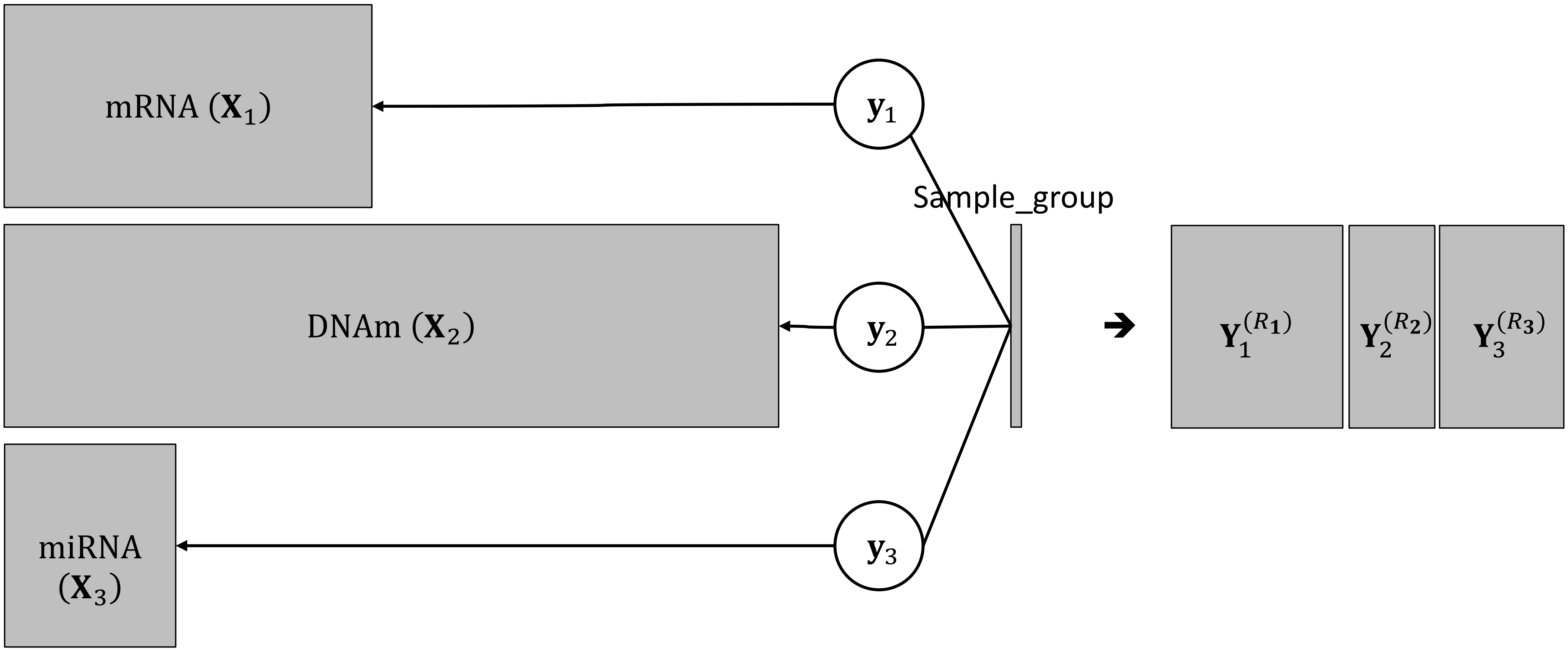

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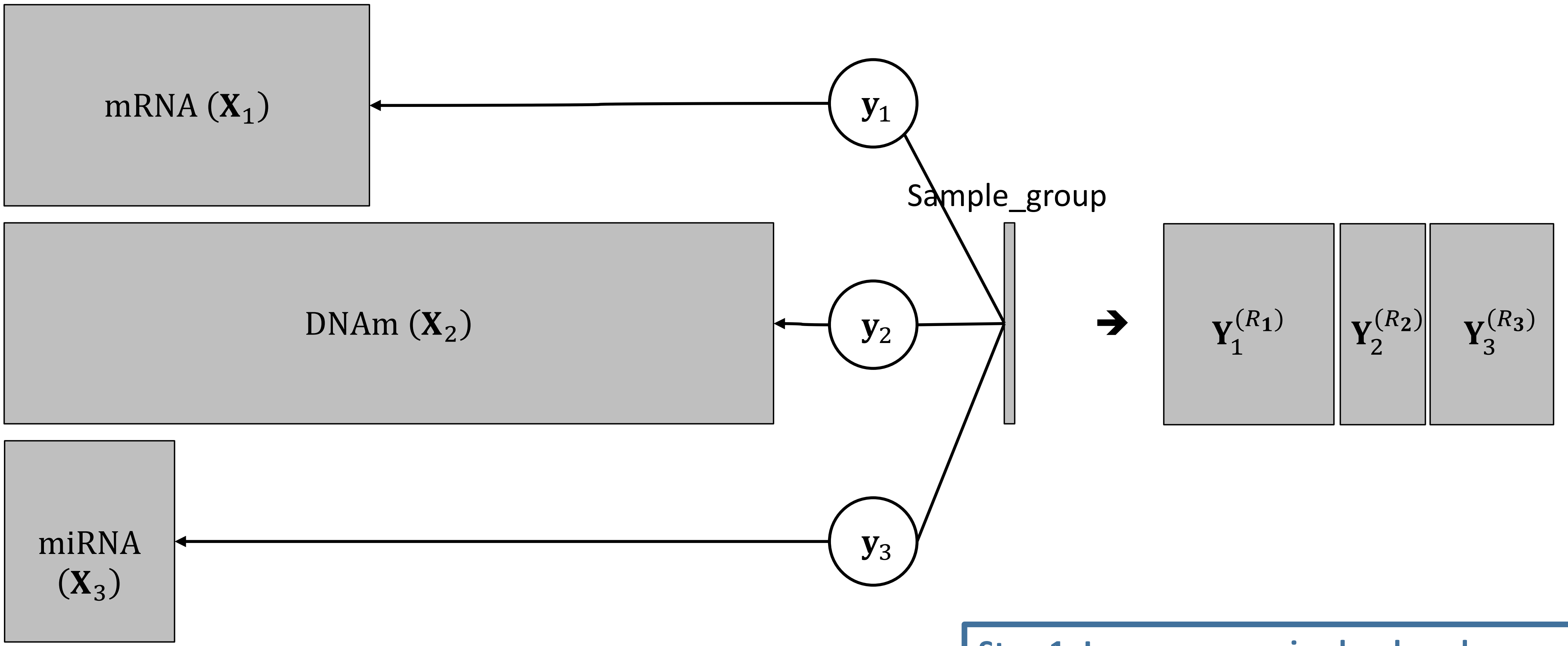
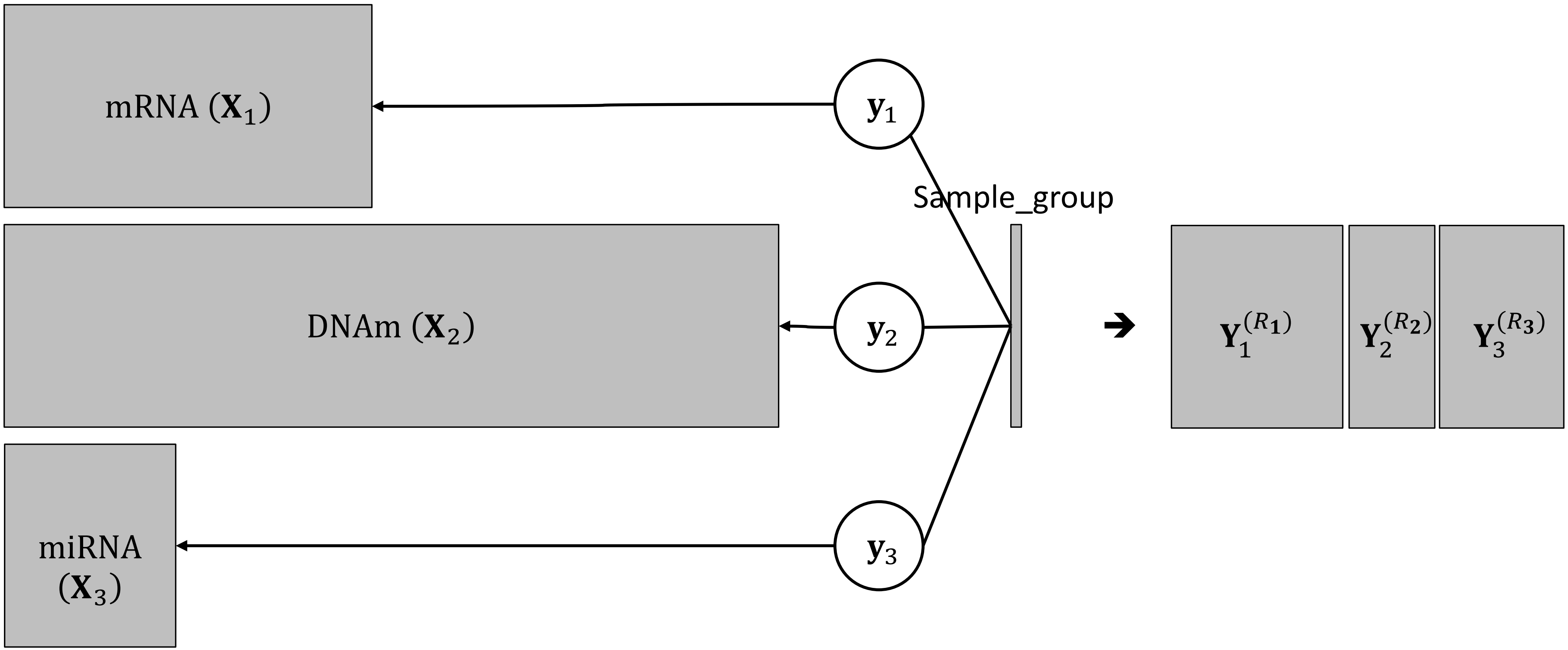


Step 1: Learn a supervised reduced space

Supervising with RGCCA



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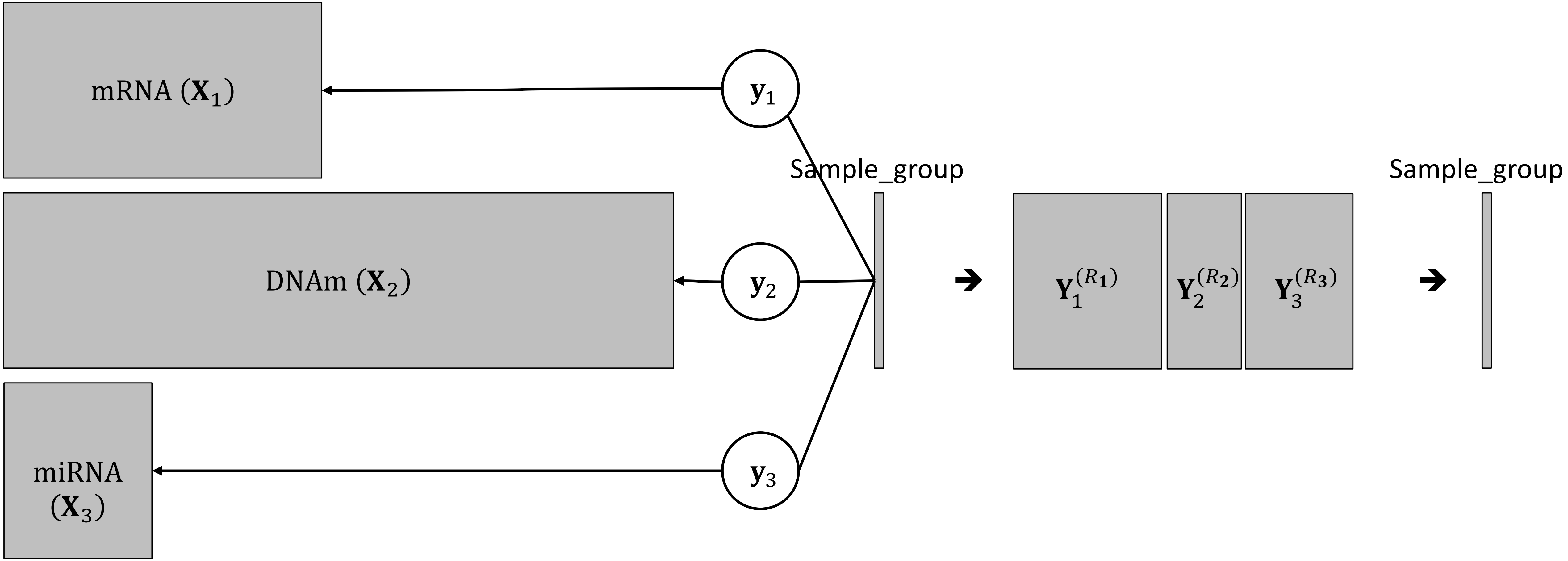

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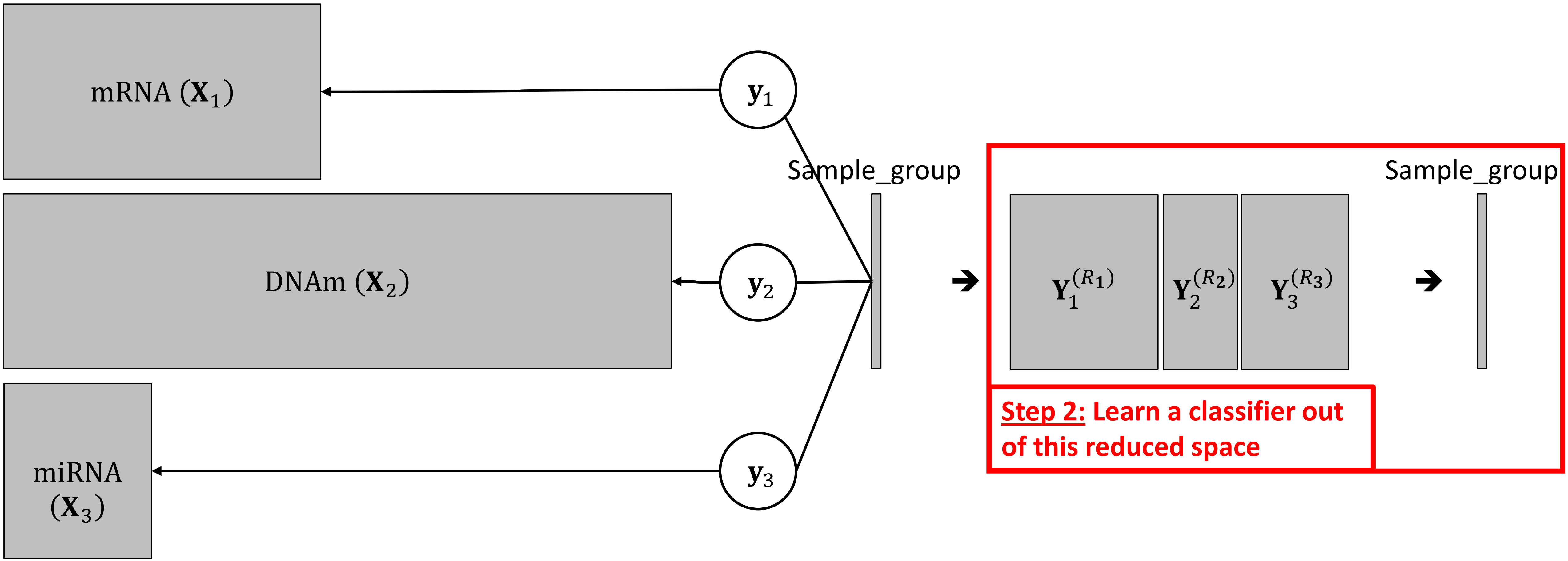
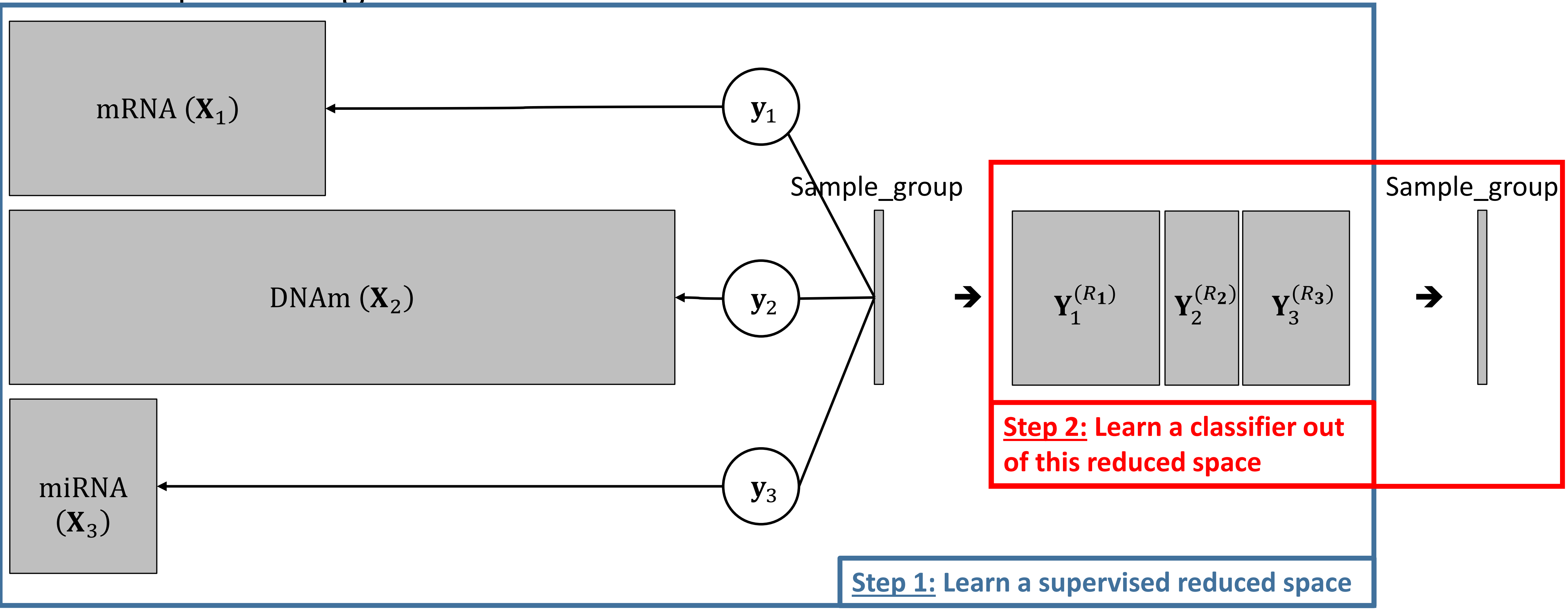
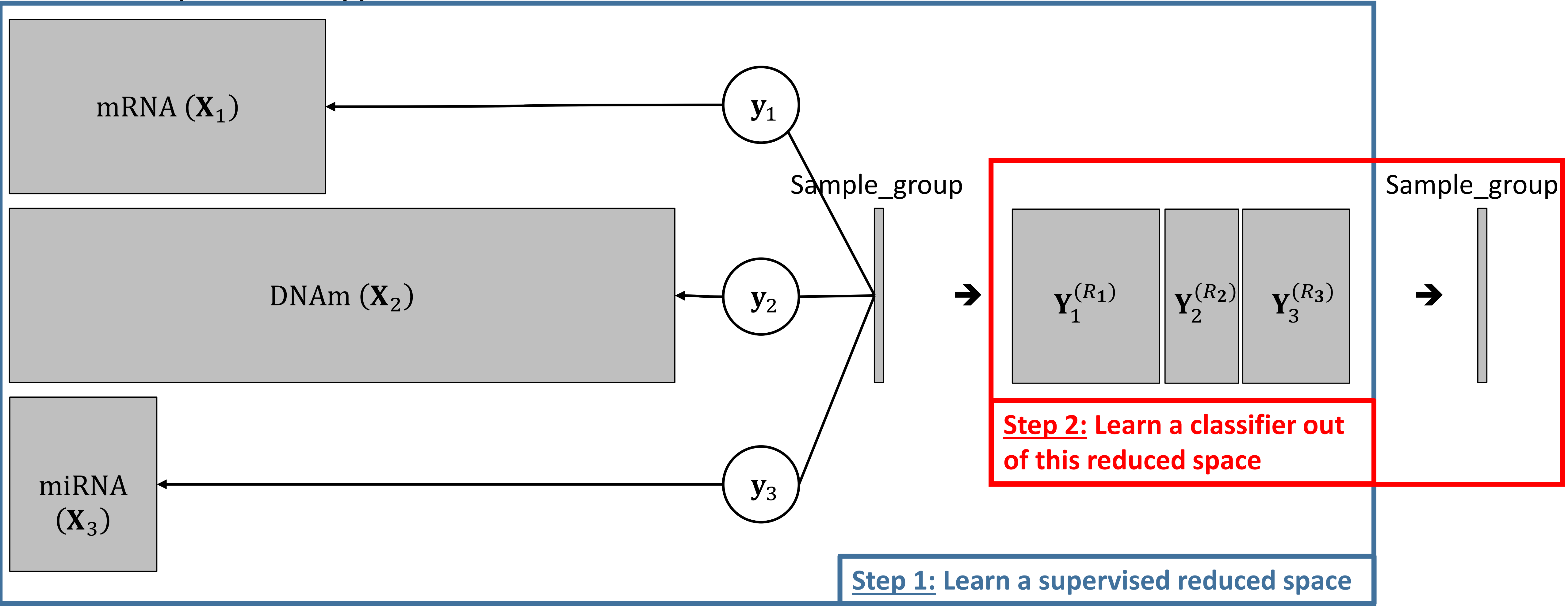


Step 2: Learn a classifier out of this reduced space

Supervising with RGCCA

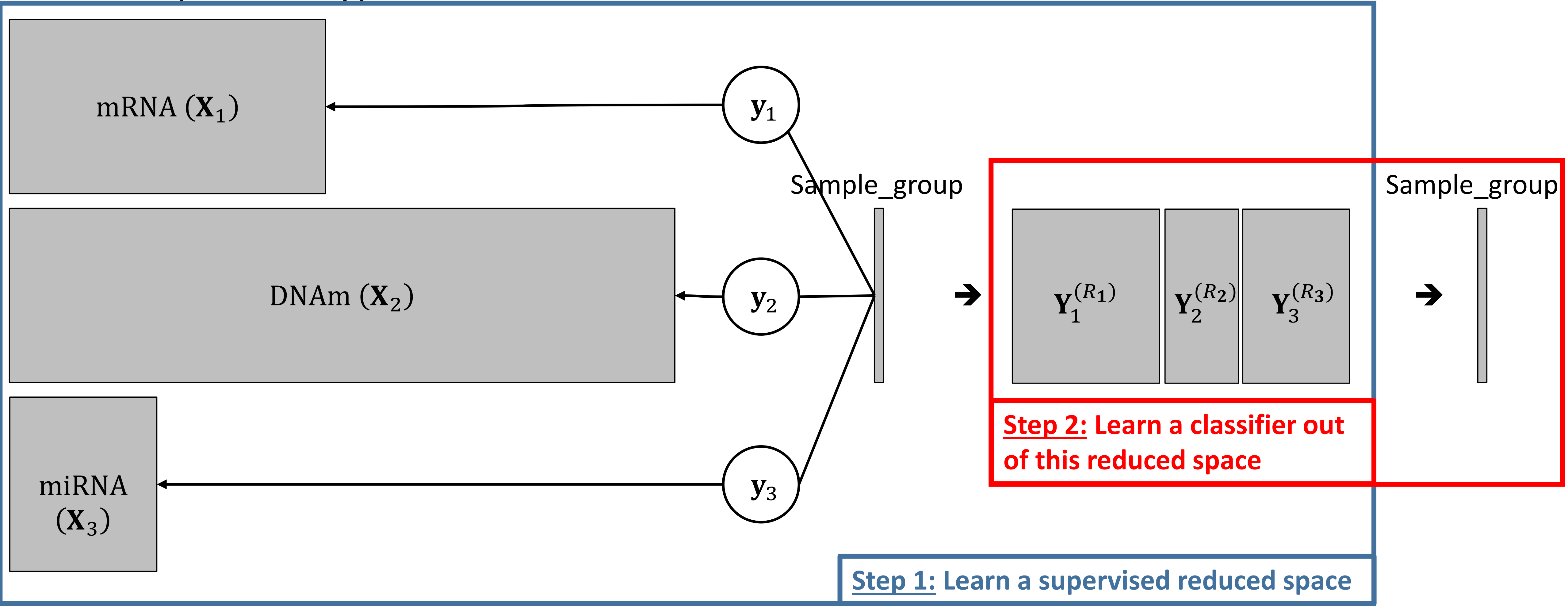


Supervising with RGCCA



The model sequentially learn block-weight vectors to compute components and a classifier.

Supervising with RGCCA



The model sequentially learn block-weight vectors to compute components and a classifier. Standard Cross-Validation can be performed.

F1-score

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Confusion Matrix:

		True labels	
		Positive	Negative
Predicted labels	Positive	True Positive (TP)	False Positive (FP)
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$$precision = \frac{TP}{TP + FP}$$

➔ How many positive predicted labels are true ?

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$$recall = \frac{TP}{TP + FN}$$

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$$F = \frac{2}{\frac{1}{recall} + \frac{1}{precision}} = \frac{2precision.recall}{recall + precision}$$

1. Introduction of the case study

2. Unsupervised analysis with one-block:
Principal Component Analysis (PCA)

3. Unsupervised analysis with two-blocks:
Partial Least Squares (PLS) and Canonical Correlation Analysis (CCA)

4. Unsupervised analysis with L-blocks:
Regularized Generalized Canonical Correlation Analysis (RGCCA)

5. Supervised analysis with RGCCA

6. Variable selection in RGCCA:
Sparse Generalized Canonical Correlation Analysis (SGCCA)

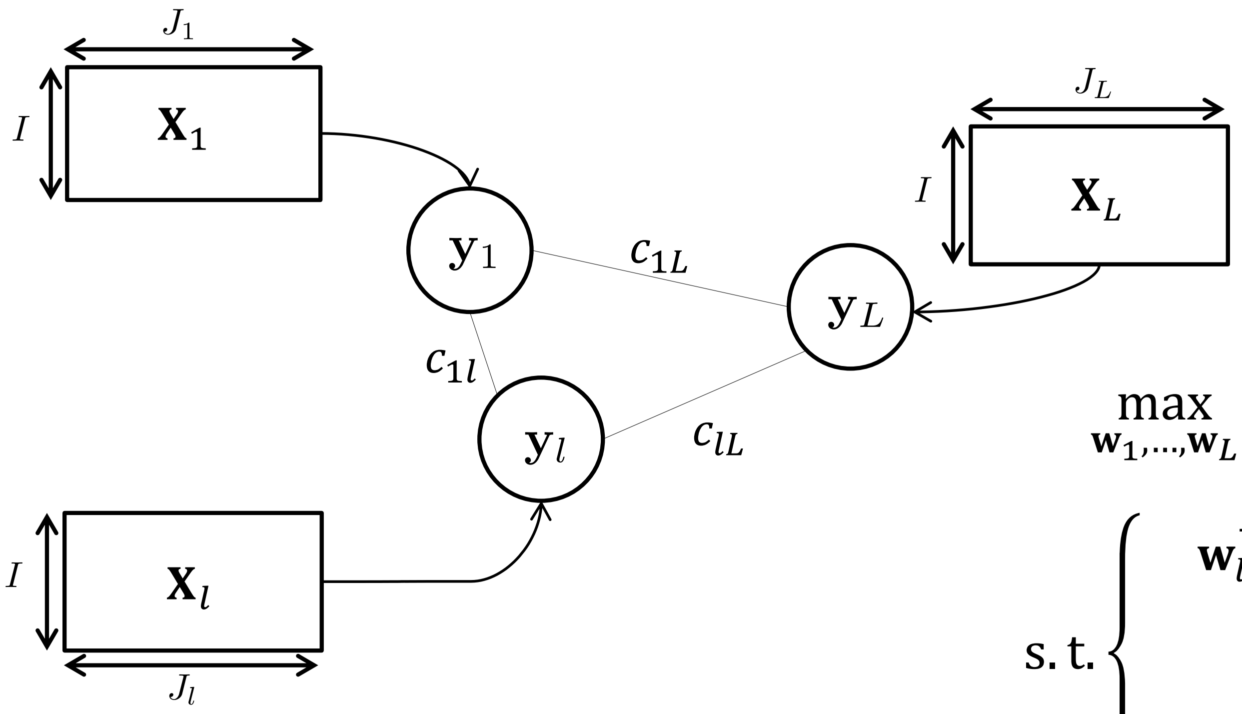
7. The flexible Optimization Framework of RGCCA

→ 7.1 The general principal

→ 7.2 Extension to multi-way analysis

→ 7.3 From Sequential to Global

Sparse Generalized Canonical Correlation Analysis (SGCCA)



$$\max_{\mathbf{w}_1,\dots,\mathbf{w}_L} \sum_{k,l=1}^{L} c_{kl}\, g\big(\mathrm{Cov}(\mathbf{X}_k\mathbf{w}_k, \mathbf{X}_l\mathbf{w}_l)\big)$$

$$\text{s.t.} \begin{cases} \mathbf{w}_l^\top \mathbf{M}_l \mathbf{w}_l = 1 \\ \\ \end{cases}, l = 1, \dots, L.$$

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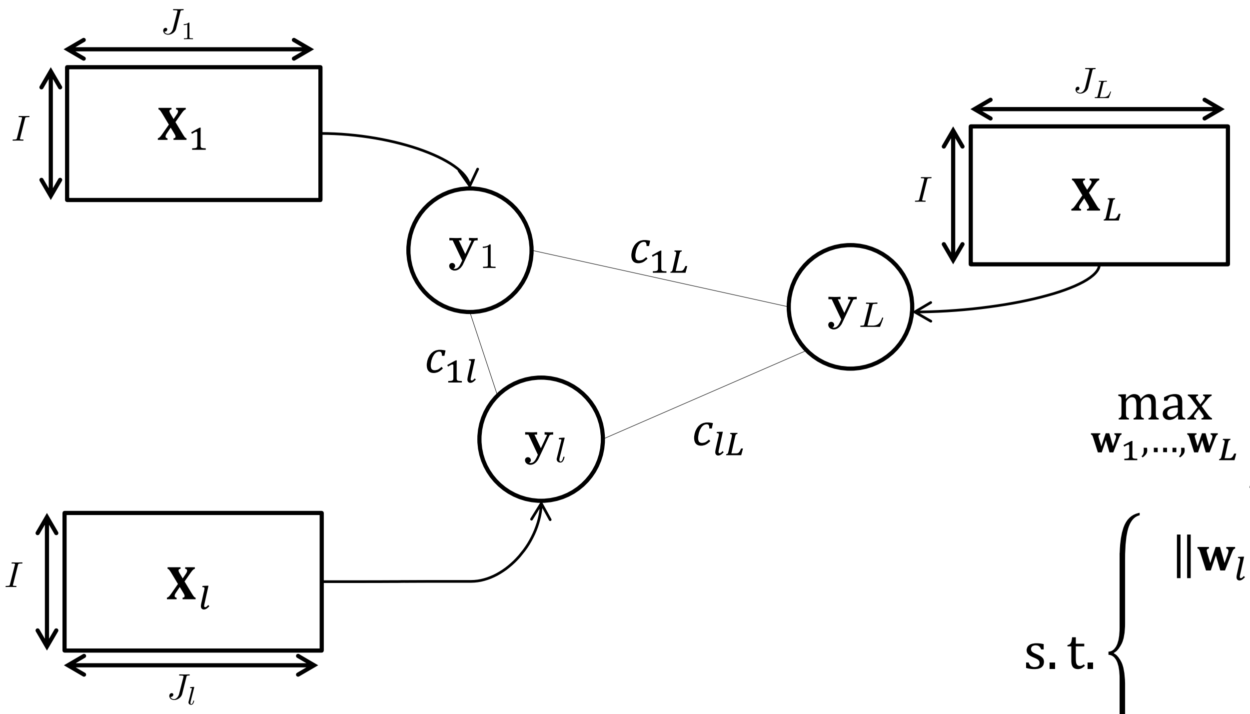

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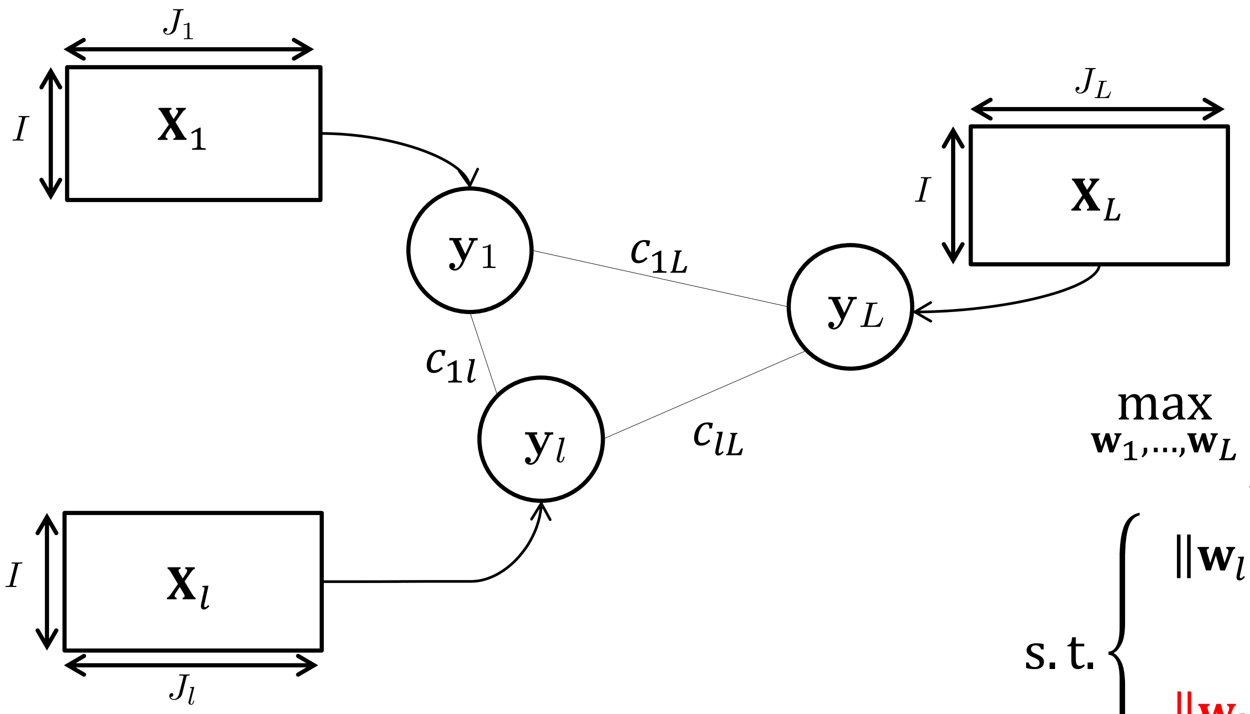

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$$\text{s.t.} \begin{cases} \|\mathbf{w}_l\|_2^2 = 1 \\ \|\mathbf{w}_l\|_1 = \sum_{j=1}^{J_l} |w_{lj}| \le s_l \end{cases}, l = 1, \ldots, L.$$

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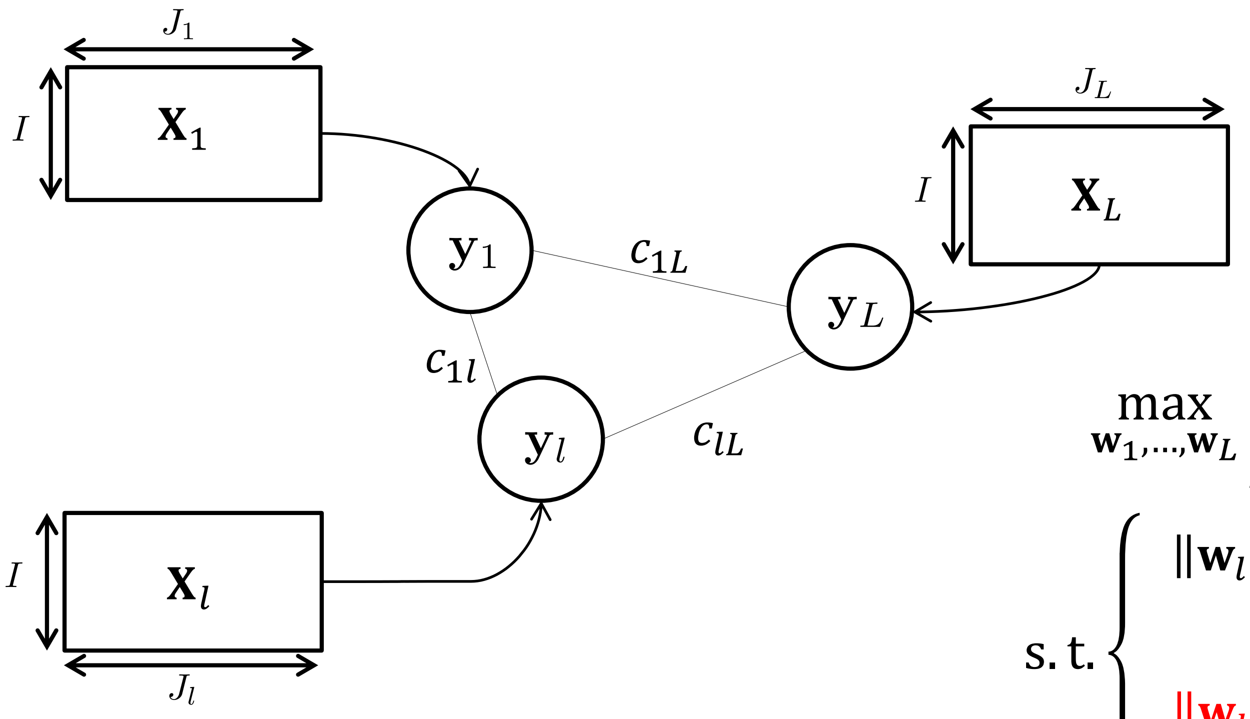

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The ℓ_1-norm regularization allows to perform variable selection.

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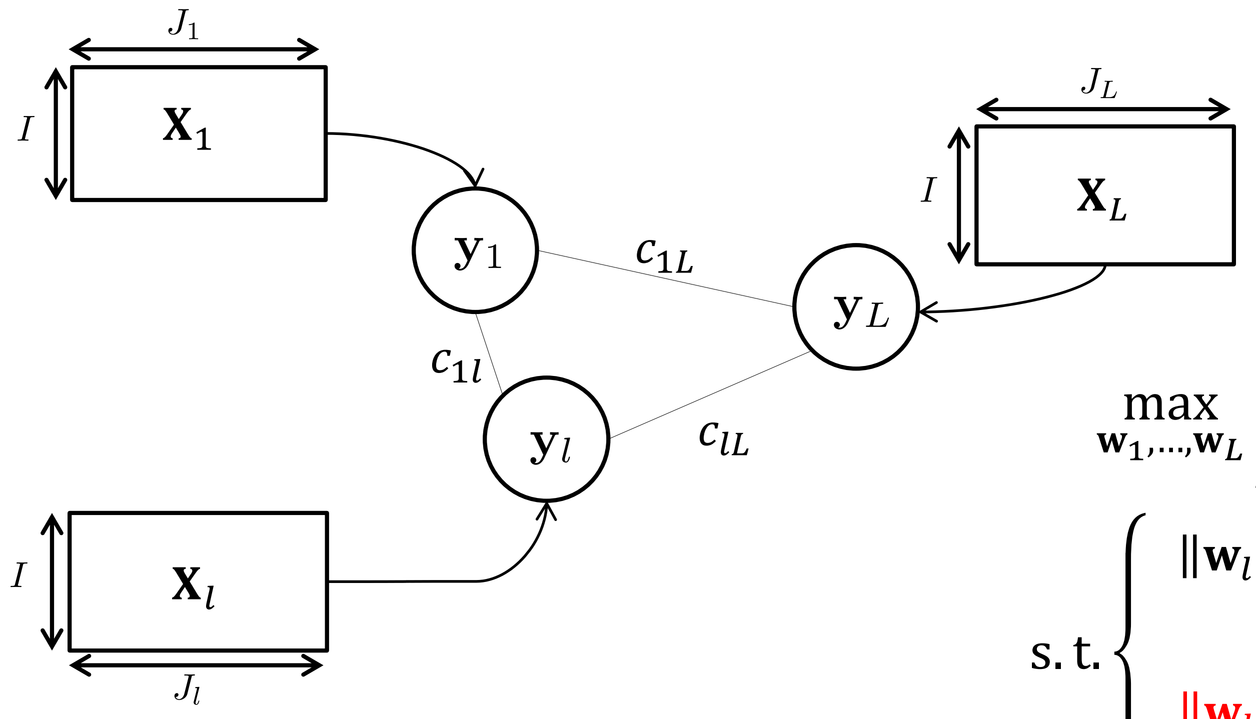

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Controls the level of sparsity (has to be tuned).

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The Variable Importance in Projection (VIP) score

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$$\mathrm{VIP}\left(\mathbf{x}_{lj}\right) = \frac{1}{R}\sum_{r=1}^{R}\left({w_{lj}^{(r)}}^2 \mathrm{AVE}\left(\mathbf{X}_l^{(r)}\right)\right)$$

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  Thus, $\mathbf{X}_l^{(r)}$ correspond to the projection of $\mathbf{X}_l^{(r-1)}$ onto the space orthogonal to $\boldsymbol{y}_l^{(r)}$:

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- ❖ Furthermore $\mathbf{X}_l^{(0)} = \mathbf{X}_l$
- ❖ The Average Variance Explained (AVE) associated with $\boldsymbol{y}_l^{(r)}$ is:

The Variable Importance in Projection (VIP) score

$$\mathrm{VIP}\left(\mathbf{x}_{lj}\right) = \frac{1}{R}\sum_{r=1}^{R}\left({w_{lj}^{(r)}}^2 \mathrm{AVE}\left(\mathbf{X}_l^{(r)}\right)\right)$$

Where:

- R is the number of extracted components.
- $\mathbf{X}_l = \left[\mathbf{x}_{l1}, \dots, \mathbf{x}_{lJ_l}\right]$ and $\mathbf{w}_l = \left[w_{l1}, \dots, w_{lJ_l}\right]^\top$.
- RGCCA uses a deflation procedure to extract the following components.
  Thus, $\mathbf{X}_l^{(r)}$ correspond to the projection of $\mathbf{X}_l^{(r-1)}$ onto the space orthogonal to $\boldsymbol{y}_l^{(r)}$:

$$\mathbf{X}_l^{(r)} = \left(\mathbf{I}_{J_l} - \frac{\boldsymbol{y}_l^{(r)}{\boldsymbol{y}_l^{(r)}}^\top}{\left\|\boldsymbol{y}_l^{(r)}\right\|_2^2}\right)\mathbf{X}_l^{(r-1)}$$

- Furthermore $\mathbf{X}_l^{(0)} = \mathbf{X}_l$
- The Average Variance Explained (AVE) associated with $\boldsymbol{y}_l^{(r)}$ is:

$$\mathrm{AVE}\left(\mathbf{X}_l^{(r)}\right) = \frac{1}{\left\|\mathbf{X}_l^{(r)}\right\|_F^2}\sum_{j=1}^{J_l}\left(\mathrm{var}\left(\mathbf{x}_{lj}^{(r)}\right) \times \mathrm{cor}^2\left(\mathbf{x}_{lj}^{(r)}, \boldsymbol{y}_l^{(r+1)}\right)\right)$$

1. Introduction of the case study

2. Unsupervised analysis with one-block:
Principal Component Analysis (PCA)

3. Unsupervised analysis with two-blocks:
Partial Least Squares (PLS) and Canonical Correlation Analysis (CCA)

4. Unsupervised analysis with L-blocks:
Regularized Generalized Canonical Correlation Analysis (RGCCA)

5. Supervised analysis with RGCCA

6. Variable selection in RGCCA:
Sparse Generalized Canonical Correlation Analysis (SGCCA)

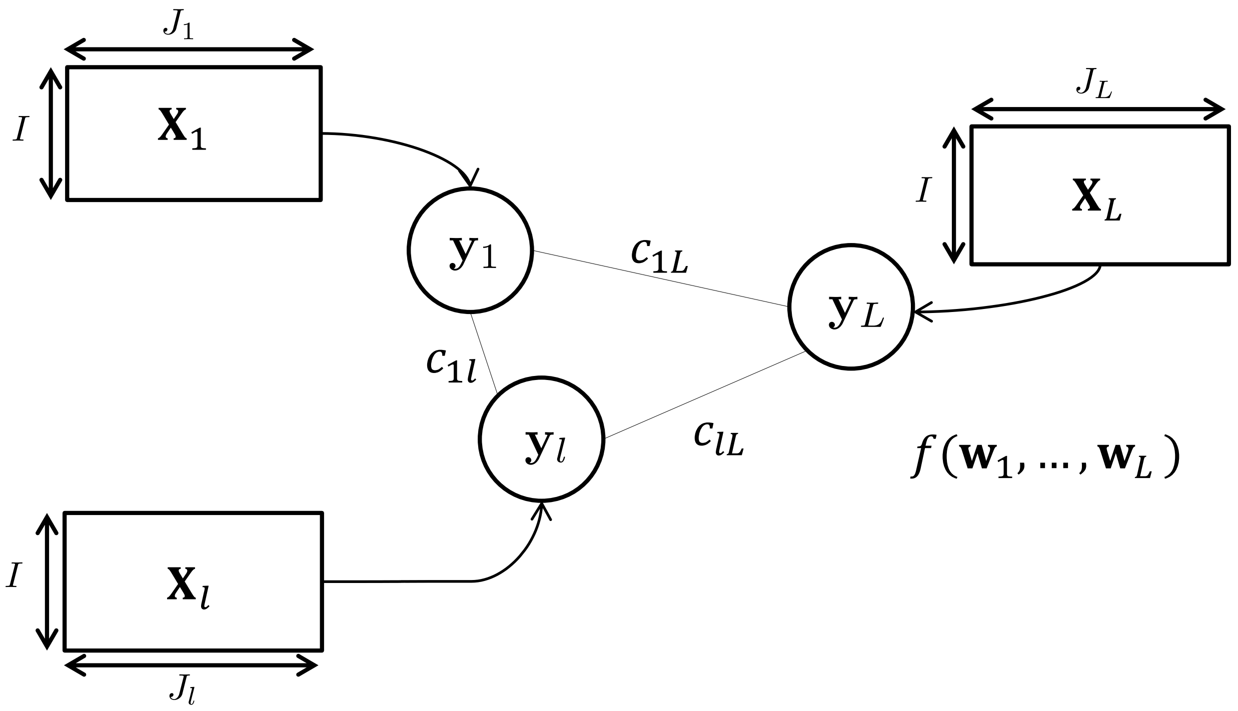
7. The flexible Optimization Framework of RGCCA

→ 7.1 The general principal

→ 7.2 Extension to multi-way analysis

→ 7.3 From Sequential to Global

Principle of the RGCCA Optimization Algorithm



$f(\mathbf{w}_1, \dots, \mathbf{w}_L)$

$$\max_{\mathbf{w}_1,\dots,\mathbf{w}_L} \sum_{k,l=1}^{L} c_{kl}\, g\big(\mathrm{Cov}(\mathbf{X}_k\mathbf{w}_k, \mathbf{X}_l\mathbf{w}_l)\big)$$

$$\text{s.t.} \begin{cases} \mathbf{w}_l^\top \mathbf{M}_l \mathbf{w}_l = 1 \end{cases}, l = 1, \dots, L.$$

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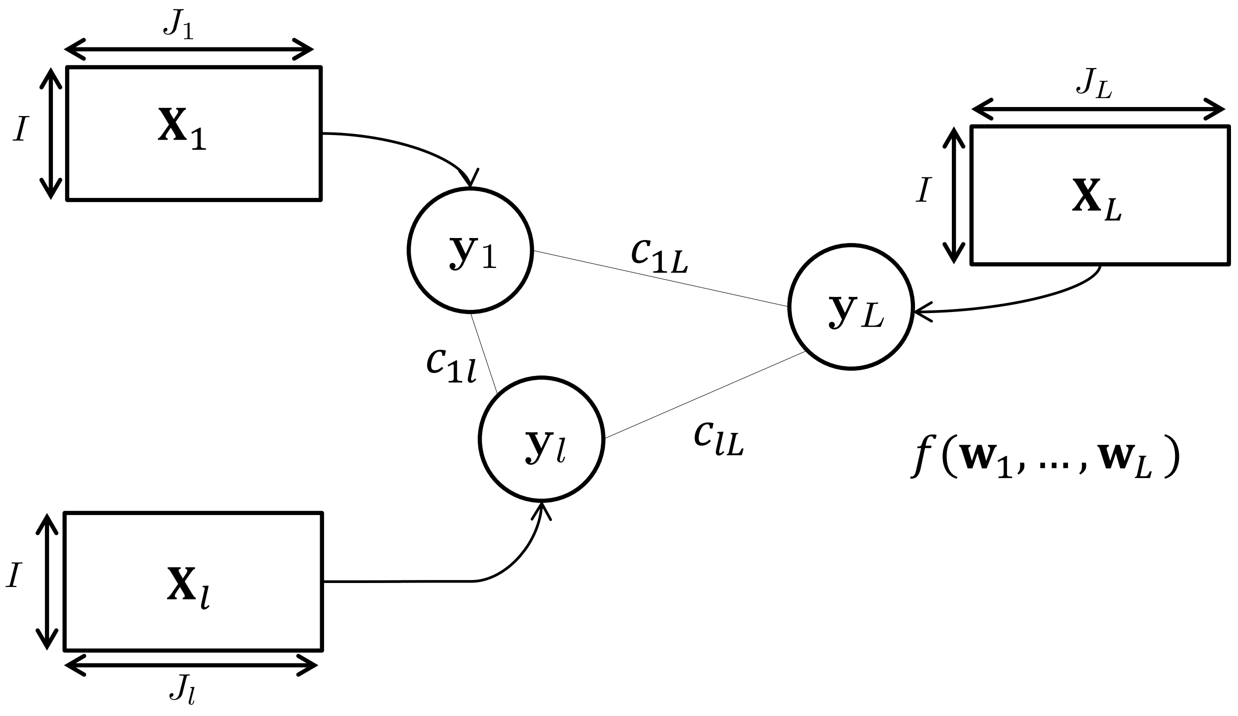

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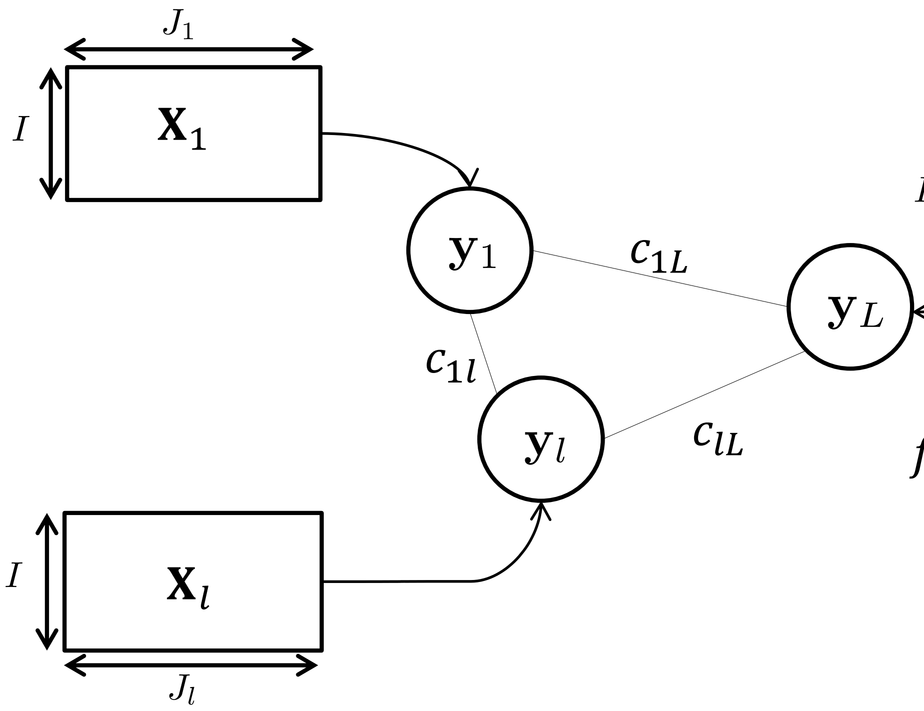

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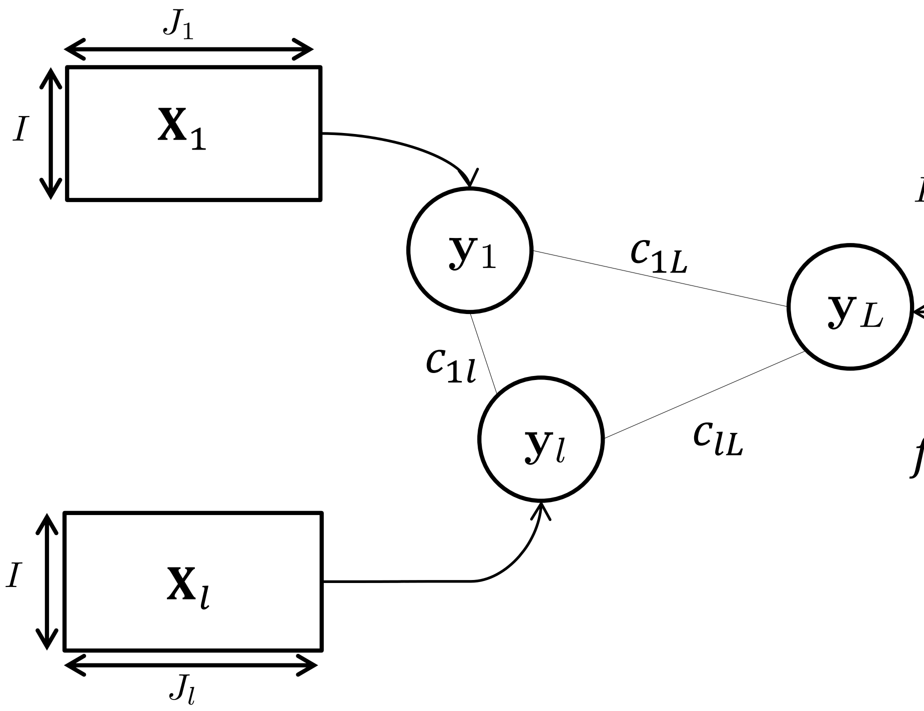

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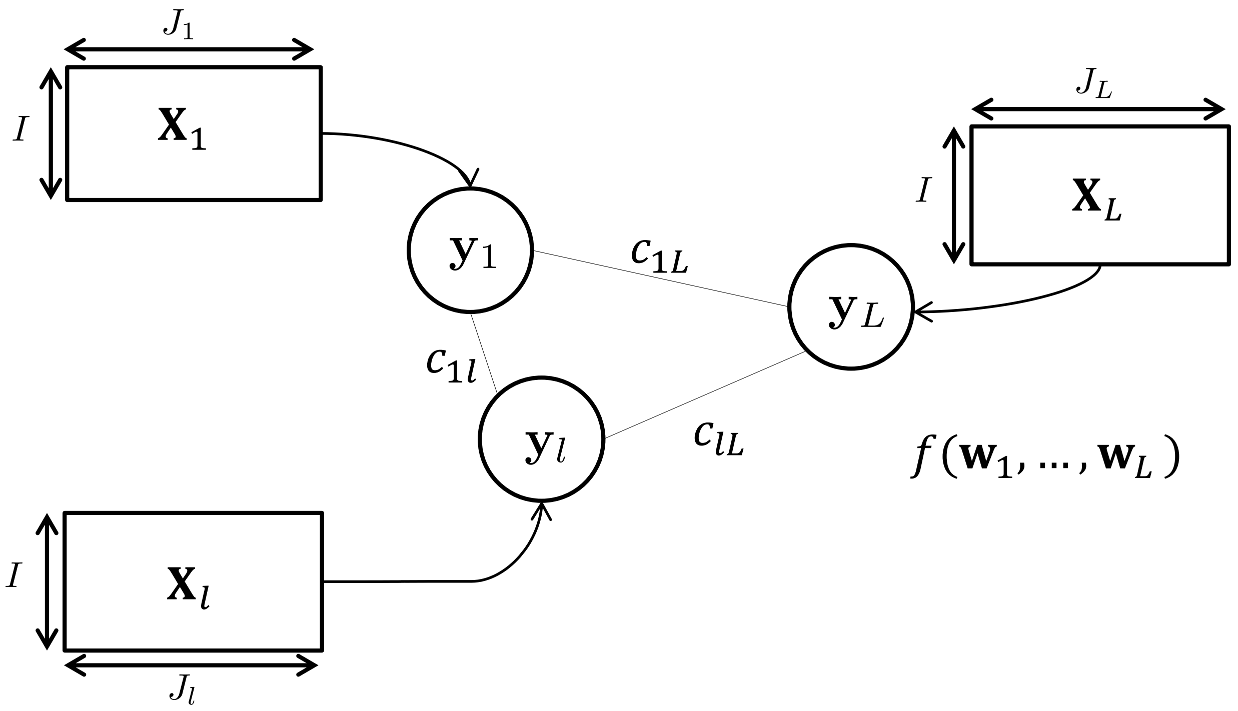
In order to maximize the multi-convex function $f(\mathbf{w}_1, \dots, \mathbf{w}_L)$, two key ingredients are used:

Principle of the RGCCA Optimization Algorithm



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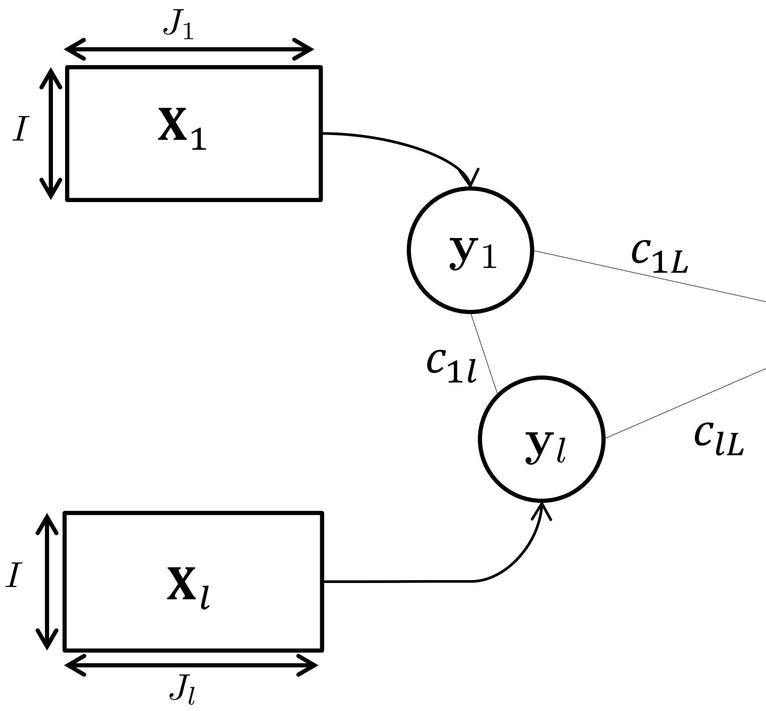
Block Coordinate Ascent (BCA).

Principle of the RGCCA Optimization Algorithm



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In order to maximize the multi-convex function $f(\mathbf{w}_1, \ldots, \mathbf{w}_L)$, two key ingredients are used:

- Block Coordinate Ascent (BCA).
- Minorize-Maximize (MM) principle.

Block Coordinate Ascent

$$\boxed{\mathbf{w}^s = (\mathbf{w}_1^s, \mathbf{w}_2^s, \dots, \mathbf{w}_L^s)}$$

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$\mathbf{w}_1^{s+1}$

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$$\mathbf{w}_1^{s+1}$$

$$\underset{\mathbf{w}_2, \mathbf{w}_2^\top \mathbf{M}_2 \mathbf{w}_2 = 1}{\operatorname{argmax}} \; f(\color{red}{\mathbf{w}_1^{s+1}}, \mathbf{w}_2, \dots, \mathbf{w}_L^s)$$

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$$\Rightarrow \mathbf{w}_1^{s+1}$$

$$\underset{\mathbf{w}_2, \mathbf{w}_2^\top \mathbf{M}_2 \mathbf{w}_2 = 1}{\operatorname{argmax}} \; f({\color{red}\mathbf{w}_1^{s+1}}, \mathbf{w}_2, \dots, \mathbf{w}_L^s)$$

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

Block Coordinate Ascent

$$\boxed{\mathbf{w}^s = (\mathbf{w}_1^s, \mathbf{w}_2^s, \dots, \mathbf{w}_L^s)}$$

$$\underset{\mathbf{w}_1, \mathbf{w}_1^\top \mathbf{M}_1 \mathbf{w}_1 = 1}{\operatorname{argmax}} \; f(\mathbf{w}_1, \mathbf{w}_2^s, \dots, \mathbf{w}_L^s) \longrightarrow \mathbf{w}_1^{s+1}$$

$$\underset{\mathbf{w}_2, \mathbf{w}_2^\top \mathbf{M}_2 \mathbf{w}_2 = 1}{\operatorname{argmax}} \; f({\color{red}\mathbf{w}_1^{s+1}}, \mathbf{w}_2, \dots, \mathbf{w}_L^s) \longrightarrow \mathbf{w}_2^{s+1}$$

$$\vdots$$

$$\underset{\mathbf{w}_l, \mathbf{w}_l^\top \mathbf{M}_l \mathbf{w}_l = 1}{\operatorname{argmax}} \; f({\color{red}\mathbf{w}_1^{s+1}, \dots, \mathbf{w}_{l-1}^{s+1}}, \mathbf{w}_l, \mathbf{w}_{l+1}^s, \dots, \mathbf{w}_L^s) \longrightarrow \mathbf{w}_l^{s+1}$$

Block Coordinate Ascent

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$$\underset{\mathbf{w}_1, \mathbf{w}_1^\top \mathbf{M}_1 \mathbf{w}_1 = 1}{\operatorname{argmax}} \; f(\mathbf{w}_1, \mathbf{w}_2^s, \ldots, \mathbf{w}_L^s) \longrightarrow \mathbf{w}_1^{s+1}$$

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Minorize-Maximize (MM) principle

$$\underset{\mathbf{w}_l, \mathbf{w}_l^\top \mathbf{M}_l \mathbf{w}_l = 1}{\operatorname{argmax}} \; f(\mathbf{w}_1^{s+1}, \dots, \mathbf{w}_{l-1}^{s+1}, \mathbf{w}_l, \mathbf{w}_{l+1}^{s}, \dots, \mathbf{w}_L^{s})$$

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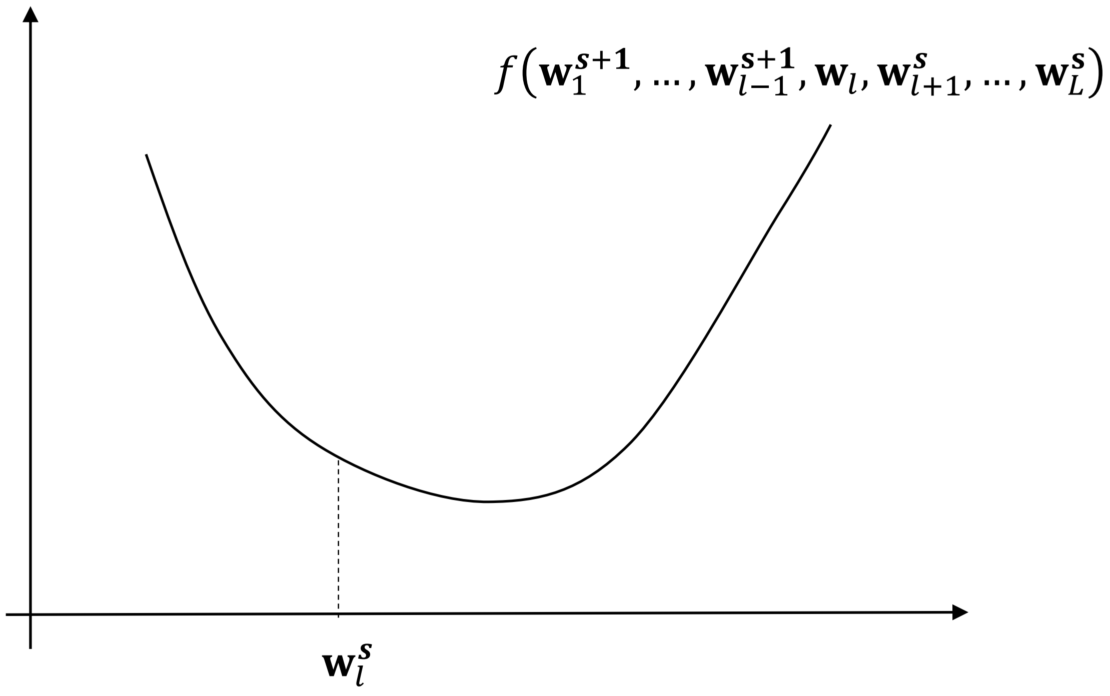

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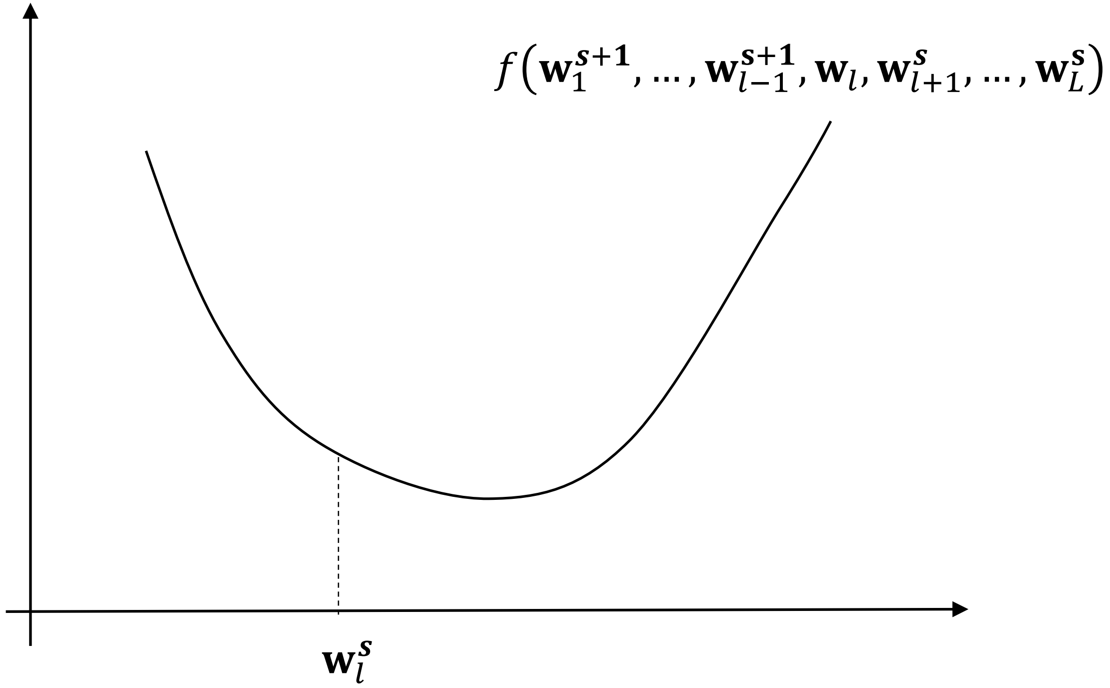

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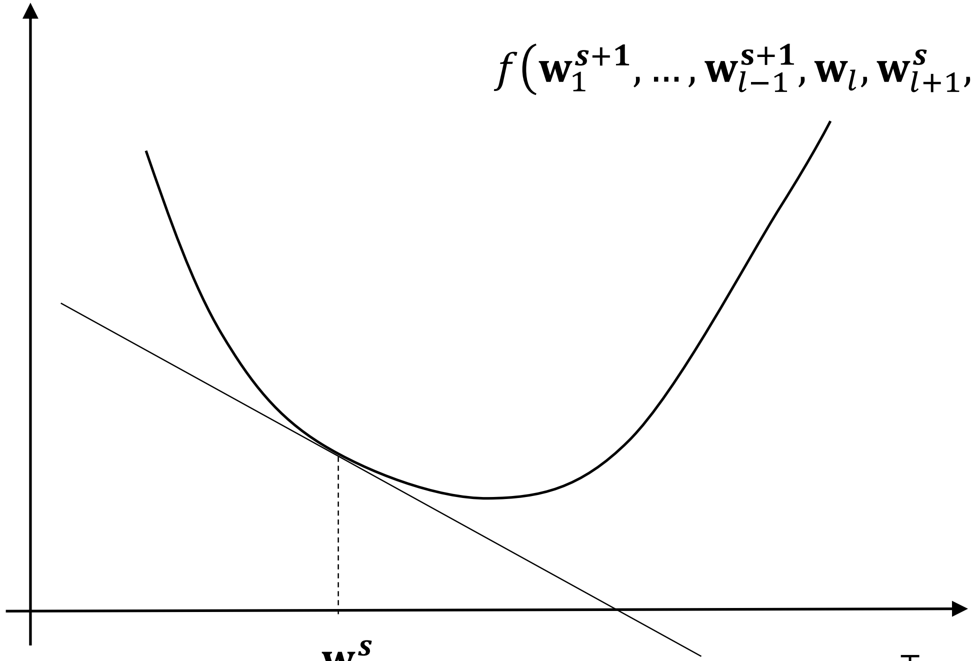

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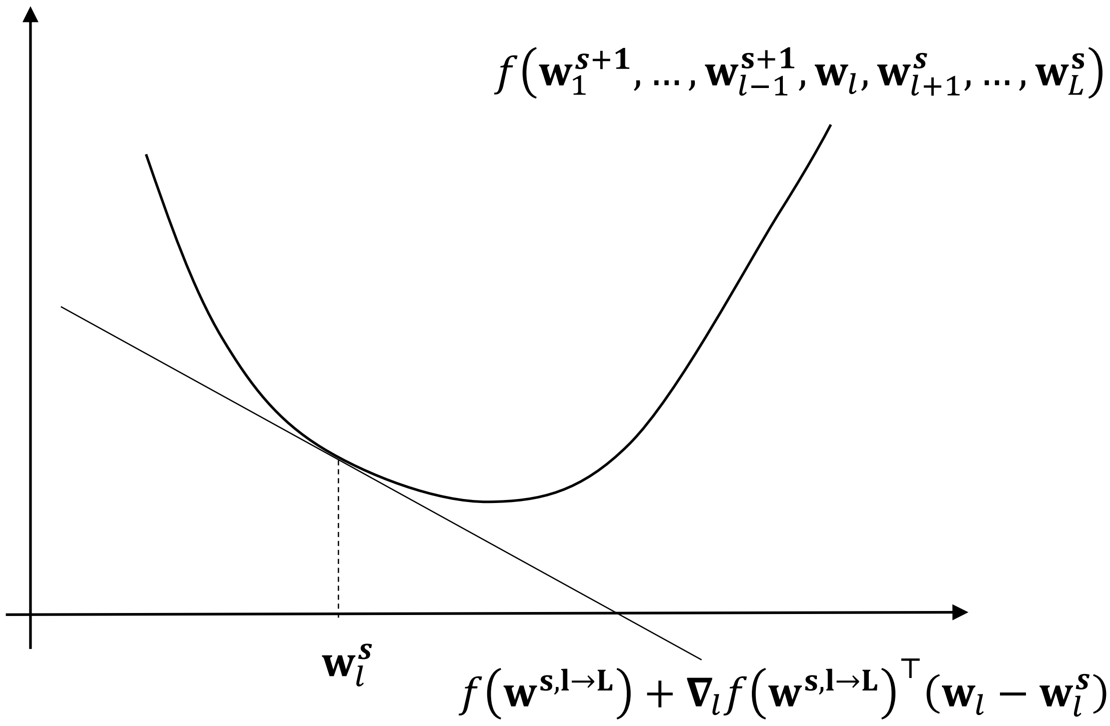

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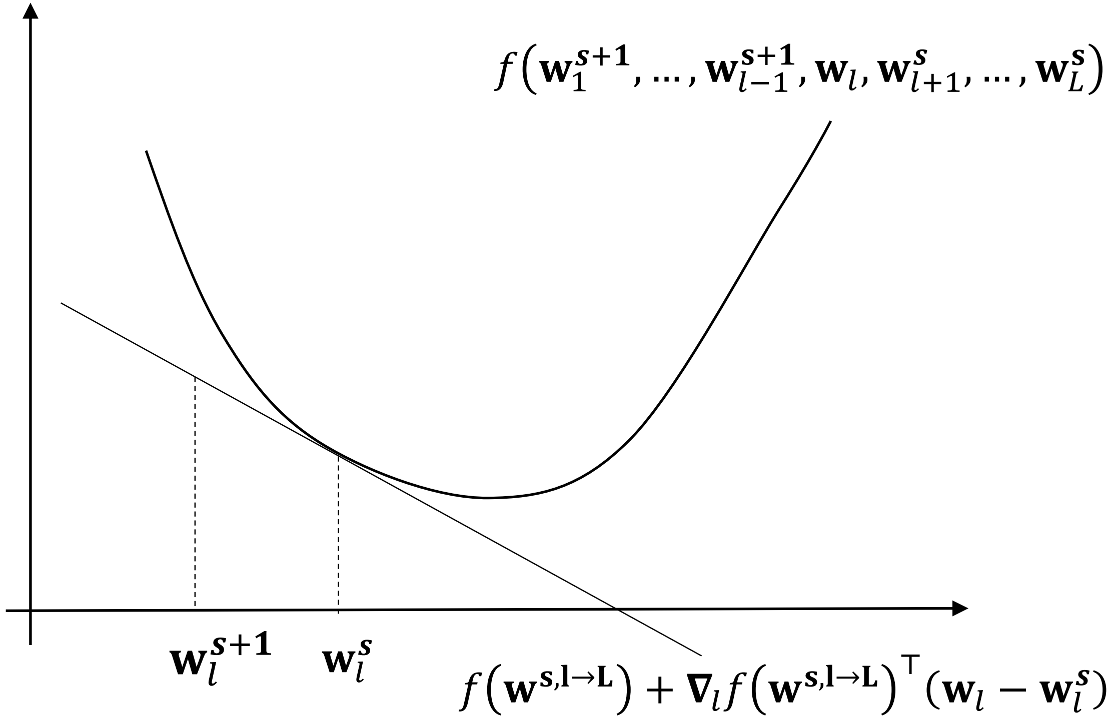

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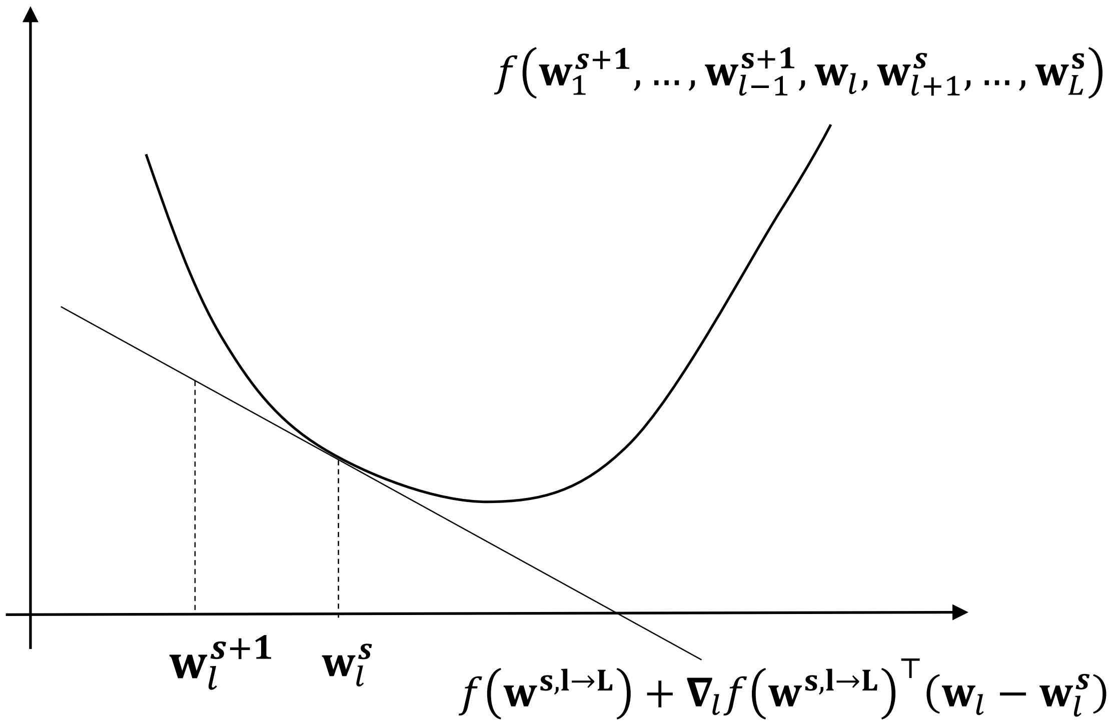

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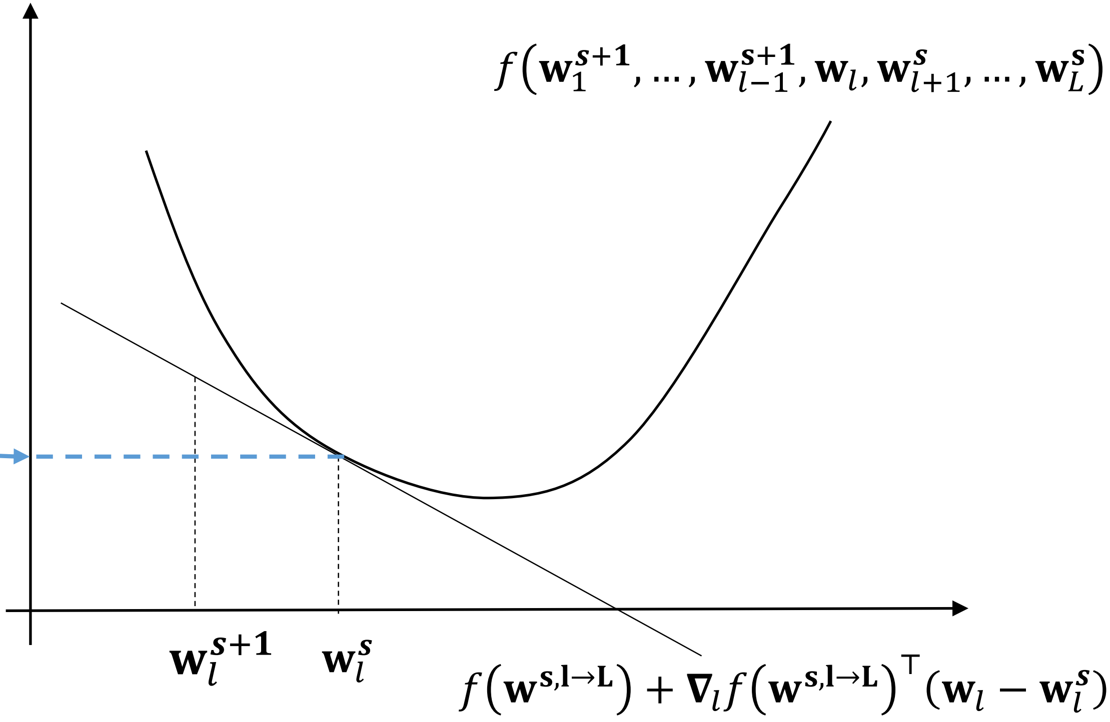

Minorize-Maximize (MM) principle

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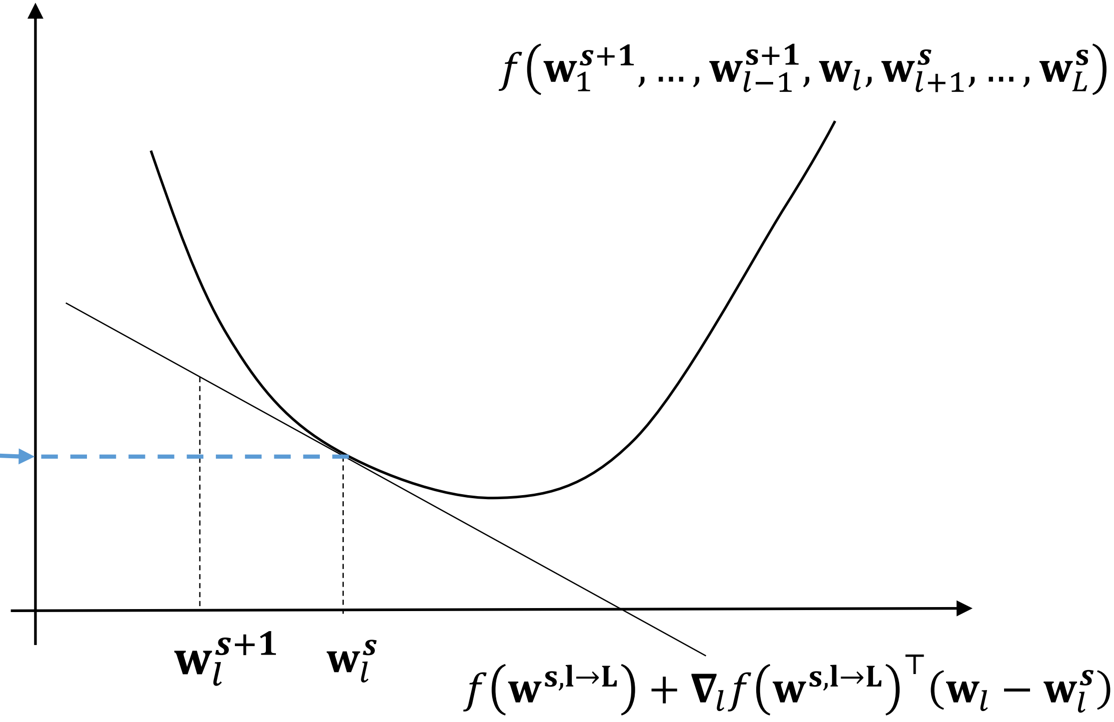
$$\begin{aligned} f\left(\mathbf{w}^{\mathbf{s},\mathbf{l}\to\mathbf{L}}\right) &= f\left(\mathbf{w}^{\mathbf{s},\mathbf{l}\to\mathbf{L}}\right) + \nabla_l f\left(\mathbf{w}^{\mathbf{s},\mathbf{l}\to\mathbf{L}}\right)^\top \left(\mathbf{w}_l^{s} - \mathbf{w}_l^{s}\right) \\ &\leq f\left(\mathbf{w}^{\mathbf{s},\mathbf{l}\to\mathbf{L}}\right) + \nabla_l f\left(\mathbf{w}^{\mathbf{s},\mathbf{l}\to\mathbf{L}}\right)^\top \left(\mathbf{w}_l^{s+1} - \mathbf{w}_l^{s}\right) \end{aligned}$$



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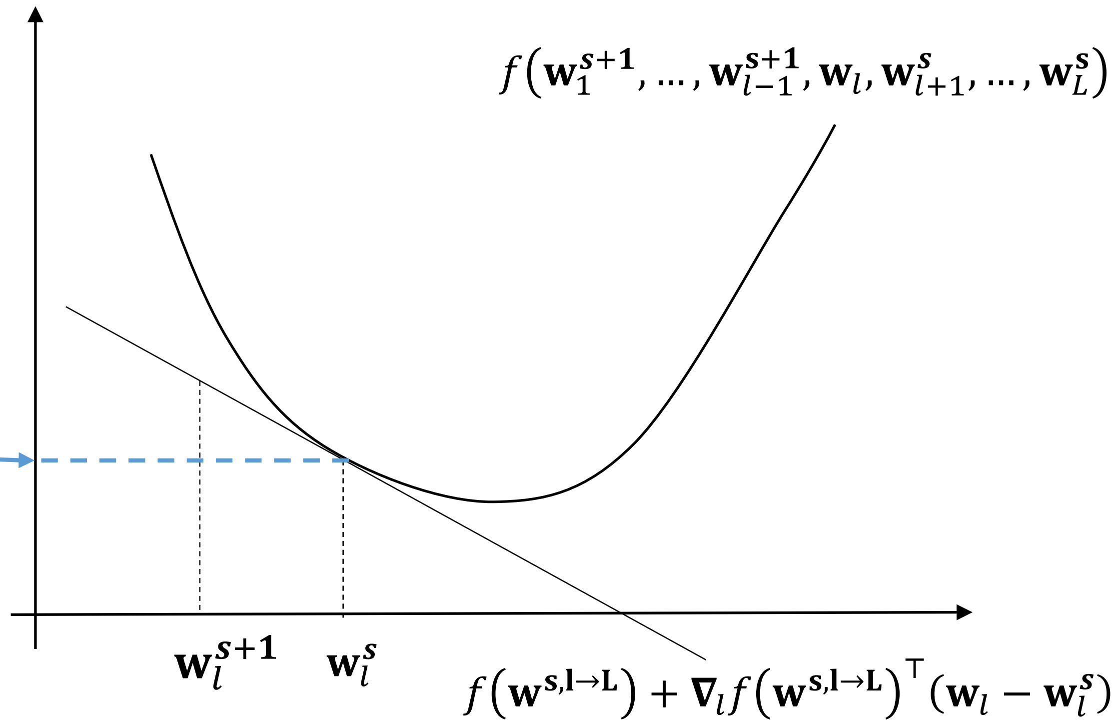

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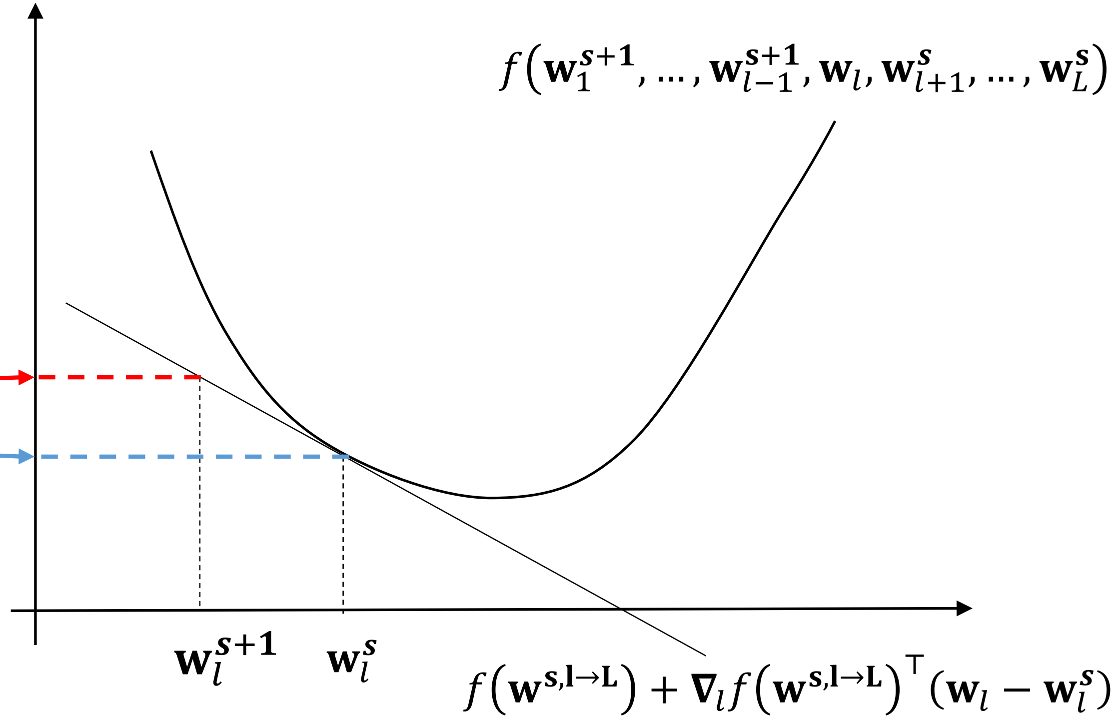

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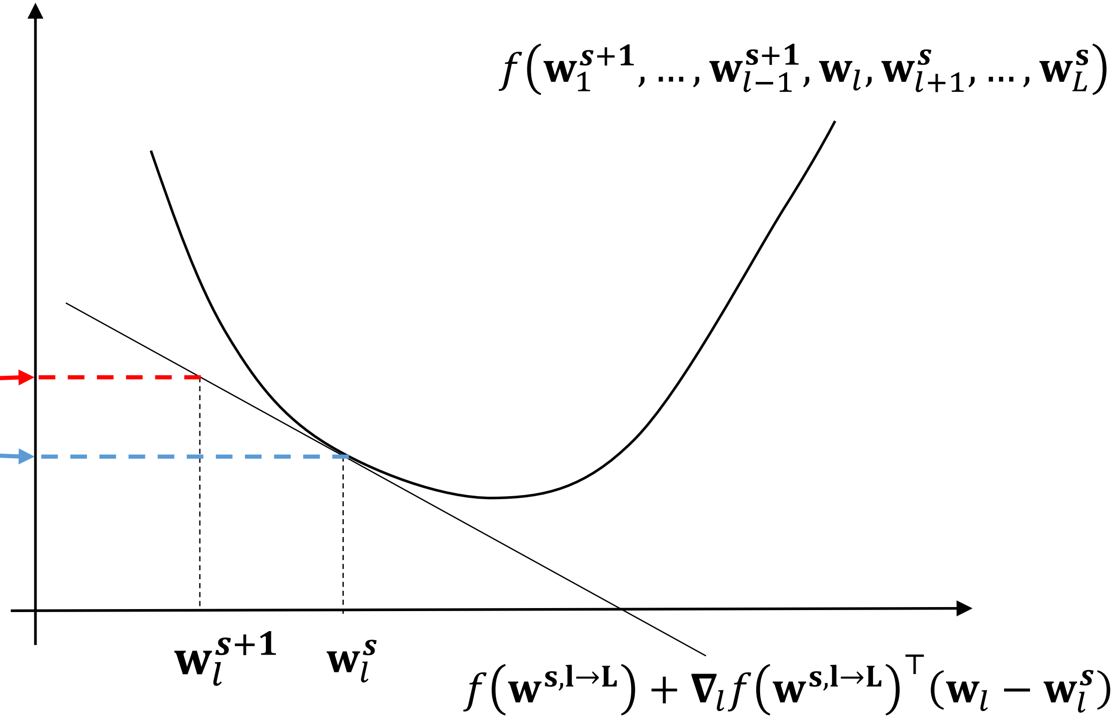

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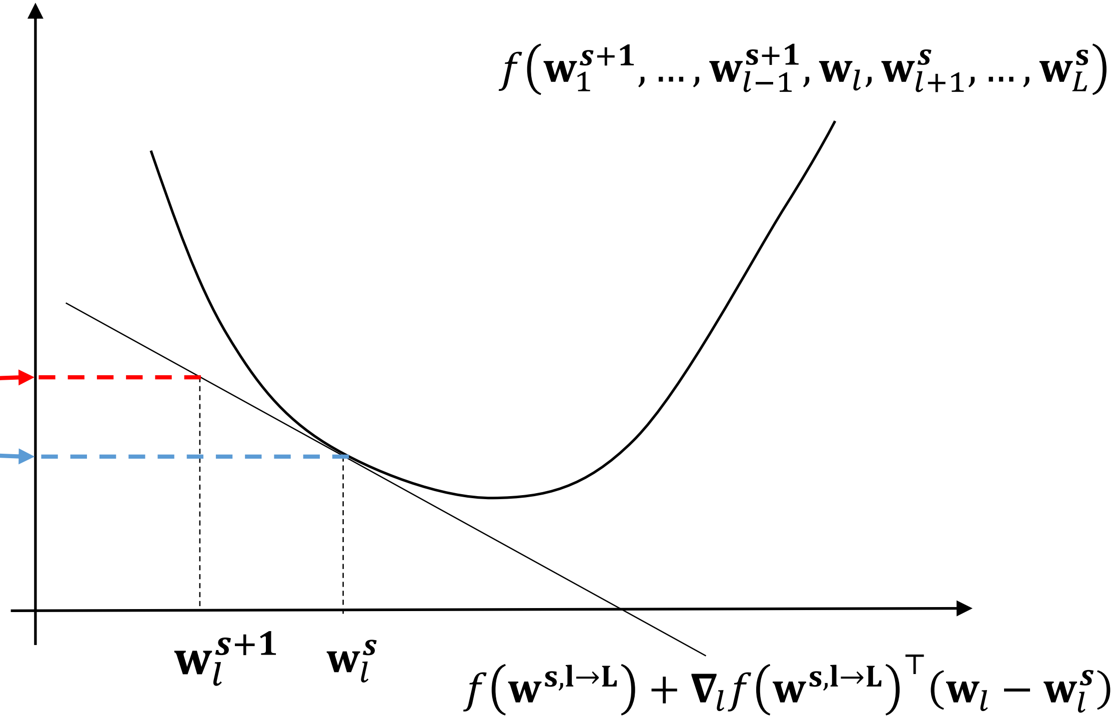

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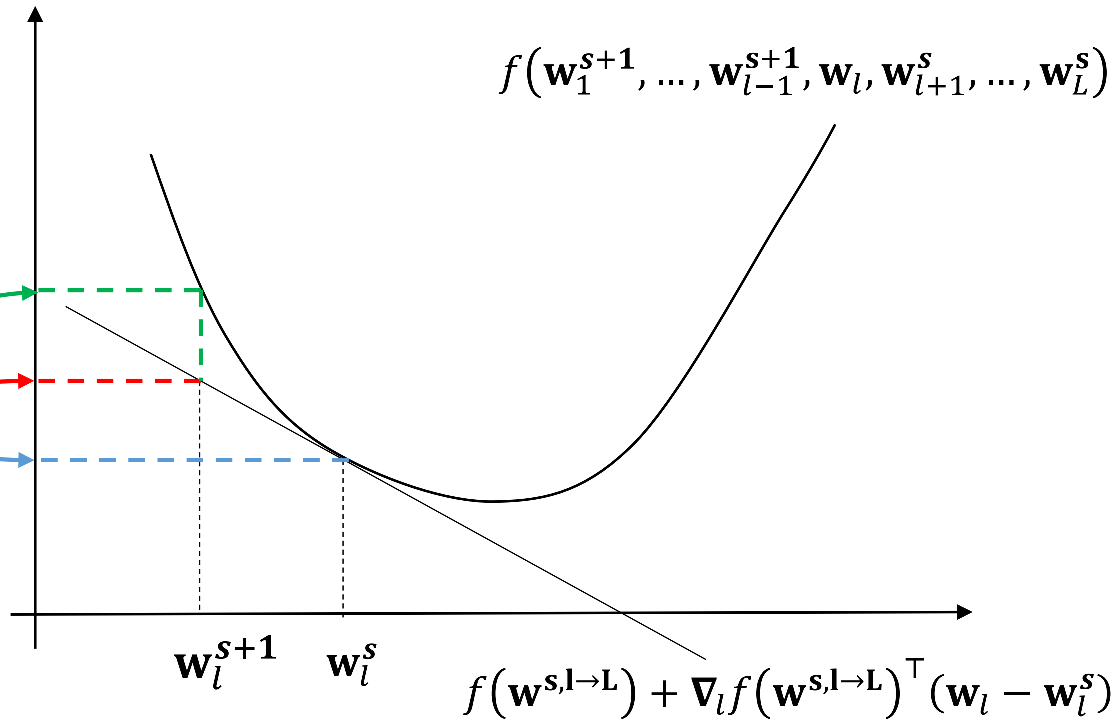

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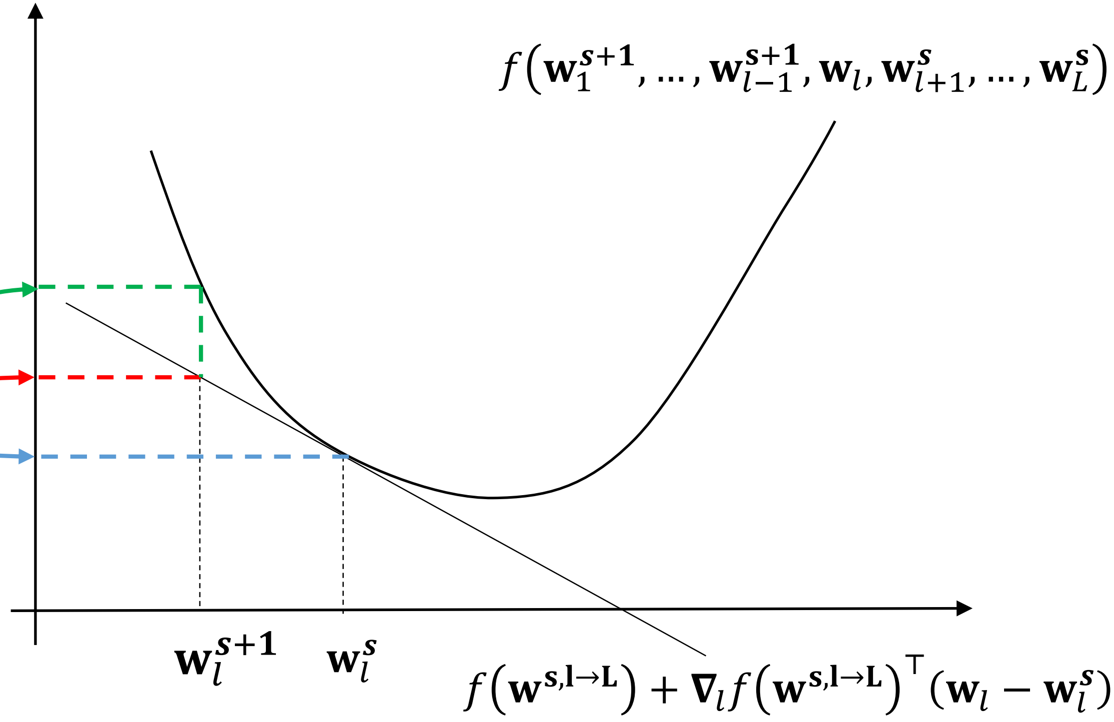

In the end $f\left(\mathbf{w}_1^{s+1}, \dots, \mathbf{w}_{l-1}^{s+1}, \color{red}{\mathbf{w}_l^{s}}, \mathbf{w}_{l+1}^{s}, \dots, \mathbf{w}_L^{s}\right) \leq f\left(\mathbf{w}_1^{s+1}, \dots, \mathbf{w}_{l-1}^{s+1}, \color{red}{\mathbf{w}_l^{s+1}}, \mathbf{w}_{l+1}^{s}, \dots, \mathbf{w}_L^{s}\right)$

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RGCCA framework - State of the Art of the **package**

	Core Optimization Problem			
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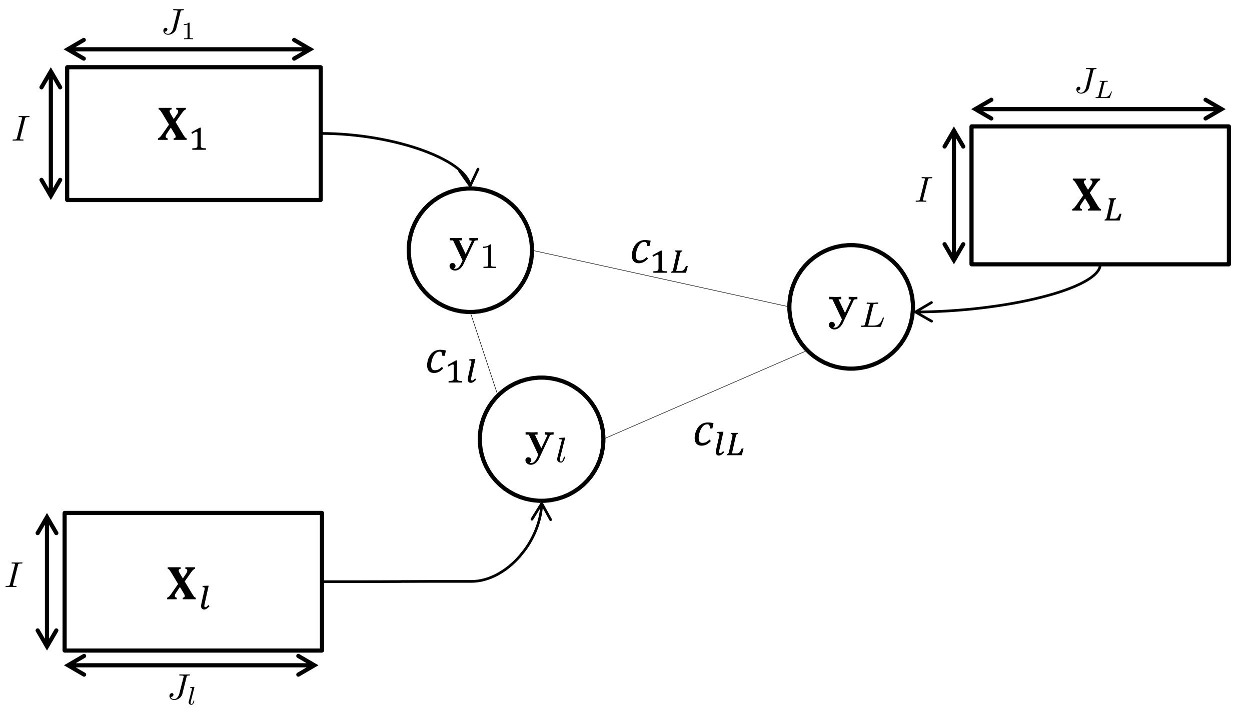
From RGCCA to Multiway GCCA



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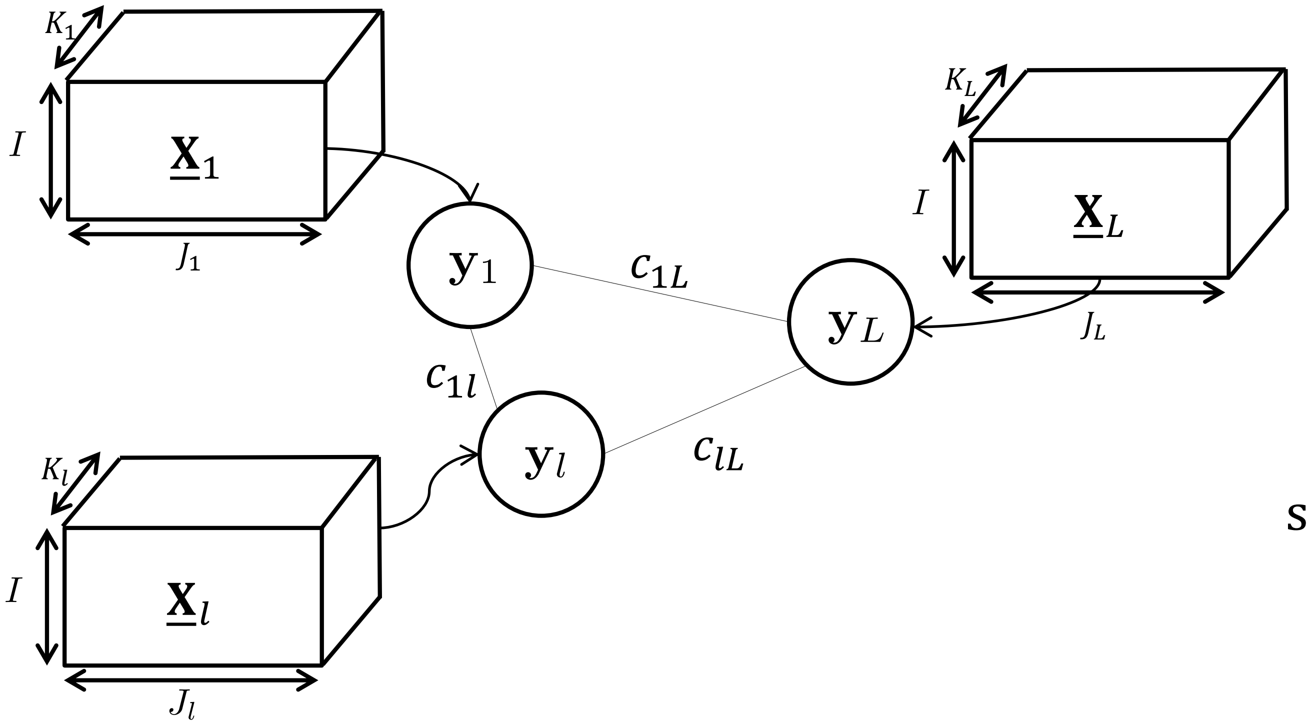

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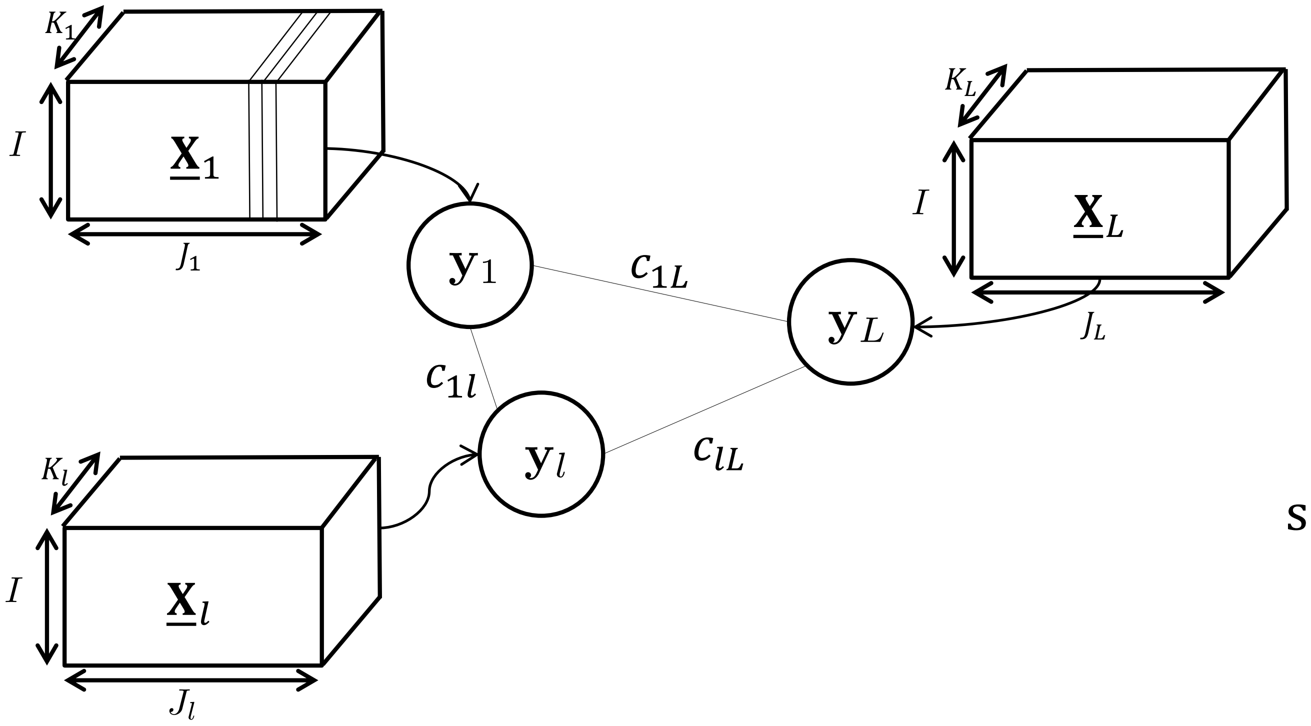

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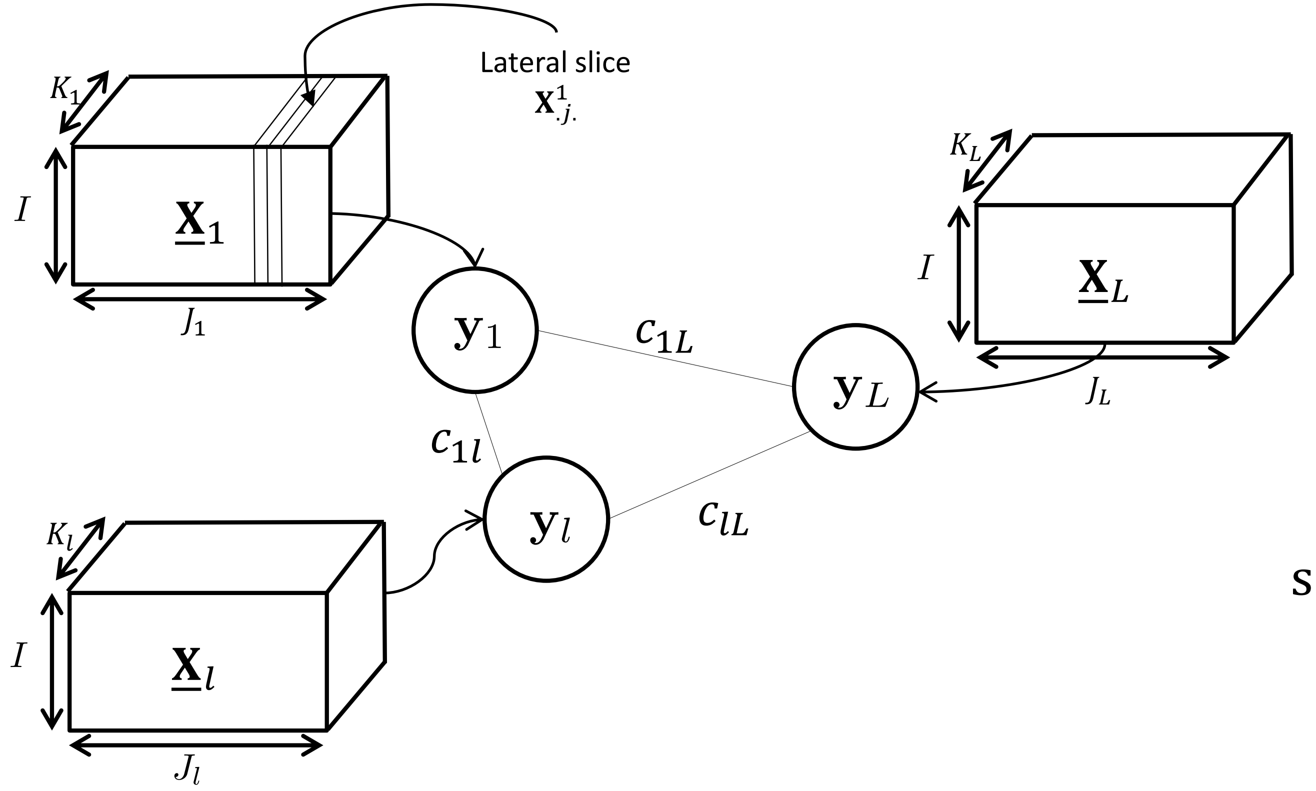

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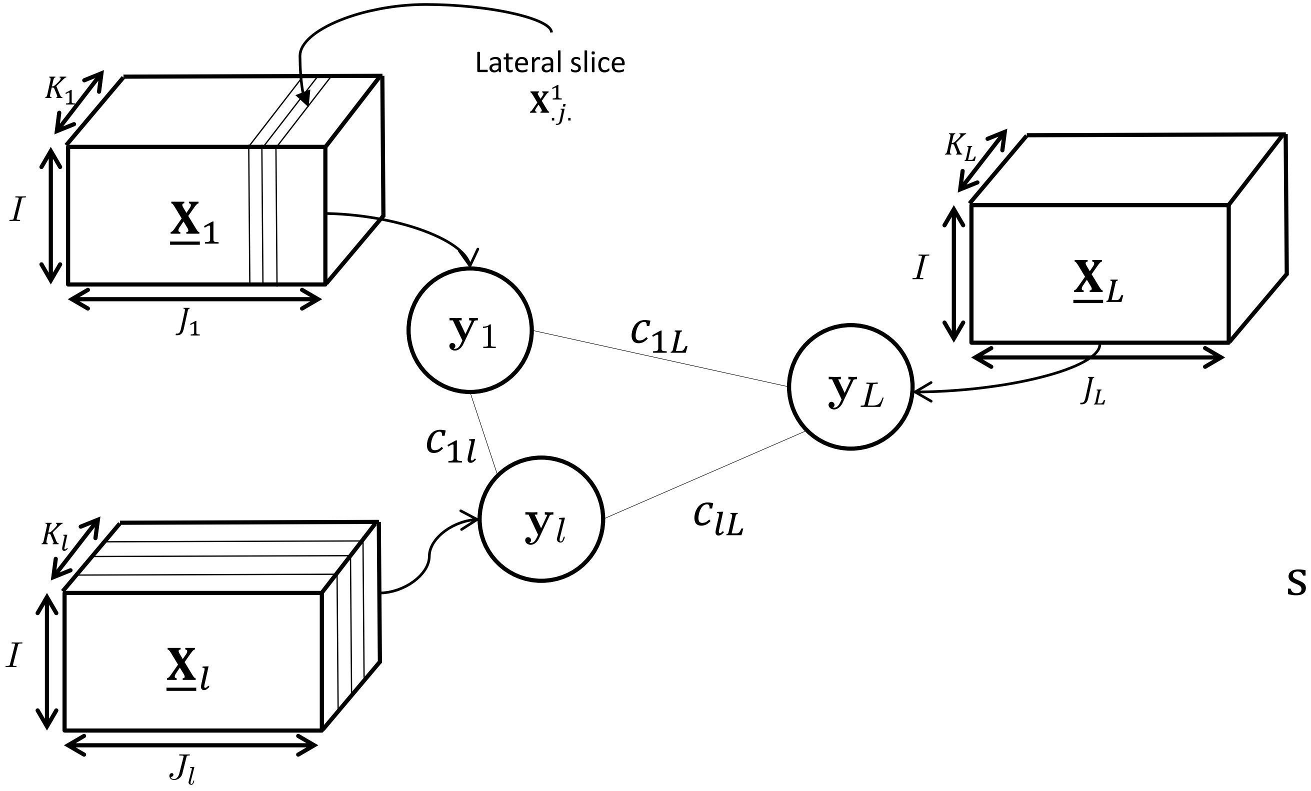

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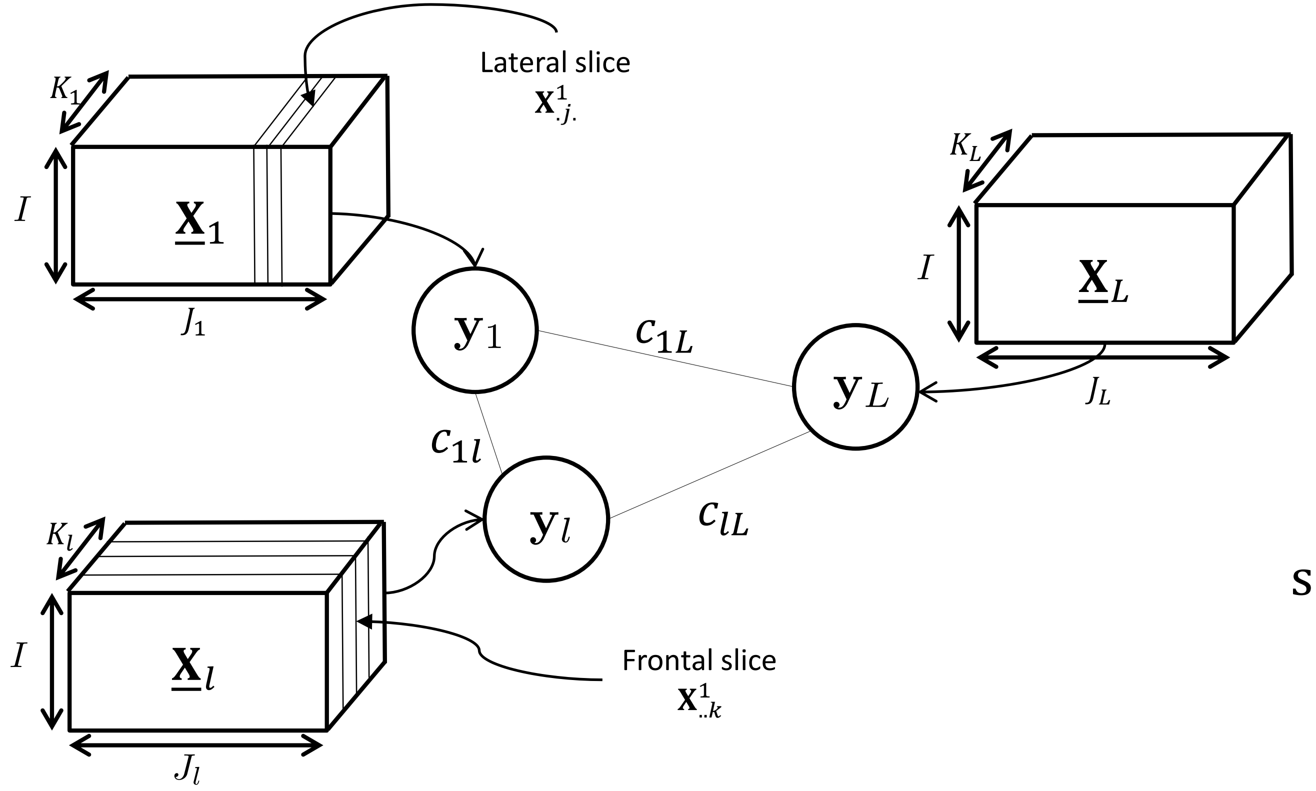

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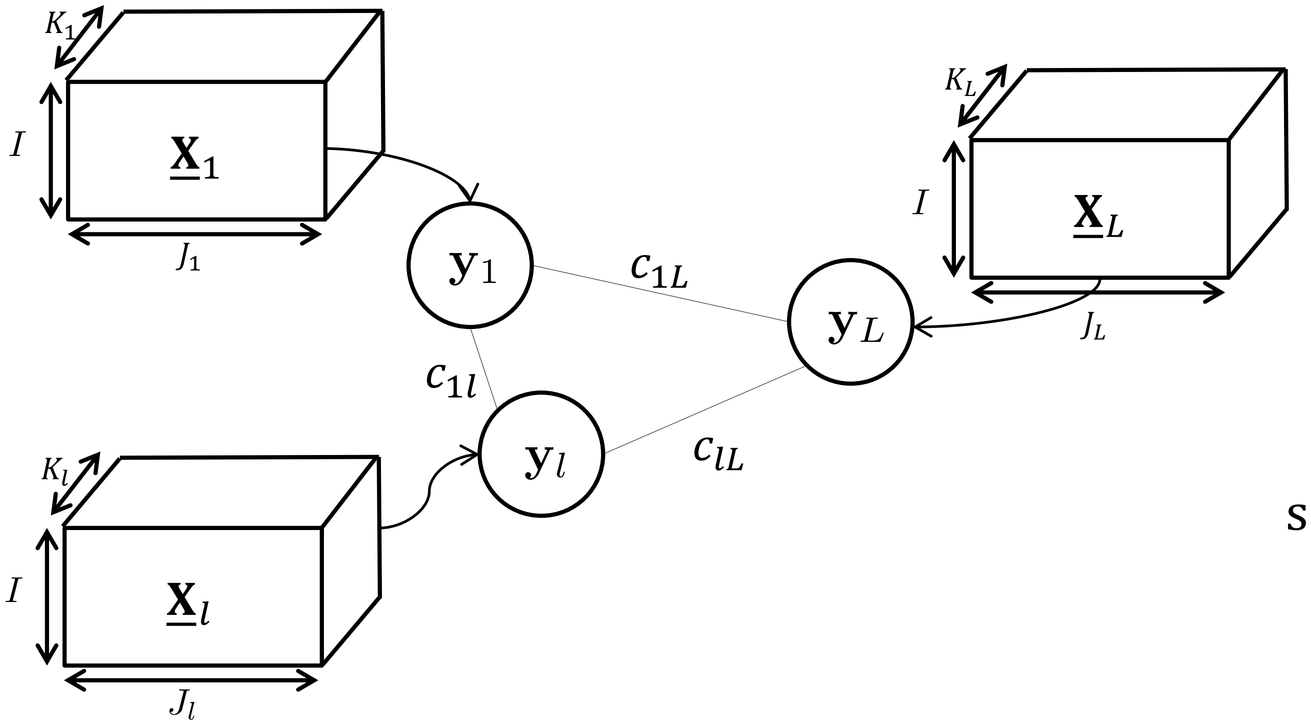

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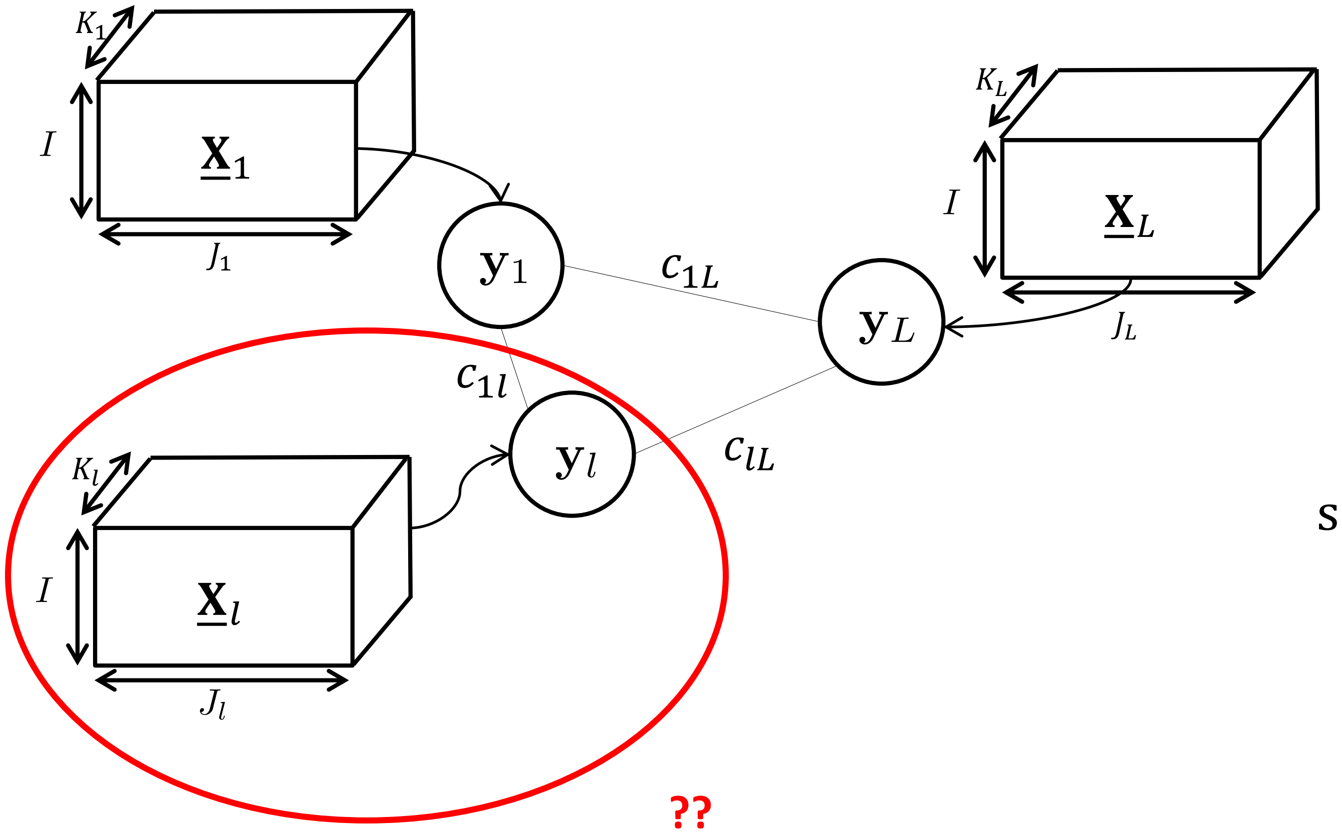

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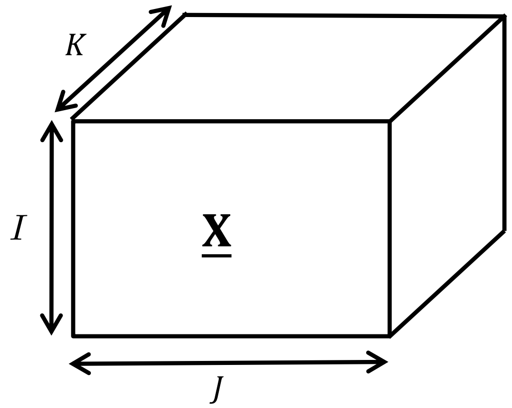

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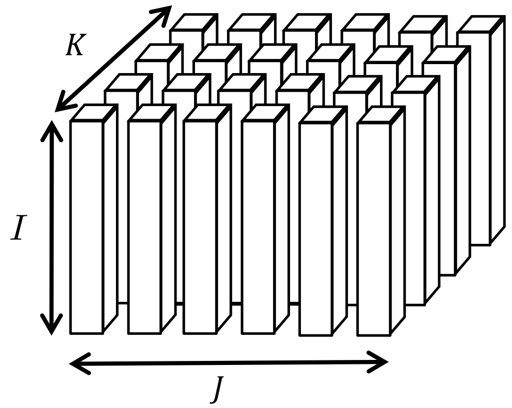

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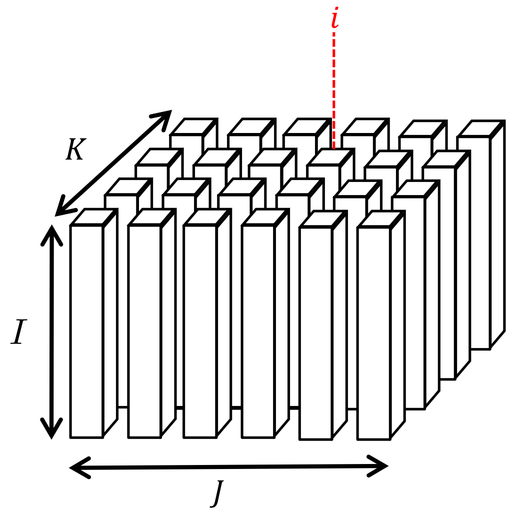

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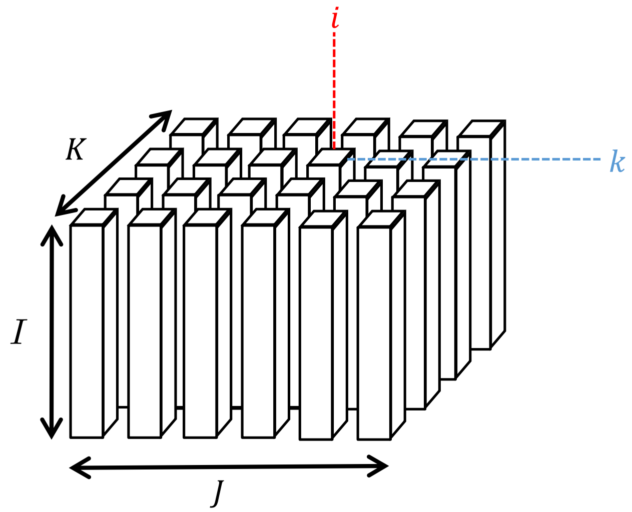

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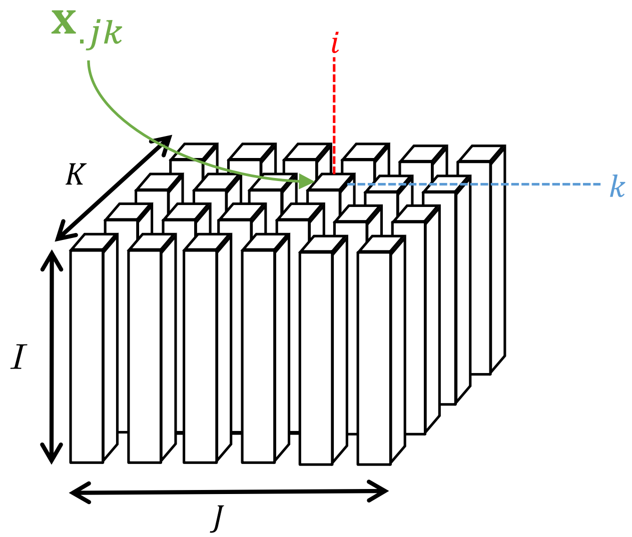

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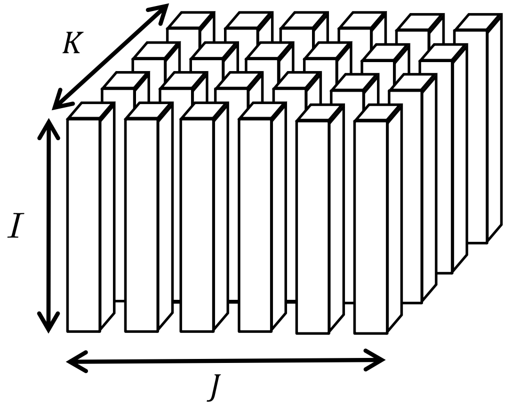

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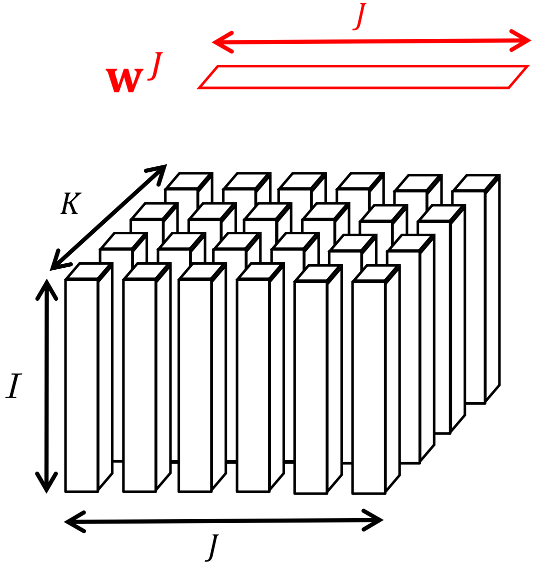

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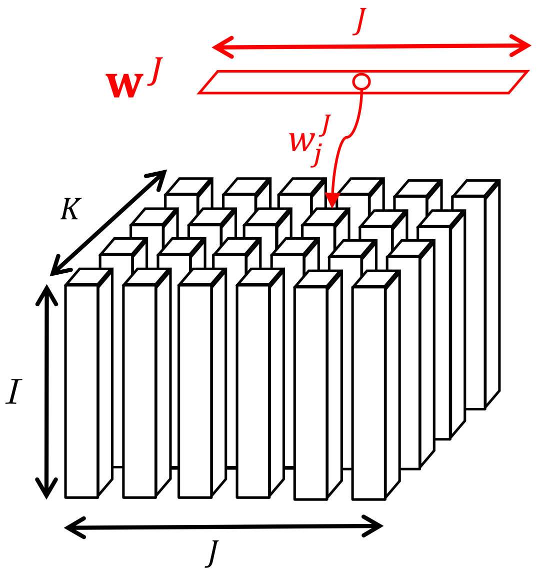
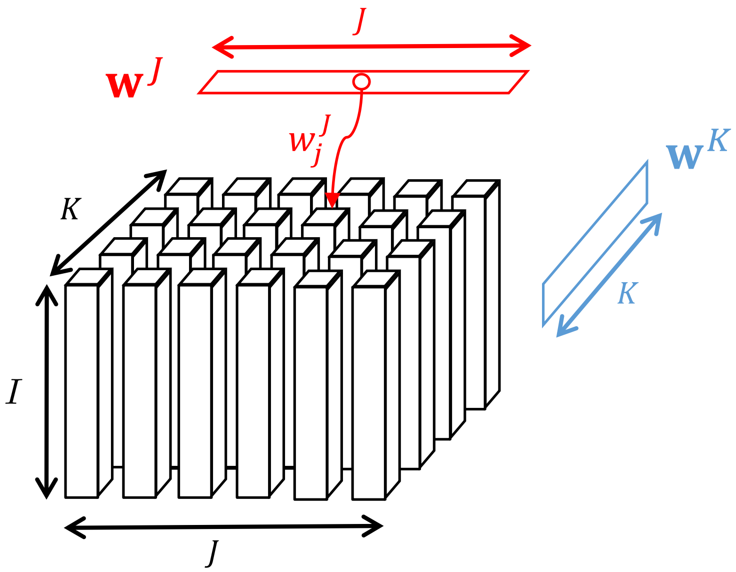


From RGCCA to Multiway GCCA



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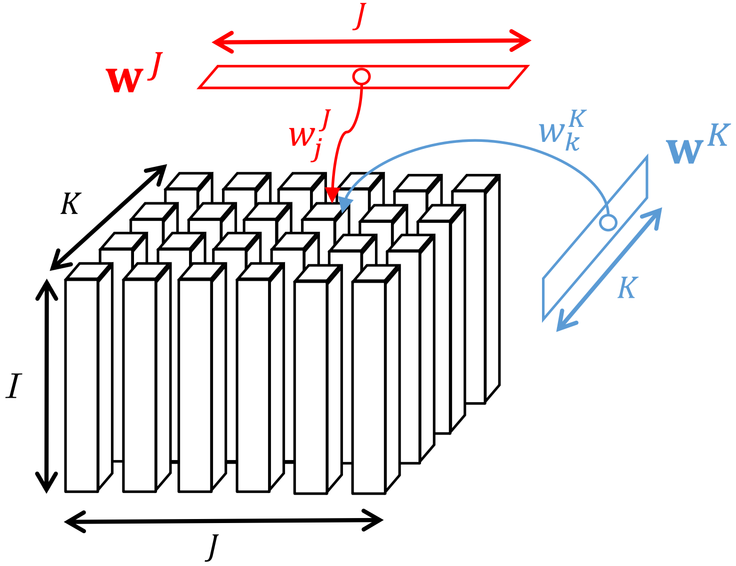

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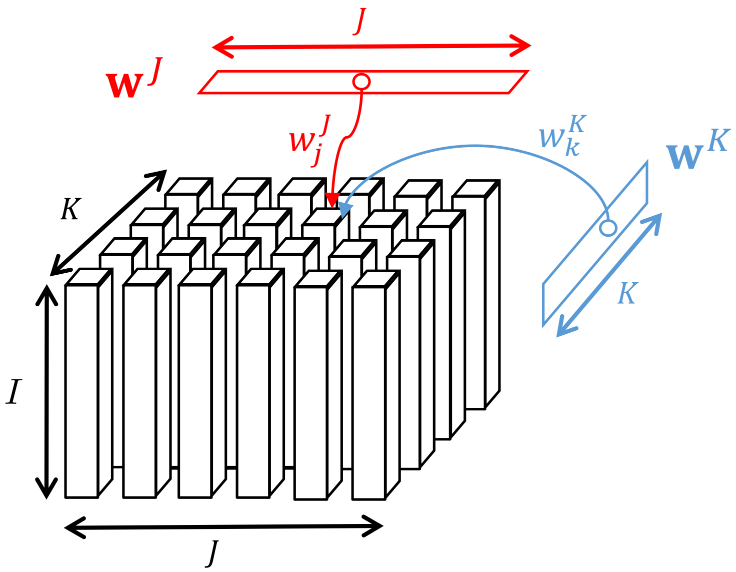

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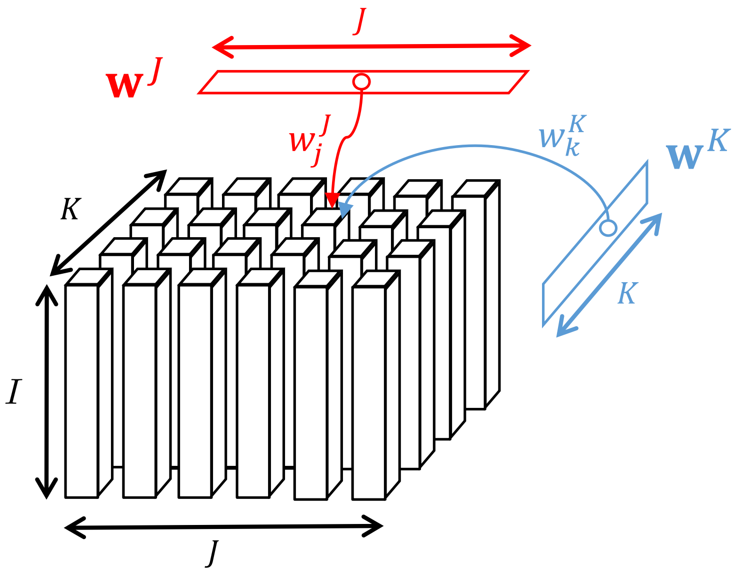
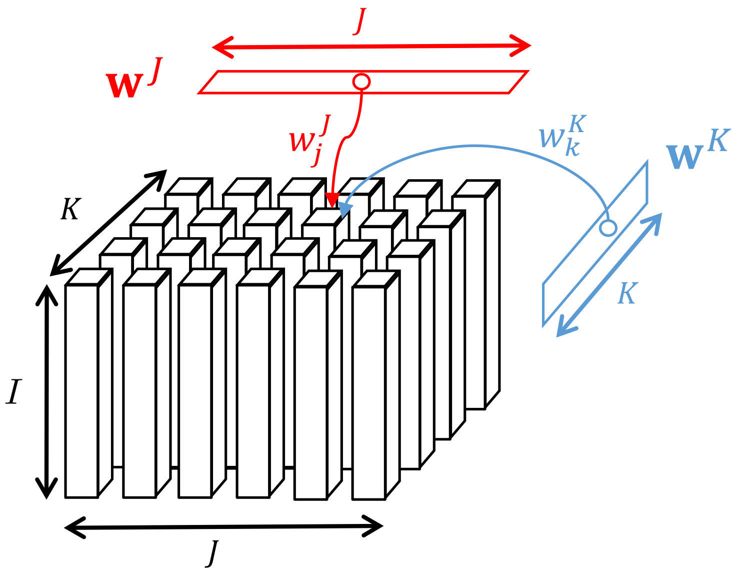


$$\mathbf{y} = \sum_{j=1}^{J} \sum_{k=1}^{K} w_k^K w_j^J \mathbf{x}_{.jk}$$

From RGCCA to Multiway GCCA



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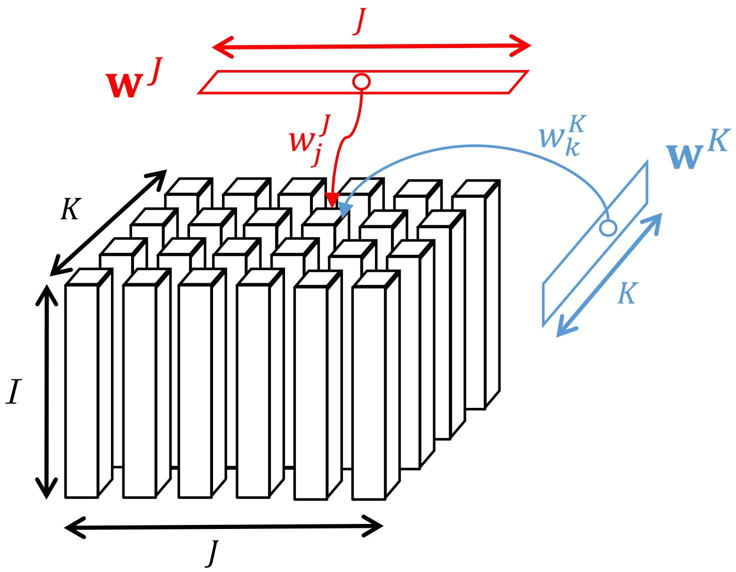
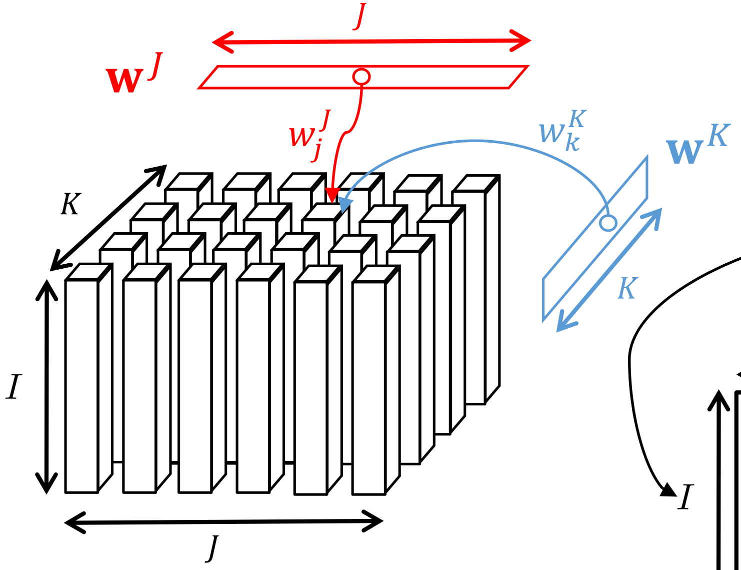


$$\mathbf{y} = \sum_{j=1}^{J} \sum_{k=1}^{K} w_k^K w_j^J \mathbf{x}_{.jk}$$

$$\mathbf{y} = \mathbf{X}(\mathbf{w}^K \otimes \mathbf{w}^J)$$

From RGCCA to Multiway GCCA



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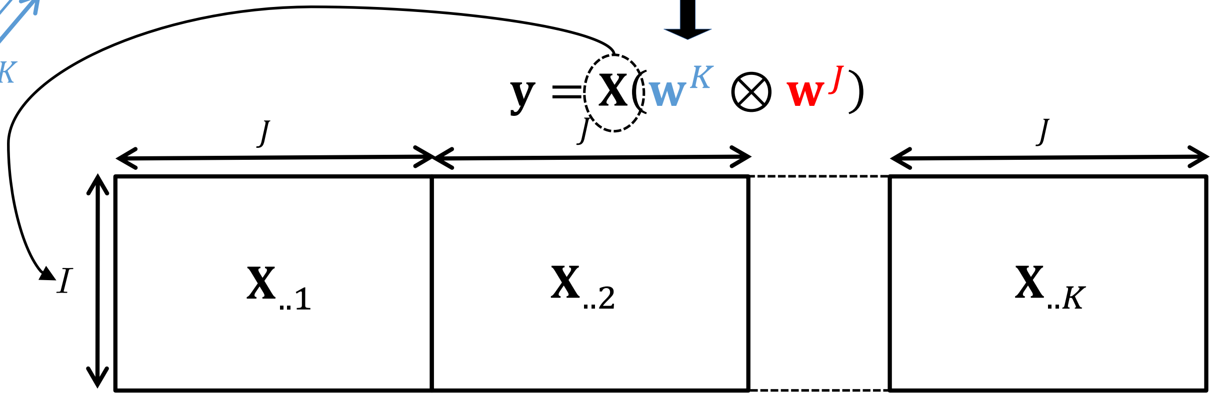

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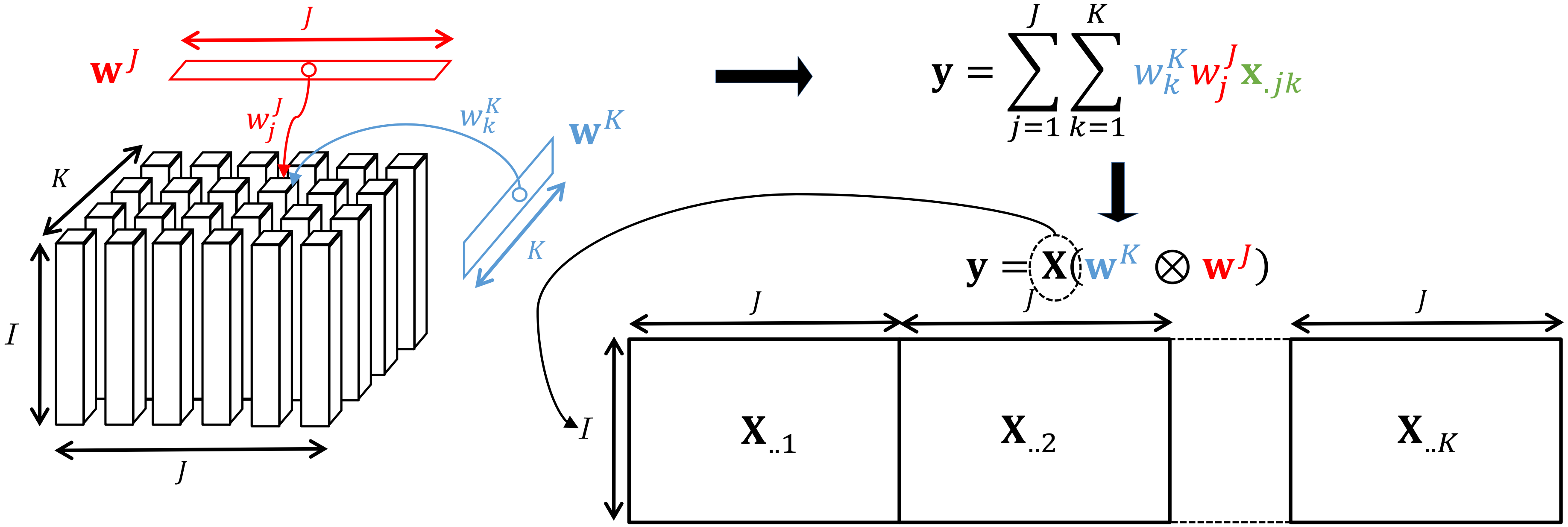
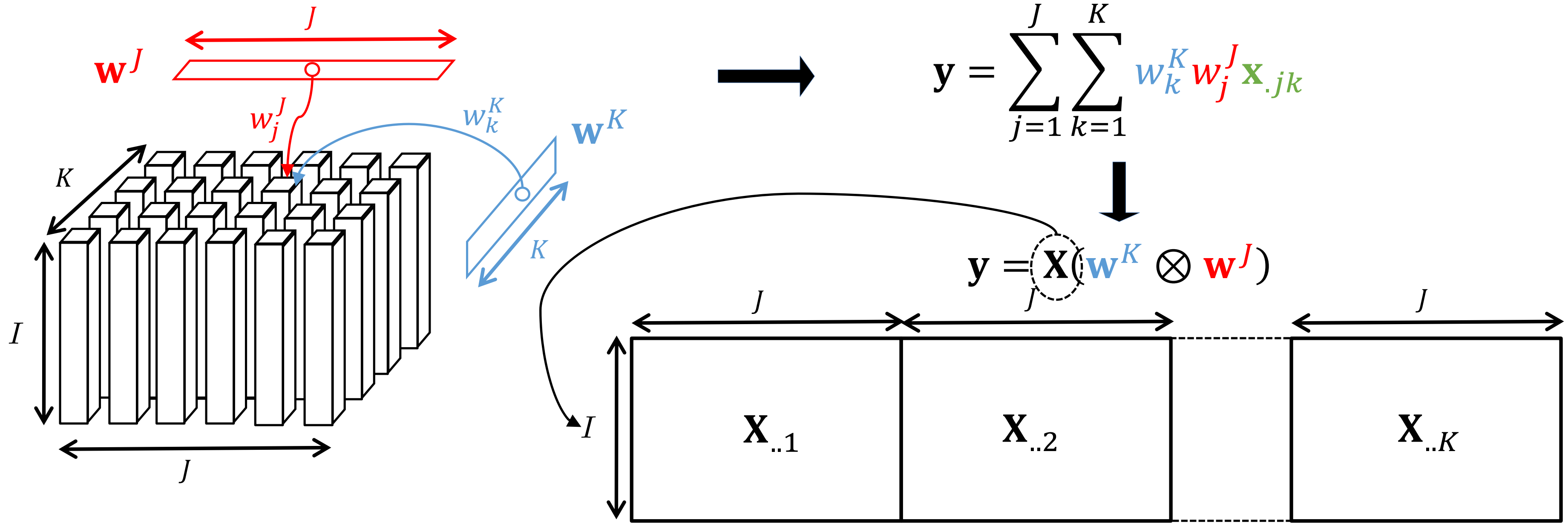


Interest in taking into account 3-way structure with the Kronecker product:

From RGCCA to Multiway GCCA



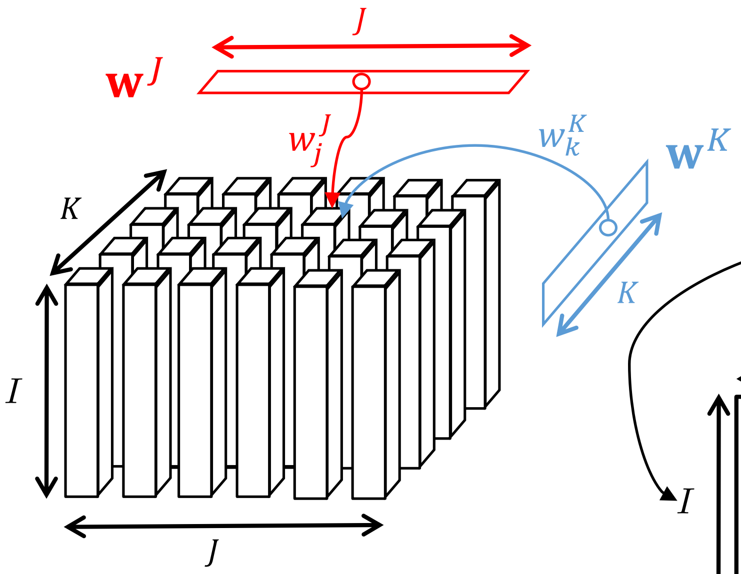
$$\mathbf{y} = \sum_{j=1}^{J} \sum_{k=1}^{K} w_k^K w_j^J \mathbf{x}_{.jk}$$

$$\mathbf{y} = \mathbf{X}(\mathbf{w}^K \otimes \mathbf{w}^J)$$

Interest in taking into account 3-way structure with the Kronecker product:

❖ Gain in interpretability thanks to vector weights specific to each dimension.

From RGCCA to Multiway GCCA



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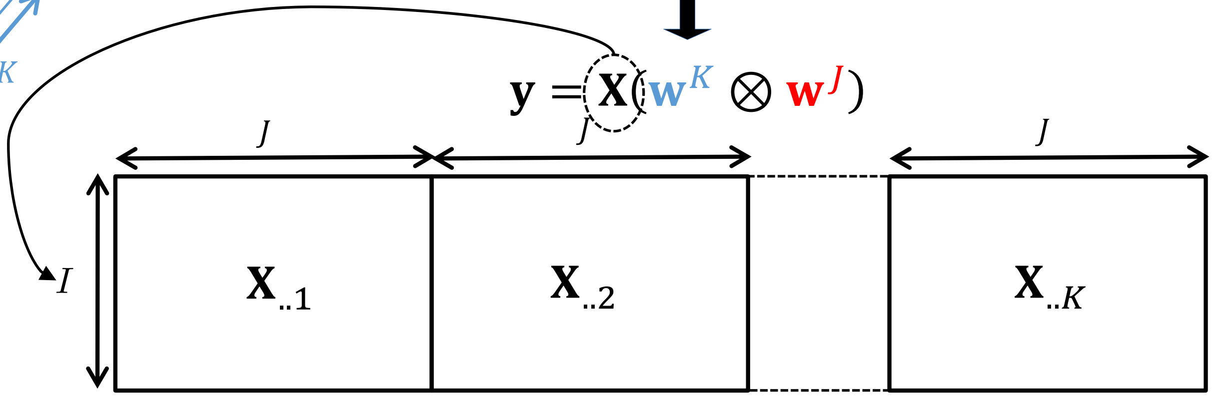
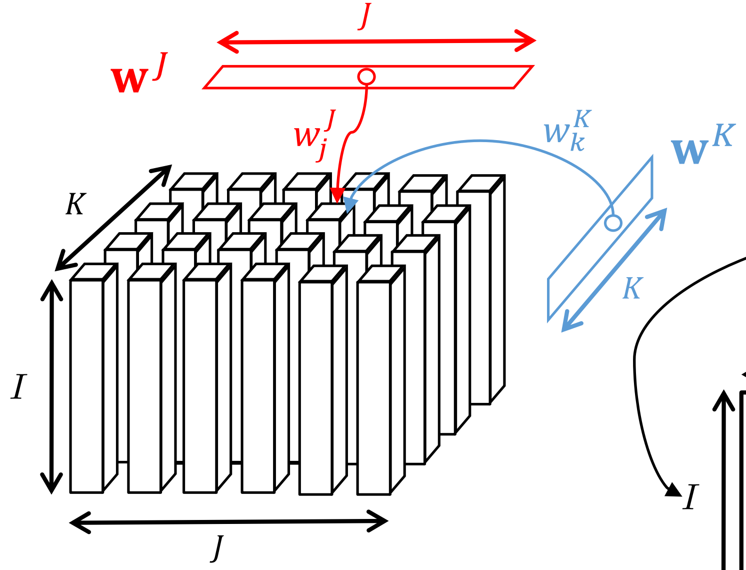


Interest in taking into account 3-way structure with the Kronecker product:

- ❖ Gain in interpretability thanks to vector weights specific to each dimension.
- ❖ Less weights to estimate: from $J \times K$ to $J + K$.

From RGCCA to Multiway GCCA



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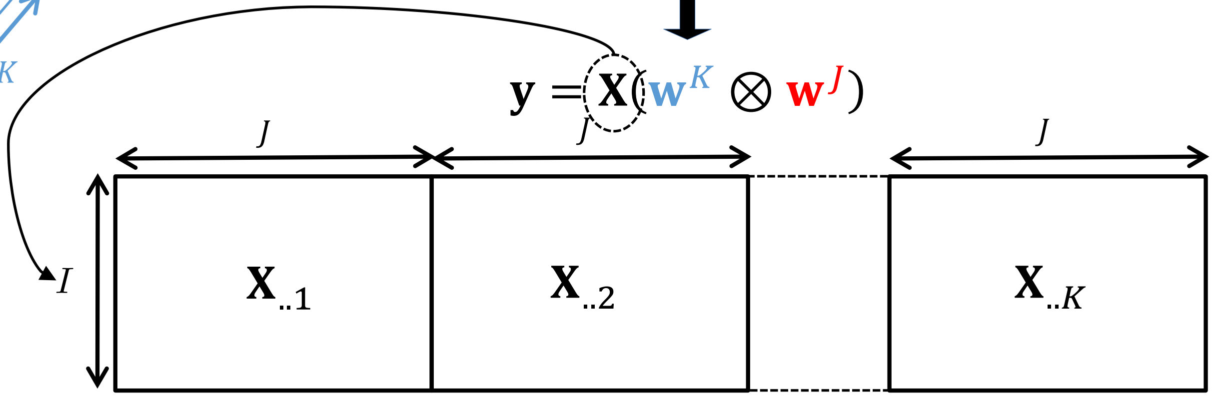

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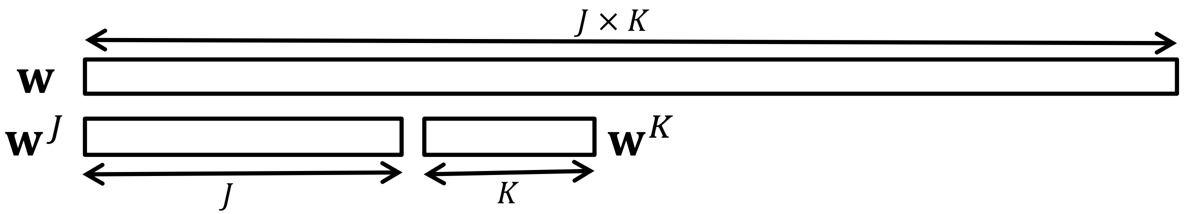
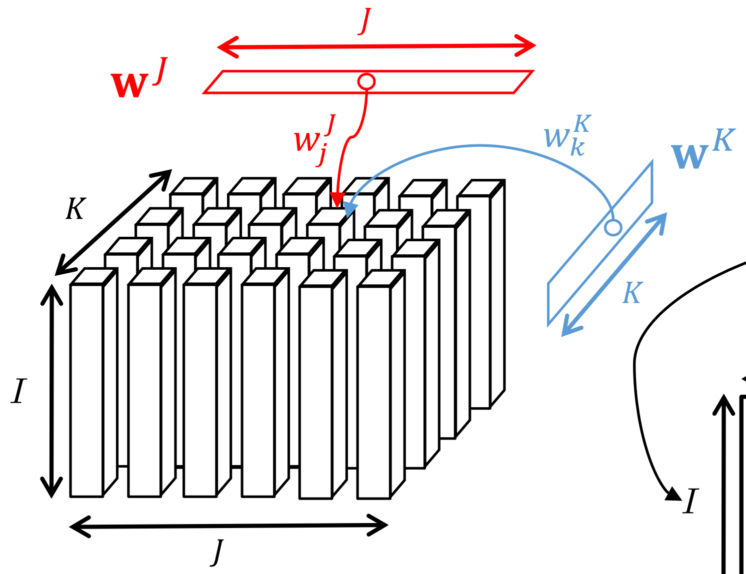


From RGCCA to Multiway GCCA



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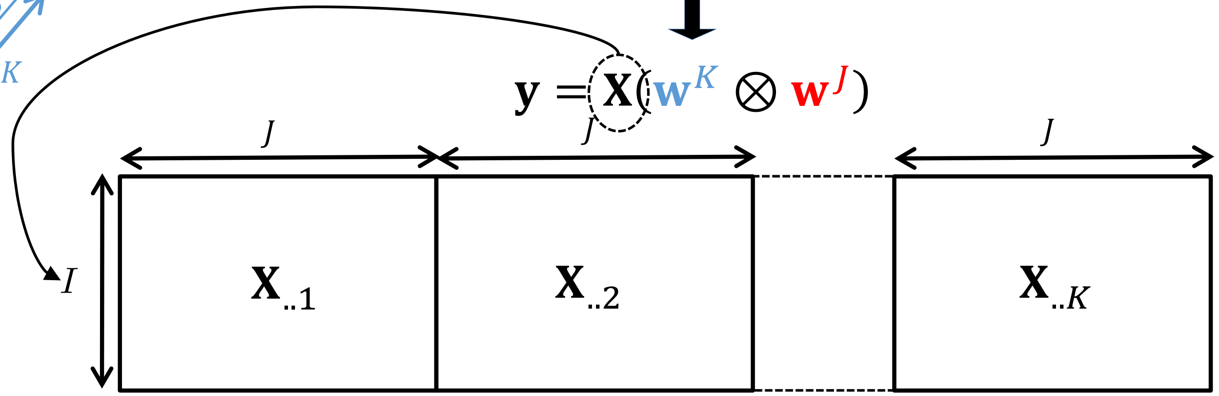

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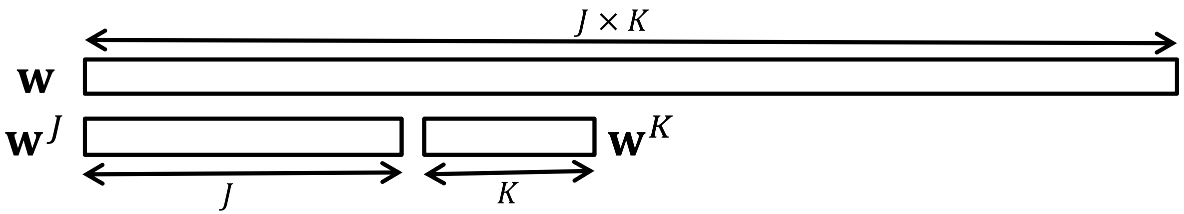
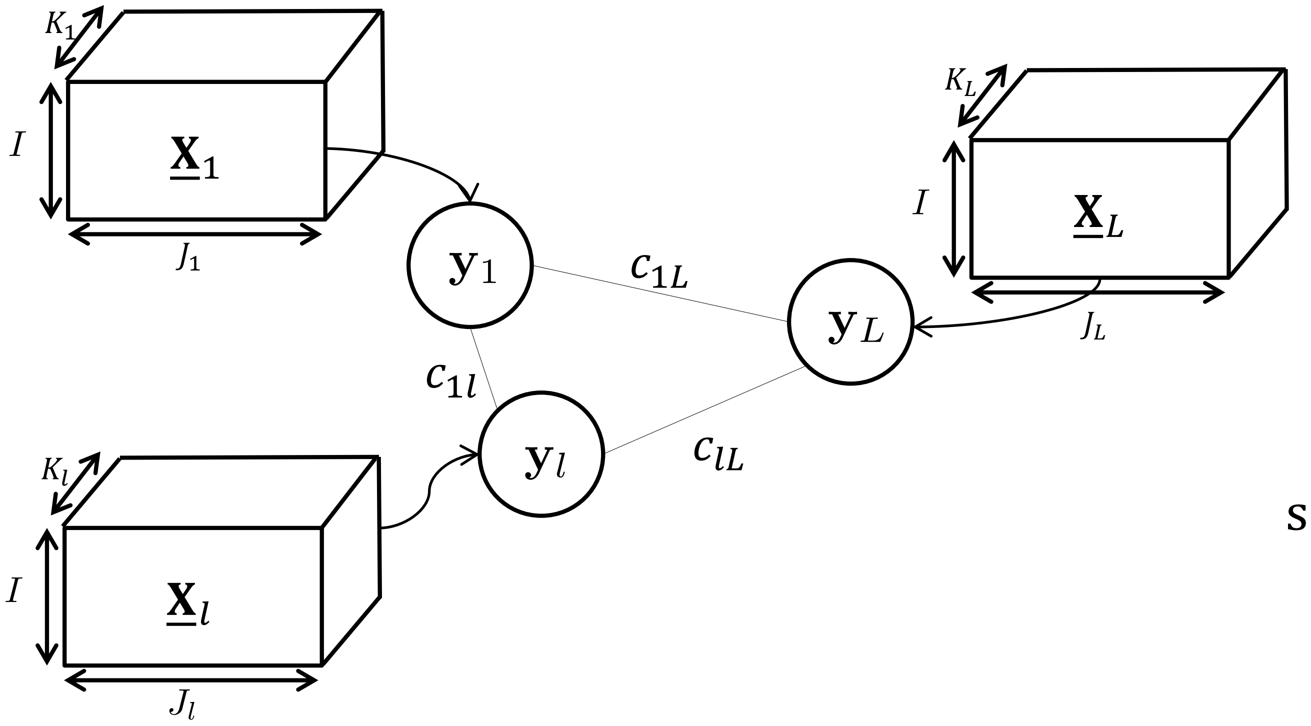


$\rightarrow$ $J \times K$ Vs $J + K$

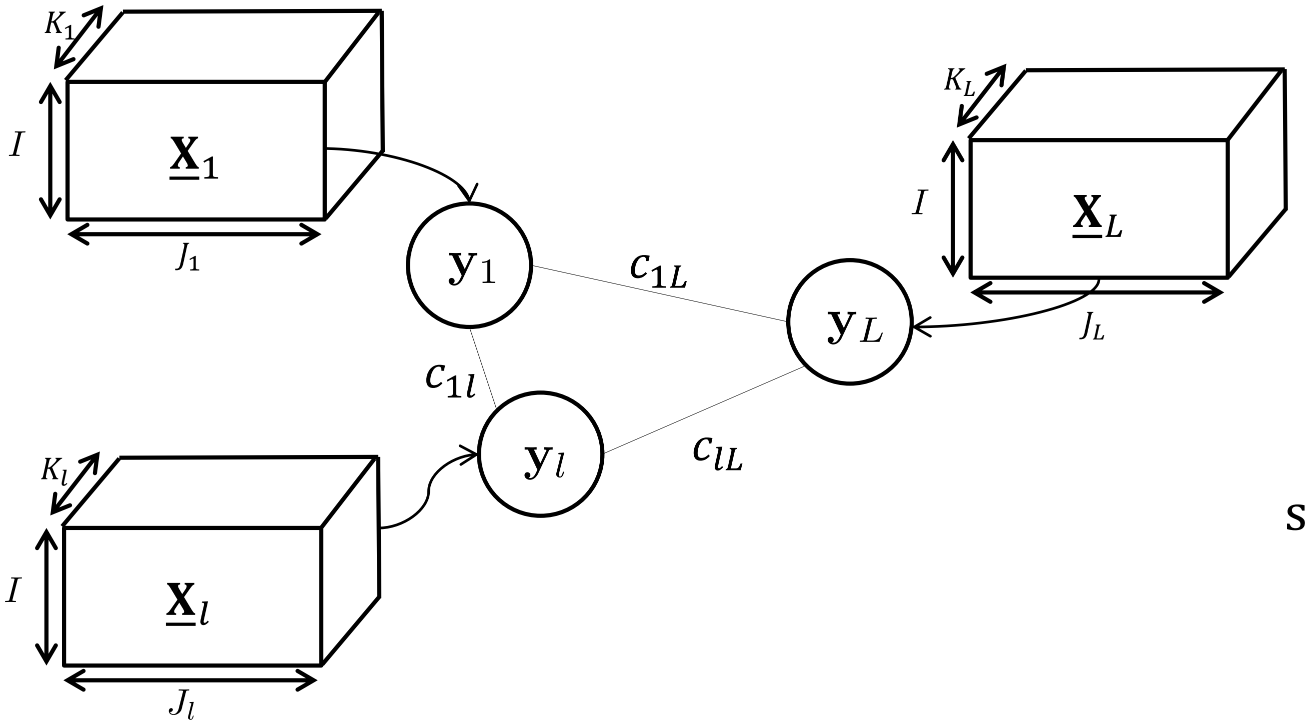
Multiway Generalized Canonical Correlation Analysis (MGCCA)



$$\max_{\mathbf{w}_1,\ldots,\mathbf{w}_L} \sum_{k,l=1}^{L} c_{kl}\, g\big(\mathrm{Cov}(\mathbf{X}_k\mathbf{w}_k, \mathbf{X}_l\mathbf{w}_l)\big)$$

$$\text{s.t.} \begin{cases} \mathbf{w}_l^\top \mathbf{M}_l \mathbf{w}_l = 1 \\ \\ \\ \end{cases} , l = 1, \ldots, L.$$

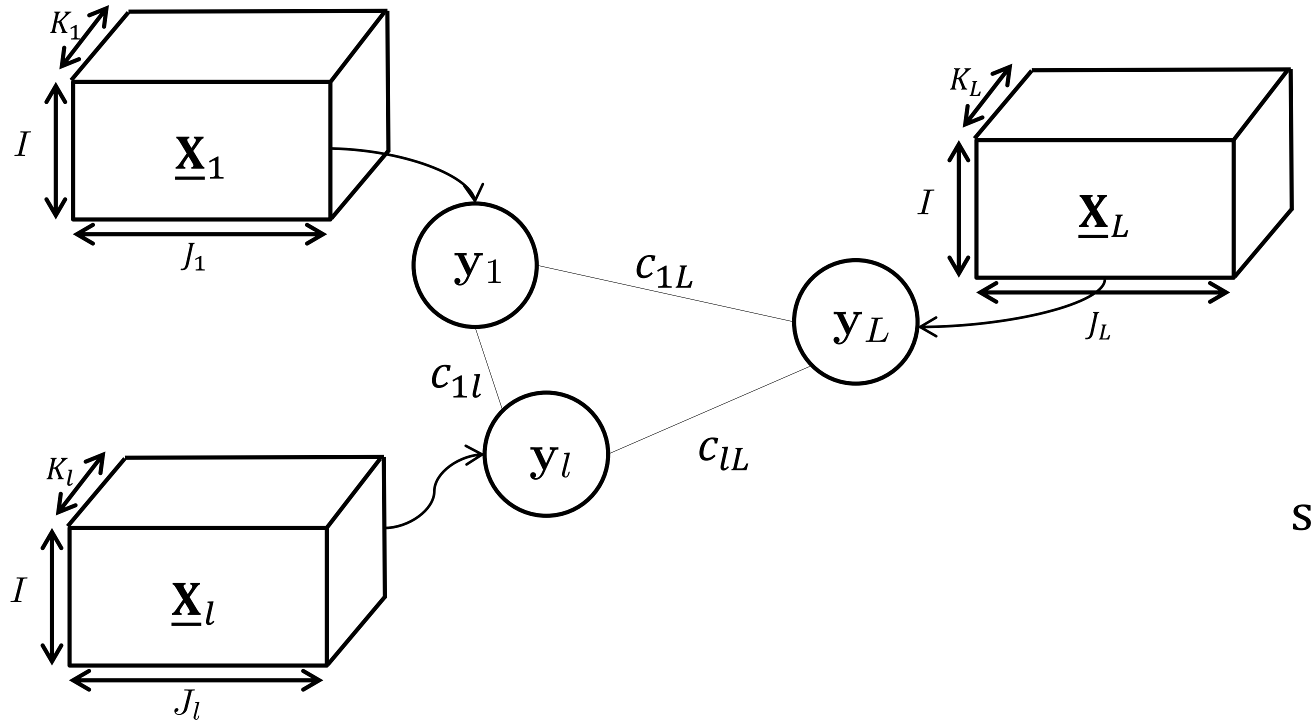
Multiway Generalized Canonical Correlation Analysis (MGCCA)



$$\max_{\mathbf{w}_1,\ldots,\mathbf{w}_L} \sum_{k,l=1}^{L} c_{kl}\, g\big(\mathrm{Cov}(\mathbf{X}_k\mathbf{w}_k, \mathbf{X}_l\mathbf{w}_l)\big)$$

$$\text{s.t.} \begin{cases} \mathbf{w}_l^\top \mathbf{M}_l \mathbf{w}_l = 1 \\ \mathbf{w}_l = \mathbf{w}_l^K \otimes \mathbf{w}_l^J \end{cases} , l = 1, \ldots, L.$$

Multiway Generalized Canonical Correlation Analysis (MGCCA)



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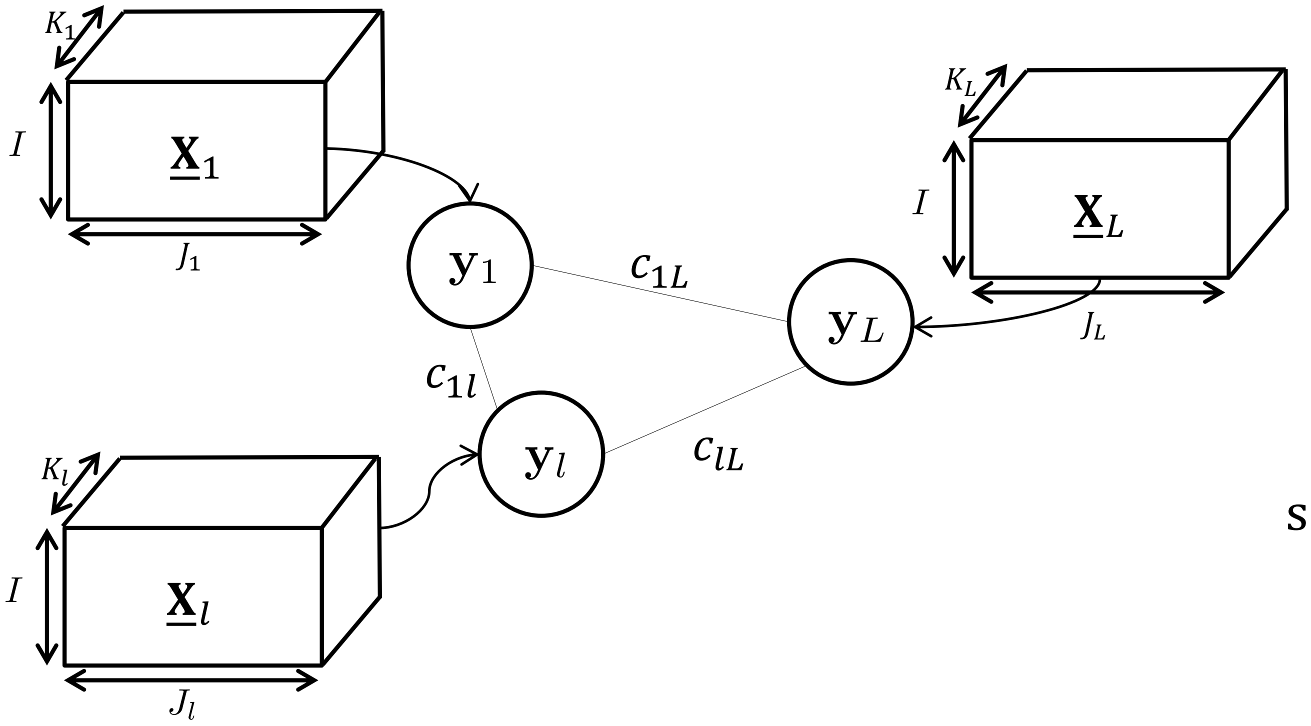

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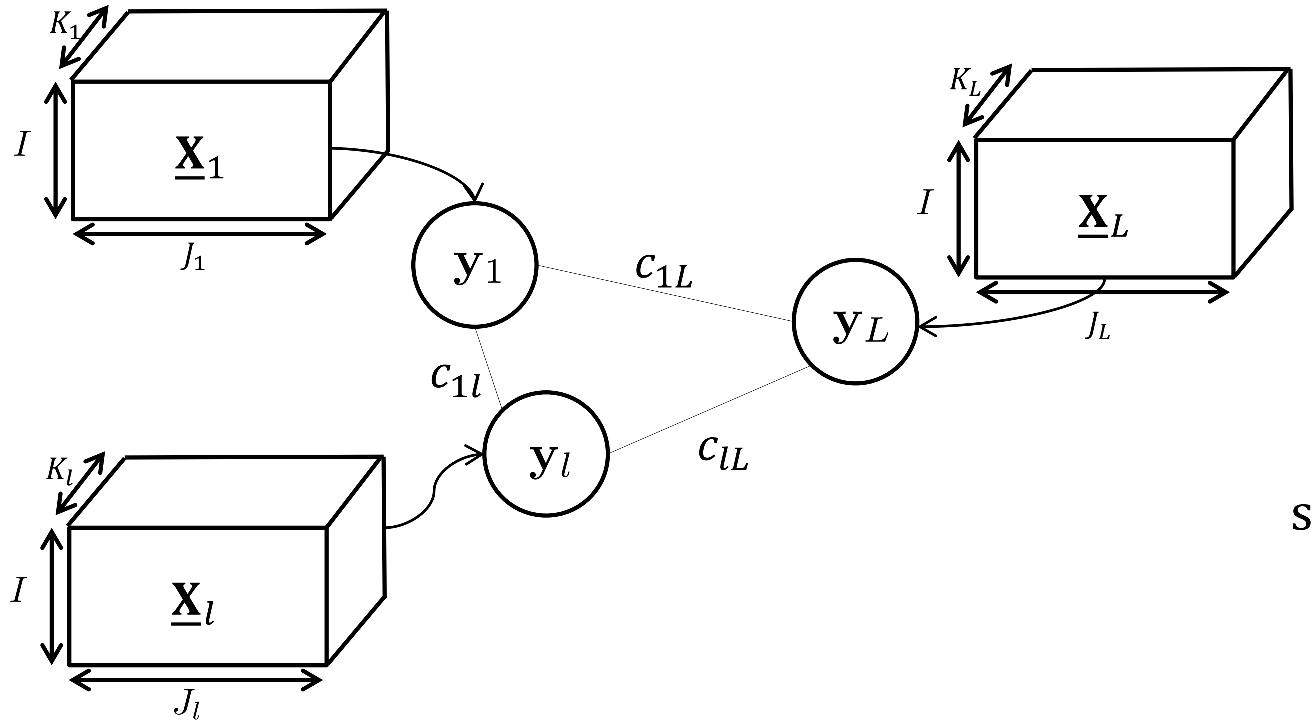
$$\text{s.t.} \begin{cases} \mathbf{w}_l^\top \mathbf{M}_l \mathbf{w}_l = 1 \\ \color{red}{\mathbf{w}_l = \mathbf{w}_l^K \otimes \mathbf{w}_l^J} \end{cases}, l = 1, \ldots, L.$$

Example of such data: Electro-EncephaloGrams.

Multiway Generalized Canonical Correlation Analysis (MGCCA)



$$\max_{\mathbf{w}_1,\ldots,\mathbf{w}_L} \sum_{k,l=1}^{L} c_{kl}\, g\big(\mathrm{Cov}(\underline{\mathbf{X}}_k \mathbf{w}_k, \underline{\mathbf{X}}_l \mathbf{w}_l)\big)$$

$$\text{s.t.} \begin{cases} \mathbf{w}_l^\top \mathbf{M}_l \mathbf{w}_l = 1 \\ \\ \mathbf{w}_l = \mathbf{w}_l^K \otimes \mathbf{w}_l^J \end{cases}, l = 1, \ldots, L.$$

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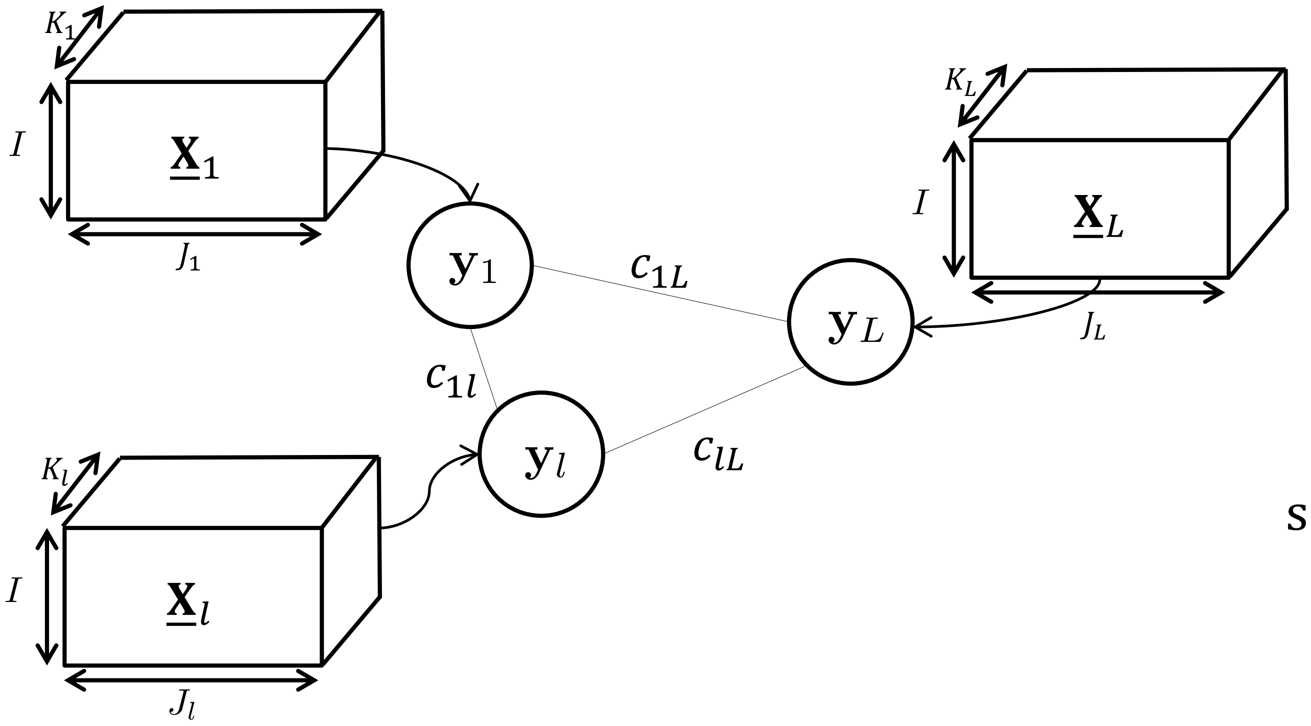
Idea of the Algorithm:

Multiway Generalized Canonical Correlation Analysis (MGCCA)



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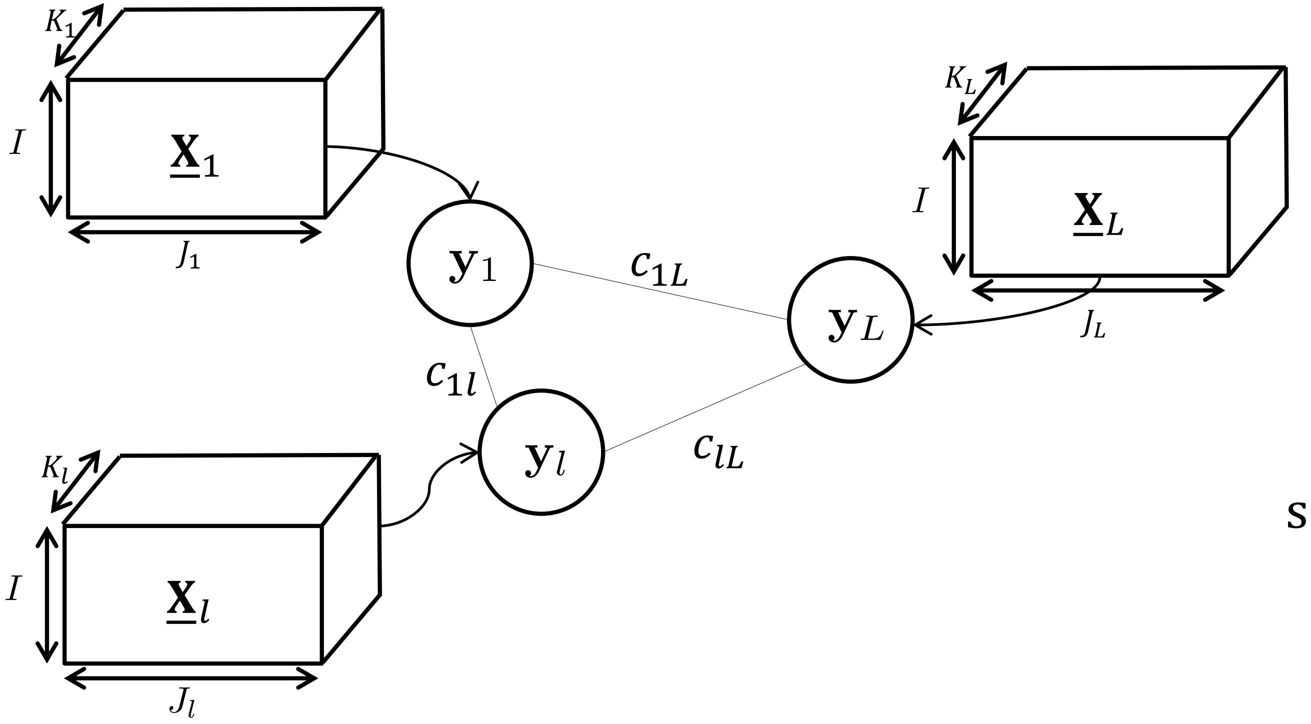
Idea of the Algorithm:

1. Block Coordinate Ascent (BCA).

Multiway Generalized Canonical Correlation Analysis (MGCCA)



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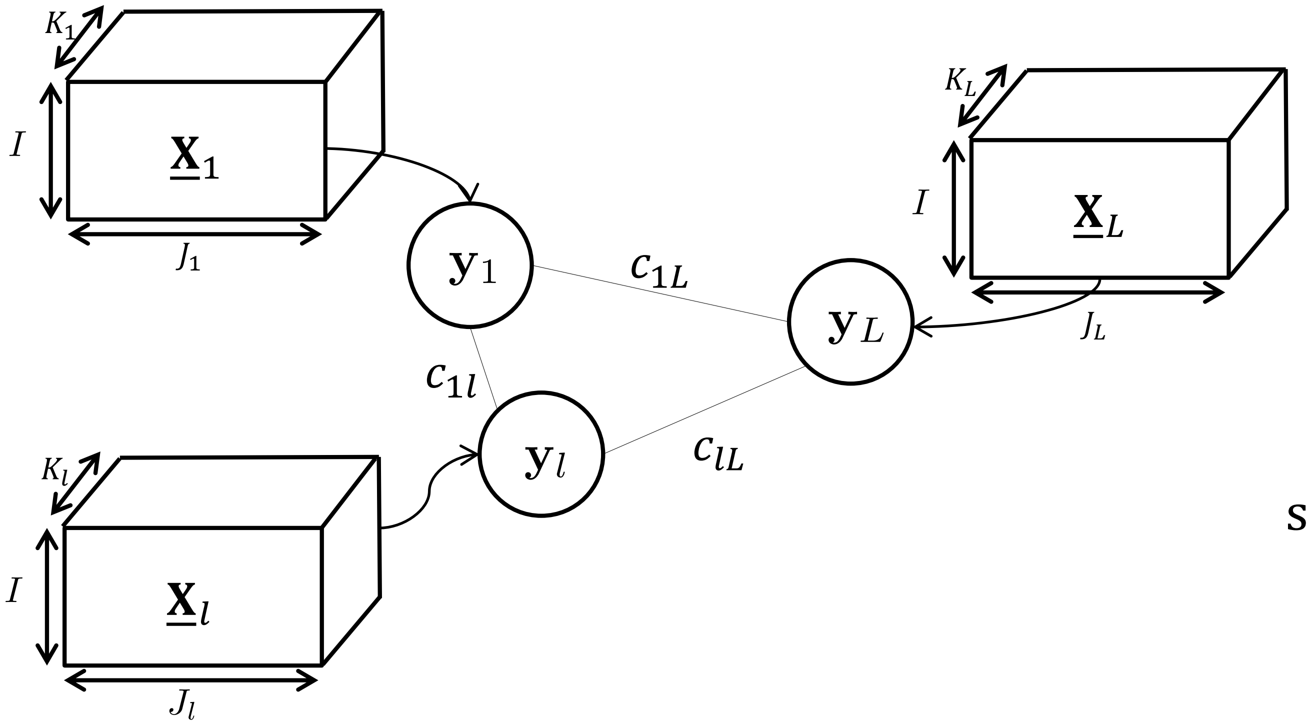
Example of such data: Electro-EncephaloGrams.

Idea of the Algorithm:

1. Block Coordinate Ascent (BCA).
2. MM principle: each update is a SVD of a specic matrix of size $K_l \times J_l$.

Multiway Generalized Canonical Correlation Analysis (MGCCA)



$$\max_{\mathbf{w}_1,\dots,\mathbf{w}_L} \sum_{k,l=1}^{L} c_{kl}\, g\big(\mathrm{Cov}(\mathbf{X}_k\mathbf{w}_k, \mathbf{X}_l\mathbf{w}_l)\big)$$

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Example of such data: Electro-EncephaloGrams.

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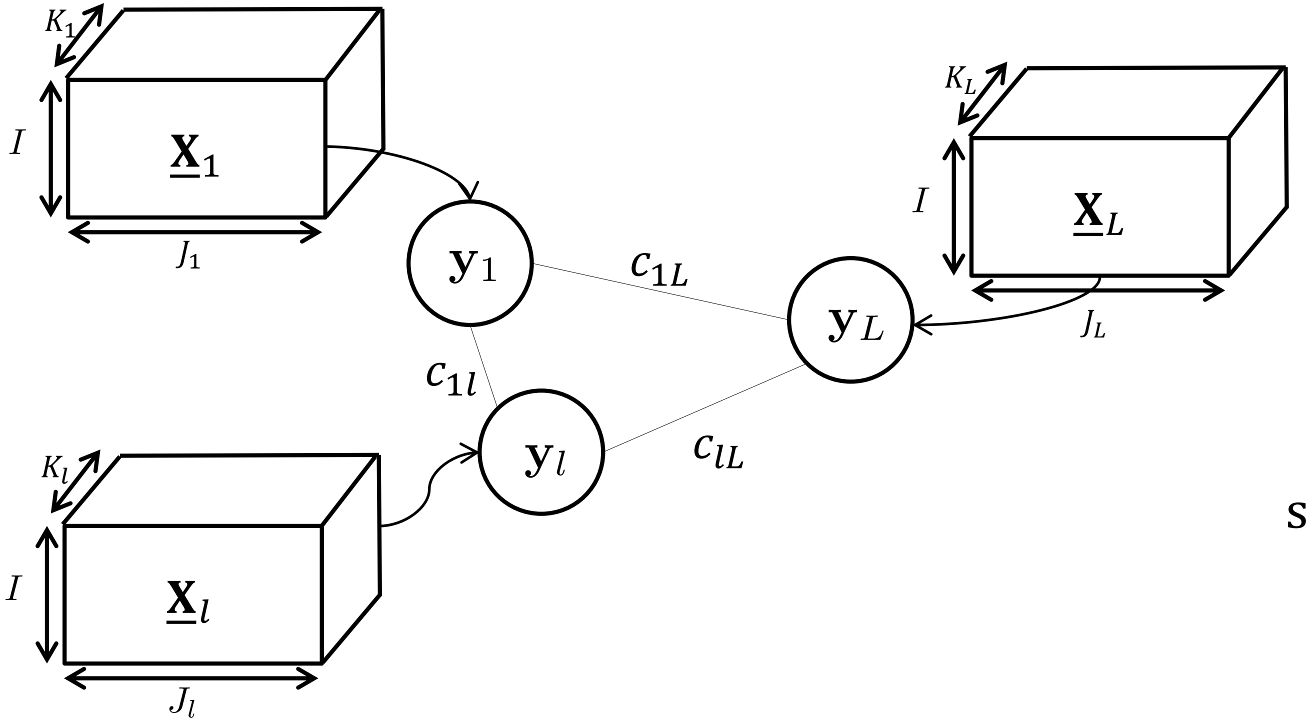
Global convergence of this algorithm was shown.

Multiway Generalized Canonical Correlation Analysis (MGCCA)



$$\max_{\mathbf{w}_1,\ldots,\mathbf{w}_L} \sum_{k,l=1}^{L} c_{kl}\, g\big(\mathrm{Cov}(\mathbf{X}_k\mathbf{w}_k, \mathbf{X}_l\mathbf{w}_l)\big)$$

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Example of such data: Electro-EncephaloGrams.

Idea of the Algorithm:

1. Block Coordinate Ascent (BCA).
2. MM principle: each update is a SVD of a specic matrix of size $K_l \times J_l$.

New extension with Tensor GCCA

Global convergence of this algorithm was shown.

RGCCA framework - State of the Art of the **package**

Constraints		Core Optimization Problem			Constraints
		$\max \nabla_l f(\mathbf{w}^s)^\top \mathbf{w}_l$			
	$\mathbf{w}_l \in \omega_l$	RGCCA[1,2]			
	$\begin{cases} \lVert \mathbf{w}_l \rVert_2^2 = 1 \\ \lVert \mathbf{w}_l \rVert_1 \leq s_l \end{cases}$	SGCCA[3]			

$$\omega_l = \left\{ \mathbf{w}_l \in \mathbb{R}^{J_l};\ \mathbf{w}_l^\top \mathbf{M}_l \mathbf{w}_l = 1 \right\}$$

1. (Tenenhaus and Tenenhaus, 2011) 2. (Tenenhaus, Tenenhaus and Groenen, 2017) 3. (Tenenhaus et al., 2014)

9. (Guigui et al., 2019) 10. (Chegraoui et al., 2023) 11. (Löfstedt et al., 2016)

RGCCA framework - State of the Art

Constraints		Core Optimization Problem			Constraints
		$\max \nabla_l f(\mathbf{w}^s)^\top \mathbf{w}_l$			
	$\mathbf{w}_l \in \omega_l$	RGCCA[1,2]			
	$\begin{cases} \|\mathbf{w}_l\|_2^2 = 1 \\ \|\mathbf{w}_l\|_1 \leq s_l \end{cases}$	SGCCA[3]			
	$\begin{cases} \mathbf{w}_l = \mathbf{w}_l^K \otimes \mathbf{w}_l^J \\ \mathbf{w}_l \in \omega_l \end{cases}$				

$$\omega_l = \{\mathbf{w}_l \in \mathbb{R}^{J_l};\ \mathbf{w}_l^\top \mathbf{M}_l \mathbf{w}_l = 1\}$$

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RGCCA framework - State of the Art

		Core Optimization Problem			
		$\max \nabla_l f(\mathbf{w}^s)^\top \mathbf{w}_l$			
Constraints	$\mathbf{w}_l \in \omega_l$	RGCCA[1,2]			Constraints
	$\begin{cases} \lVert \mathbf{w}_l \rVert_2^2 = 1 \\ \lVert \mathbf{w}_l \rVert_1 \leq s_l \end{cases}$	SGCCA[3]			
	$\begin{cases} \mathbf{w}_l = \mathbf{w}_l^K \otimes \mathbf{w}_l^J \\ \mathbf{w}_l \in \omega_l \end{cases}$	MGCCA[4]/TGCCA[5]			

$$\omega_l = \left\{\mathbf{w}_l \in \mathbb{R}^{J_l};\ \mathbf{w}_l^\top \mathbf{M}_l \mathbf{w}_l = 1\right\}$$

1. (Tenenhaus and Tenenhaus, 2011) 2. (Tenenhaus, Tenenhaus and Groenen, 2017) 3. (Tenenhaus et al., 2014) 4. (Gloaguen et al., 2022)

5. (Girka et al., 2024)

9. (Guigui et al., 2019) 10. (Chegraoui et al., 2023) 11. (Löfstedt et al., 2016)

Optimization criterion: From Sequential to Global

$$\underset{\mathbf{w}_1,\ldots,\mathbf{w}_L}{\operatorname{argmax}} \sum_{k,l=1}^{L} c_{kl} \quad g\left(\operatorname{Cov}\left(\mathbf{X}_k\mathbf{w}_k^{(r)}, \mathbf{X}_l\mathbf{w}_l^{(r)}\right)\right)$$

$$\text{s.t.} \begin{cases} \mathbf{w}_l{}^\top \mathbf{M}_l \mathbf{w}_l = 1 \\ \end{cases}, l = 1, \ldots, L.$$

Where:

❖ $\mathbf{w}_l \in \mathbb{R}^{J_l}$ is a block-weight vector.

Optimization criterion: From Sequential to Global

$$\underset{\mathbf{w}_1^{(1)},\ldots,\mathbf{w}_L^{(1)}}{\text{argmax}} \sum_{k,l=1}^{L} c_{kl} \quad g\left(\text{Cov}\left(\mathbf{X}_k\mathbf{w}_k^{(1)}, \mathbf{X}_l\mathbf{w}_l^{(1)}\right)\right)$$

$$\text{s.t.} \begin{cases} \mathbf{w}_l^{(1)\top}\mathbf{M}_l\mathbf{w}_l^{(1)} = 1 \\ \end{cases} \quad , l = 1, \ldots, L.$$

Where:

❖ $\mathbf{w}_l^{(1)} \in \mathbb{R}^{J_l}$ is a the first block-weight vector.

Optimization criterion: From Sequential to Global

$$\underset{\mathbf{w}_1^{(2)},\dots,\mathbf{w}_L^{(2)}}{\operatorname{argmax}} \sum_{k,l=1}^{L} c_{kl} \quad g\left(\operatorname{Cov}\left(\mathbf{X}_k\mathbf{w}_k^{(2)}, \mathbf{X}_l\mathbf{w}_l^{(2)}\right)\right)$$

$$\text{s.t.} \begin{cases} \mathbf{w}_l^{(2)\top}\mathbf{M}_l\mathbf{w}_l^{(2)} = 1 \\ \mathbf{y}_l^{(1)\top}\mathbf{X}_l\mathbf{w}_l^{(2)} = 0 \end{cases} \quad , l = 1, \dots, L.$$

Where:

- $\mathbf{w}_l^{(1)} \in \mathbb{R}^{J_l}$ is a the first block-weight vector.
- $\mathbf{w}_l^{(2)} \in \mathbb{R}^{J_l}$is a the second block–weight vector.

Optimization criterion: From Sequential to Global

$$\underset{\mathbf{w}_1^{(2)},\dots,\mathbf{w}_L^{(2)}}{\operatorname{argmax}} \sum_{k,l=1}^{L} c_{kl} \quad g\left(\operatorname{Cov}\left(\mathbf{X}_k\mathbf{w}_k^{(2)}, \mathbf{X}_l\mathbf{w}_l^{(2)}\right)\right)$$

$$\text{s.t.} \begin{cases} \mathbf{w}_l^{(2)\top}\mathbf{M}_l\mathbf{w}_l^{(2)} = 1 \\ \mathbf{y}_l^{(1)\top}\mathbf{X}_l\mathbf{w}_l^{(2)} = 0 \end{cases} \quad , l = 1, \dots, L.$$

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- …

Optimization criterion: From Sequential to Global

$$\underset{\mathbf{w}_1^{(1)},\dots,\mathbf{w}_L^{(1)}}{\operatorname{argmax}} \sum_{k,l=1}^{L} c_{kl} \quad g\left(\mathrm{Cov}\left(\mathbf{X}_k\mathbf{w}_k^{(1)}, \mathbf{X}_l\mathbf{w}_l^{(1)}\right)\right)$$

Where:

❖ $\mathbf{w}_l^{(1)} \in \mathbb{R}^{J_l}$ is a the first block−weight vector.

Optimization criterion: From Sequential to Global

$$\underset{\mathbf{w}_1^{(r)},\ldots,\mathbf{w}_L^{(r)}}{\operatorname{argmax}} \sum_{k,l=1}^{L} c_{kl} \sum_{r=1}^{R} g\left(\mathrm{Cov}\left(\mathbf{X}_k \mathbf{w}_k^{(r)}, \mathbf{X}_l \mathbf{w}_l^{(r)}\right)\right)$$

Where:

❖ $\mathbf{w}_l^{(\mathrm{r})} \in \mathbb{R}^{J_l}$ is a the r^{th} block–weight vector.

Optimization criterion: From Sequential to Global

$$\underset{\mathbf{W}_1,\ldots,\mathbf{W}_L}{\operatorname{argmax}} \sum_{k,l=1}^{L} c_{kl} \mathrm{Trace}\left(g\left(\mathrm{Cov}(\mathbf{X}_k\mathbf{W}_k, \mathbf{X}_l\mathbf{W}_l)\right)\right)$$

Where:

- $\mathbf{w}_l^{(\mathrm{r})} \in \mathbb{R}^{J_l}$ is a the r^{th} block–weight vector.
- $\mathbf{W}_l = \left[\mathbf{w}_l^{(1)}, \ldots, \mathbf{w}_l^{(\mathrm{R})}\right] \in \mathbb{R}^{J_l \times R}$ is a block–weight matrix.

Optimization criterion: From Sequential to Global

$$\underset{\mathbf{W}_1,\ldots,\mathbf{W}_L}{\text{argmax}} \sum_{k,l=1}^{L} c_{kl} \text{Trace}\Big(g\big(\text{Cov}(\mathbf{X}_k\mathbf{W}_k, \mathbf{X}_l\mathbf{W}_l)\big)\Big)$$

$$\text{s.t.} \qquad \mathbf{W}_l^\top \mathbf{M}_l \mathbf{W}_l = \mathbf{I}_R \qquad , l = 1, \ldots, L.$$

Where:

- ❖ $\mathbf{w}_l^{(\mathrm{r})} \in \mathbb{R}^{J_l}$ is a the r^{th} block−weight vector.
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Optimization criterion: From Sequential to Global

$$\underset{\mathbf{W}_1,\ldots,\mathbf{W}_L}{\operatorname{argmax}} \sum_{k,l=1}^{L} c_{kl} \operatorname{Trace}\Big(g\big(\operatorname{Cov}(\mathbf{X}_k \mathbf{W}_k, \mathbf{X}_l \mathbf{W}_l)\big)\Big) \qquad f(\mathbf{W}_1, \ldots, \mathbf{W}_L)$$

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Following the optimization framework of RGCCA, the core optimization problem is:

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- It is possible now to add constraints across components.

Cons:

- In this form, we have to extract the same number of component per block.

RGCCA framework - State of the Art

Constraints		Core Optimization Problem			Constraints
		$\max \nabla_l f(\mathbf{w}^s)^\top \mathbf{w}_l$			
	$\mathbf{w}_l \in \omega_l$	RGCCA[1,2]			
	$\begin{cases} \Vert\mathbf{w}_l\Vert_2^2 = 1 \\ \Vert\mathbf{w}_l\Vert_1 \leq s_l \end{cases}$	SGCCA[3]			
	$\begin{cases} \mathbf{w}_l = \mathbf{w}_l^K \otimes \mathbf{w}_l^J \\ \mathbf{w}_l \in \omega_l \end{cases}$	MGCCA[4]/TGCCA[5]			

$$\omega_l = \left\{\mathbf{w}_l \in \mathbb{R}^{J_l};\ \mathbf{w}_l^\top \mathbf{M}_l \mathbf{w}_l = 1\right\}$$

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RGCCA framework - State of the Art

Constraints	Core Optimization Problem		Constraints
	Sequential	Global	
	$\max \nabla_l f(\mathbf{w}^s)^\top \mathbf{w}_l$		
$\mathbf{w}_l \in \omega_l$	RGCCA[1,2]		
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Constraints	Core Optimization Problem			Constraints
	Sequential	**Global**		
	$\max \nabla_l f(\mathbf{w}^\mathbf{s})^\top \mathbf{w}_l$	$\max \mathbf{Tr}(\nabla_l f(\mathbf{W}^\mathbf{s})^\top \mathbf{W}_l)$		
$\mathbf{w}_l \in \omega_l$	RGCCA[1,2]			
$\begin{cases} \Vert\mathbf{w}_l\Vert_2^2 = 1 \\ \Vert\mathbf{w}_l\Vert_1 \leq s_l \end{cases}$	SGCCA[3]			
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		Core Optimization Problem			
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		$\max \boldsymbol{\nabla}_l f(\mathbf{w}^{\mathbf{s}})^\top \mathbf{w}_l$	$\max \mathbf{Tr}(\boldsymbol{\nabla}_l f(\mathbf{W}^{\mathbf{s}})^\top \mathbf{W}_l)$		
Constraints	$\mathbf{w}_l \in \omega_l$	RGCCA[1,2]	Global RGCCA[6,7]	$\mathbf{W}_l \in \Omega_l$	Constraints
	$\begin{cases} \lVert\mathbf{w}_l\rVert_2^2 = 1 \\ \lVert\mathbf{w}_l\rVert_1 \leq s_l \end{cases}$	SGCCA[3]			
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	$\max \boldsymbol{\nabla}_l f(\mathbf{w}^{\mathbf{s}})^\top \mathbf{w}_l$	$\max \mathbf{Tr}(\boldsymbol{\nabla}_l f(\mathbf{W}^{\mathbf{s}})^\top \mathbf{W}_l)$	
Constraints: $\mathbf{w}_l \in \omega_l$	RGCCA[1,2]	Global RGCCA[6,7]	Constraints: $\mathbf{W}_l \in \Omega_l$
$\begin{cases} \Vert\mathbf{w}_l\Vert_2^2 = 1 \\ \Vert\mathbf{w}_l\Vert_1 \leq s_l \end{cases}$	SGCCA[3]		
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		$\max \boldsymbol{\nabla}_l f(\mathbf{w}^s)^\top \mathbf{w}_l$	$\max \mathbf{Tr}(\boldsymbol{\nabla}_l f(\mathbf{W}^s)^\top \mathbf{W}_l)$		
Constraints	$\mathbf{w}_l \in \omega_l$	RGCCA[1,2]	Global RGCCA[6,7]	$\mathbf{W}_l \in \Omega_l$	Constraints
	$\begin{cases} \Vert\mathbf{w}_l\Vert_2^2 = 1 \\ \Vert\mathbf{w}_l\Vert_1 \leq s_l \end{cases}$	SGCCA[3]			
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		Core Optimization Problem			
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		$\max \boldsymbol{\nabla}_l f(\mathbf{w^s})^\top \mathbf{w}_l$	$\max \mathbf{Tr}(\boldsymbol{\nabla}_l f(\mathbf{W^s})^\top \mathbf{W}_l)$		
Constraints	$\mathbf{w}_l \in \omega_l$	RGCCA[1,2]	Global RGCCA[6,7]	$\mathbf{W}_l \in \Omega_l$	Constraints
	$\begin{cases} \lVert\mathbf{w}_l\rVert_2^2 = 1 \\ \lVert\mathbf{w}_l\rVert_1 \leq s_l \end{cases}$	SGCCA[3]			
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	Structured Sparsity				

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Core Optimization Problem

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$\mathbf{w}_l \in \omega_l$	RGCCA[1,2]	Global RGCCA[6,7]	$\mathbf{W}_l \in \Omega_l$
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Structured Sparsity	(i). Group-Lasso in the same framework[8] (ii). Other structured sparse penalties in other frameworks[6,9,10,11]		

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Constraints	Core Optimization Problem: Sequential	Core Optimization Problem: Global	Constraints
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<u>Missing Values in RGCCA (Peltier et al., 2023).</u>

RGCCA

https://github.com/rgcca-factory/RGCCA

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Here are the contributors of the actual version of the package !!

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Laboratoire Des Signaux Et Systèmes, CentraleSupélec
➔ Soon in Cantini's Lab at Pasteur (and PhD since yesterday!!)

Laurent LE BRUSQUET
Laboratoire Des Signaux Et Systèmes, CentraleSupélec

Etienne Camenen
INSERM, Hôpital Saint-Louis AP-HP

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Vincent GUILLEMOT
Institut Pasteur, Bioinformatics and Biostatistics Hub

Arnaud GLOAGUEN
Centre National de Recherche en Génomique Humaine, CEA

Other perpectives ?

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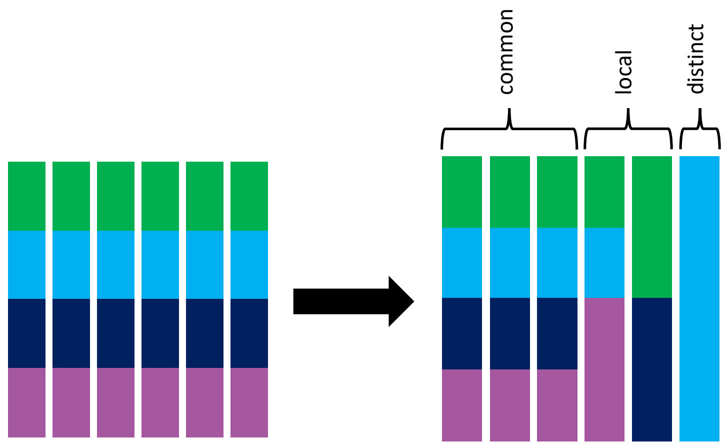
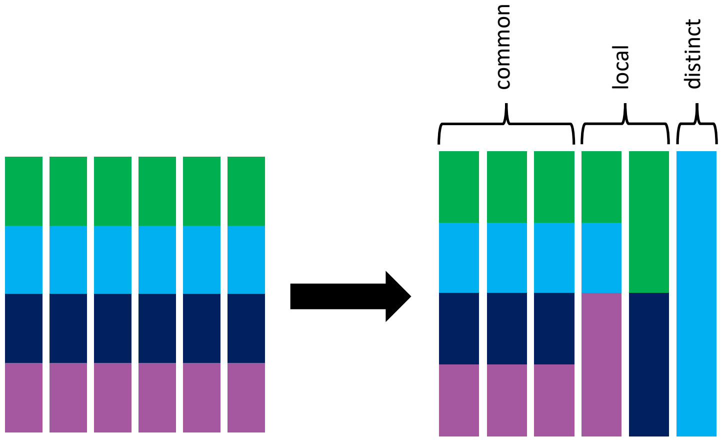
<u>Axe 1: Use comon and specific information</u>



Other perpectives ?

Axe 1: Use comon and specific information

Vary the combination of omics data from which components are built.



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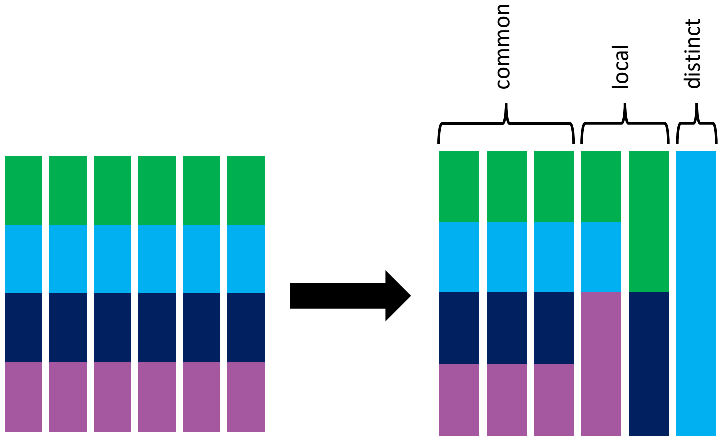

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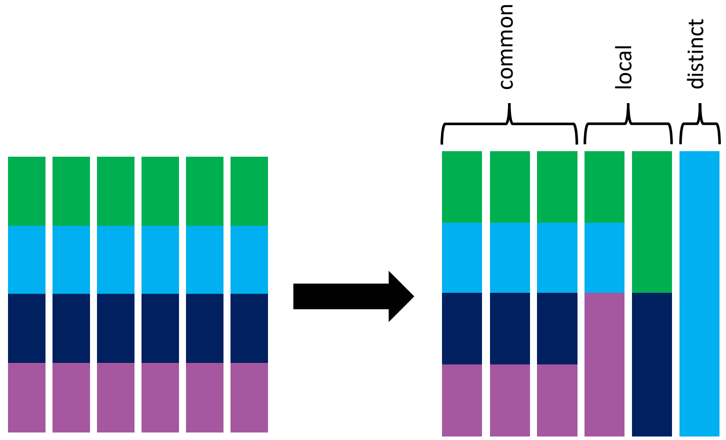
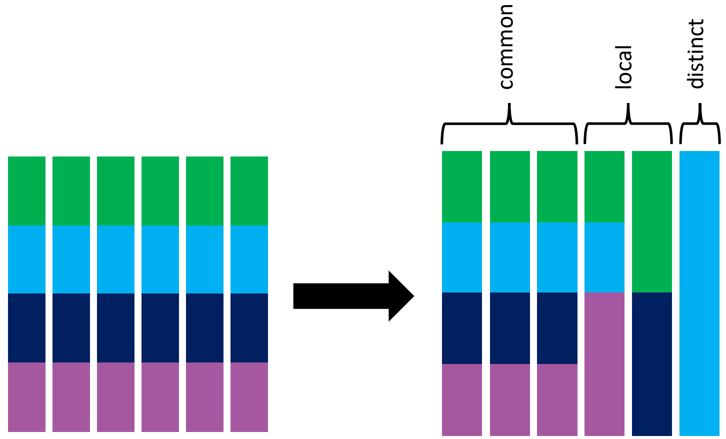


Axe 2: Include the appartenance of each variable to a biological pathway.

Divide each omic matrix by biological pathways.

Allow to identify most important pathways (With L1 norm).

Other perpectives ?



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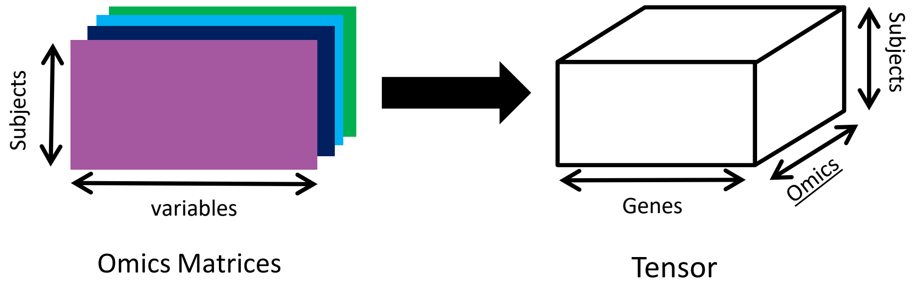
Axe 3: Link variables across different omics

Regroup omic matrices along the third dimension (ex: by genes) to create a tensor.

Permet d'ajouter une notion biologique dans la définition du modèle



Courtesy to Vincent Le Goff.

Other perpectives ?

PhD of Vincent LE GOFF

Supervised by:

- **Edith Le Floch**
- **Vincent Guillemot**
- **Arnaud Gloaguen**

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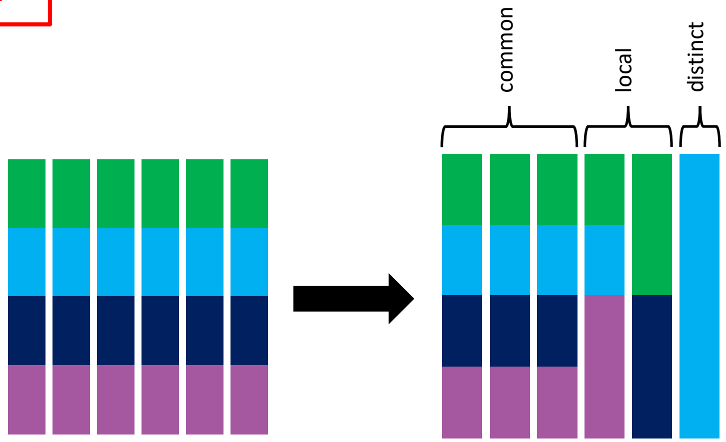

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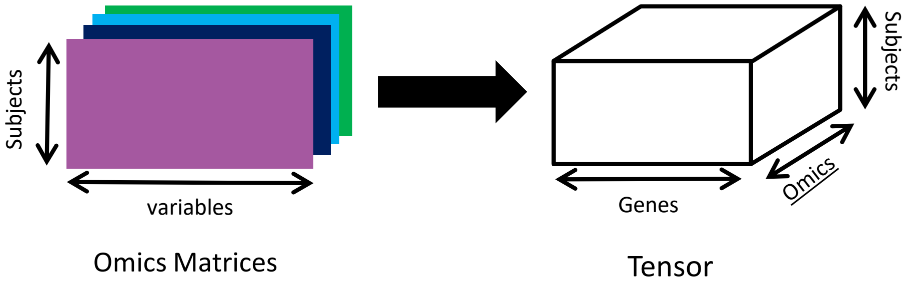

Courtesy to Vincent Le Goff.

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David Cohen
Bruno Etain
Cynthia Marie-Clair
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Belzeaux Raoul
Gascon Gonzalo
Isabelle Mansuy

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Olivier Sand
Grégoire Rossier
Jimmy Vandel
Guillemette Marot
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Morgane Terezol
Anaïs Baudot
Maxime Delmas
Jean-Clément Gallardo
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Julie Aubert
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Helene Touzet
Justine Merlan

Slides:

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Laurent Le Brusquet
Julien Bect
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QUESTIONS ?