Analysis of a cohort of Major Depressive Disorder (MDD) with Regularized Generalized Canonical Correlation Analysis (RGCCA)

Arnaud Gloaguen, Jimmy Vandel

1. Introduction of the case study

Case Study: Major Depressive Disorder (MDD)

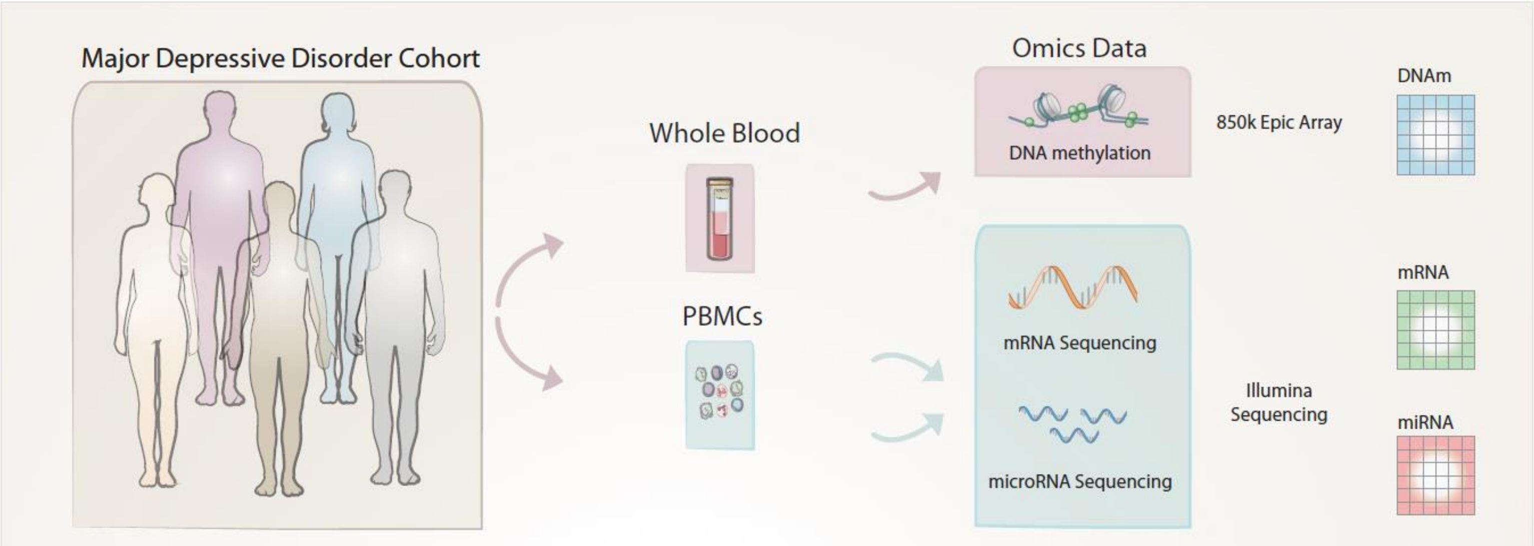
Cohort Description

a

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**							

Data Collection

b



Taken from Amazigh Mokhtari's PhD manuscript.

Case Study: Covariates

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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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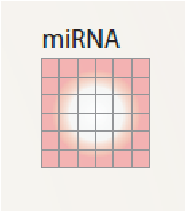

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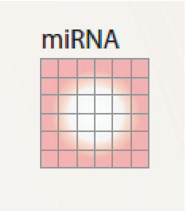

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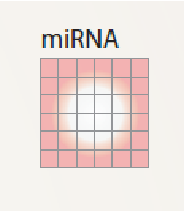

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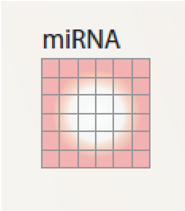

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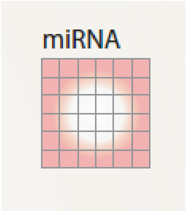

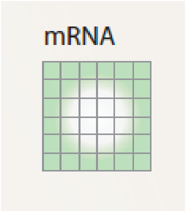

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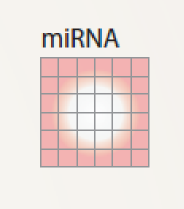

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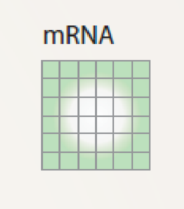

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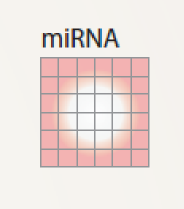

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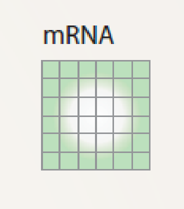

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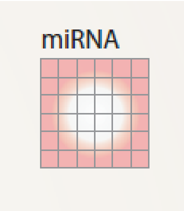

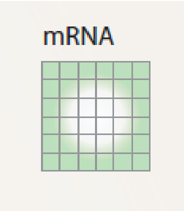

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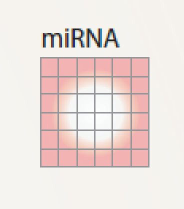

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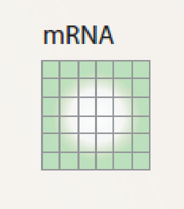

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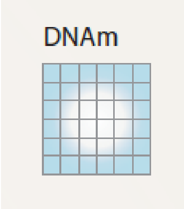

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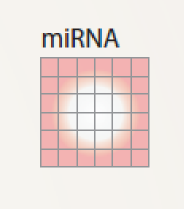

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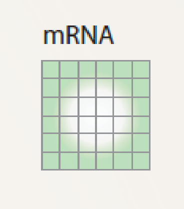

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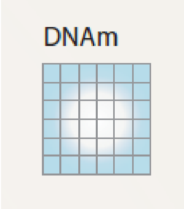

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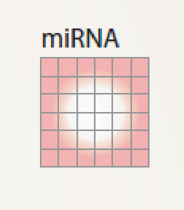

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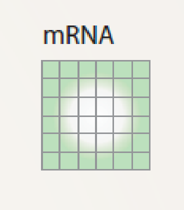

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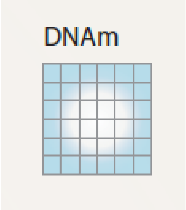

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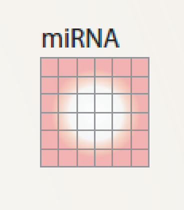

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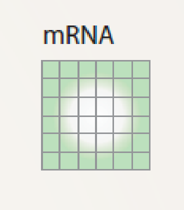

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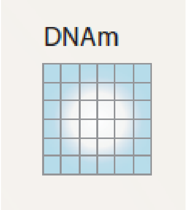

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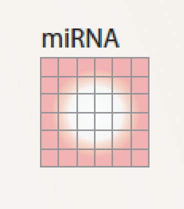

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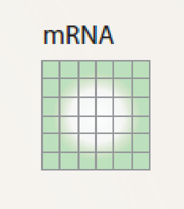

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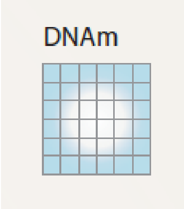

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Finally: individuals common to ALL omics data are kept.

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2. Unsupervised analysis with one-block

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Let us consider two samples $(x_1, \dots, x_n)$ and $(y_1, \dots, y_m)$. They both represent the same continuous variable but are separated by the value of the discrete one.

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$$\begin{cases} \mathrm{H_0}: (\mathrm{x_1}, \dots, \mathrm{x_n}) \text{ and } (\mathrm{y_1}, \dots, \mathrm{y_m}) \text{ comes from the same distribution.} \\ \end{cases}$$

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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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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 ➔ $RSS_0 \sim RSS_1$ ➔ $F \sim 0$

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: $\begin{cases} \mathrm{H}_0: \beta_1 = 0, \\ \mathrm{H}_1: \beta_1 \neq 0 \end{cases}$

With the statistic:

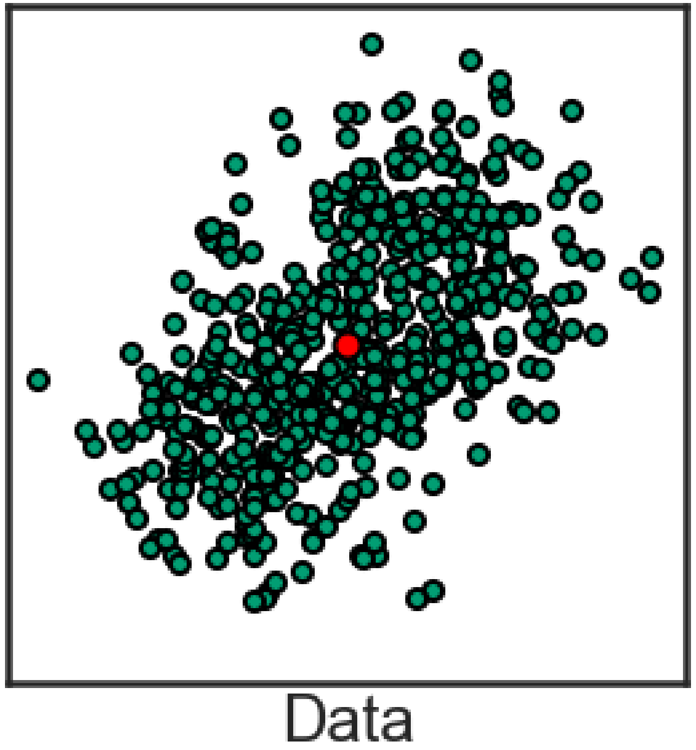
$$F = \frac{(RSS_0 - RSS_1)}{1} \times \frac{(n-2)}{RSS_1} = \frac{(\sum_i (y_i - \beta_0)^2 - \sum_i (y_i - \beta_0 - \beta_1 x_i)^2)}{1} \times \frac{(n-2)}{\sum_i (y_i - \beta_0 - \beta_1 x_i)^2}$$

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

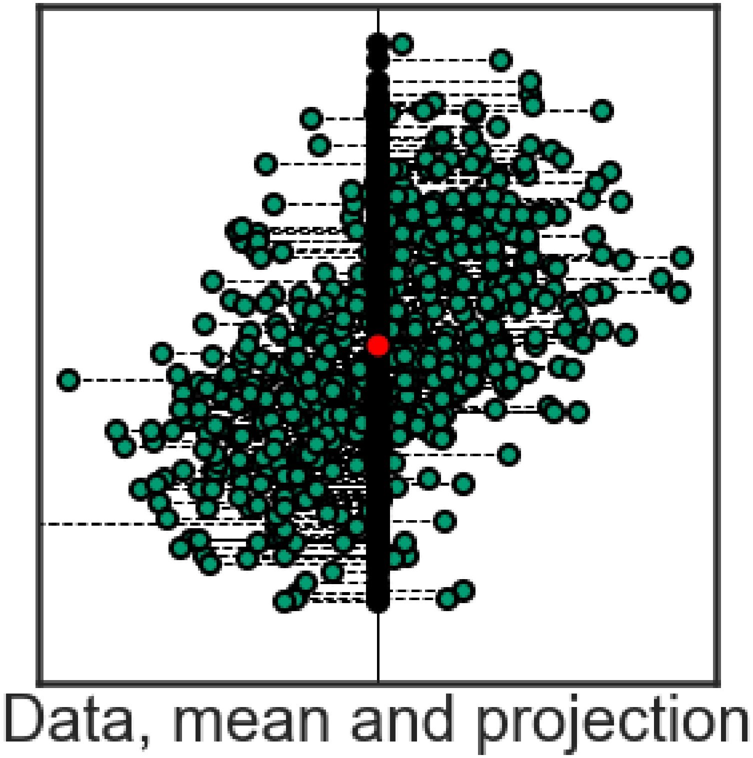
If the variables are strongly linked ➔ $RSS_0 \gg RSS_1$ ➔ $F \sim \frac{RSS_0}{RSS_1} \times (n-2) \gg n-2$ ➔ The test is likely to be rejected.

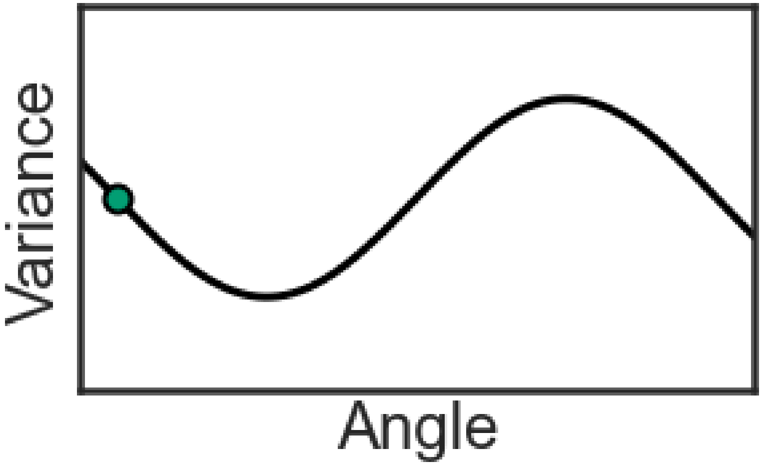
If the variables are NOT strongly linked ➔ $RSS_0 \sim RSS_1$ ➔ $F \sim 0$ ➔ The test is likely to be accepted.

Principle of Principal Component Analysis (PCA)

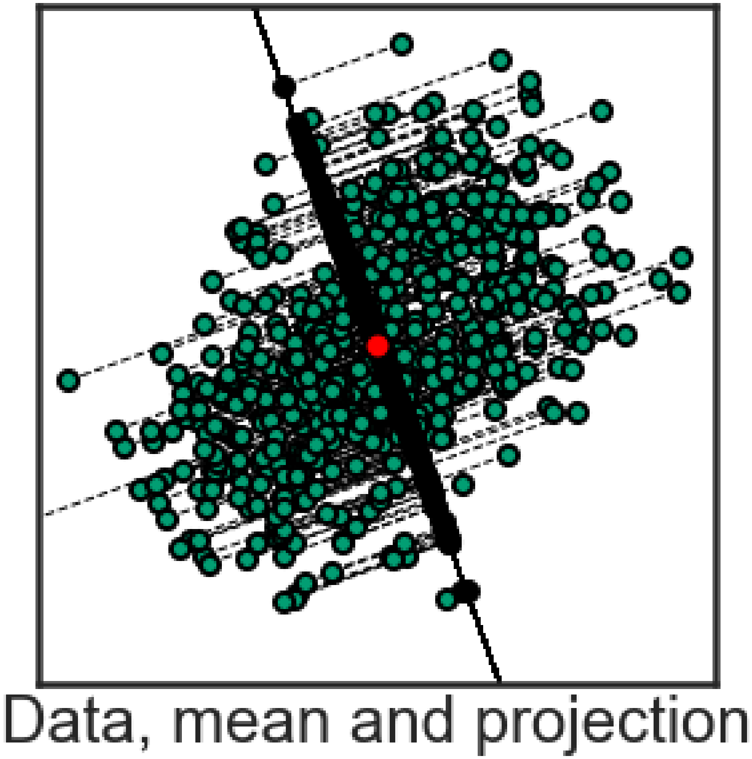


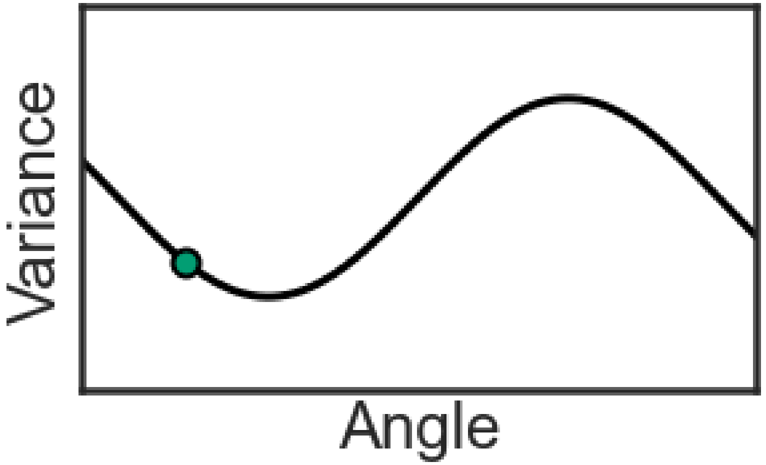
Principle of Principal Component Analysis (PCA)





Principle of Principal Component Analysis (PCA)





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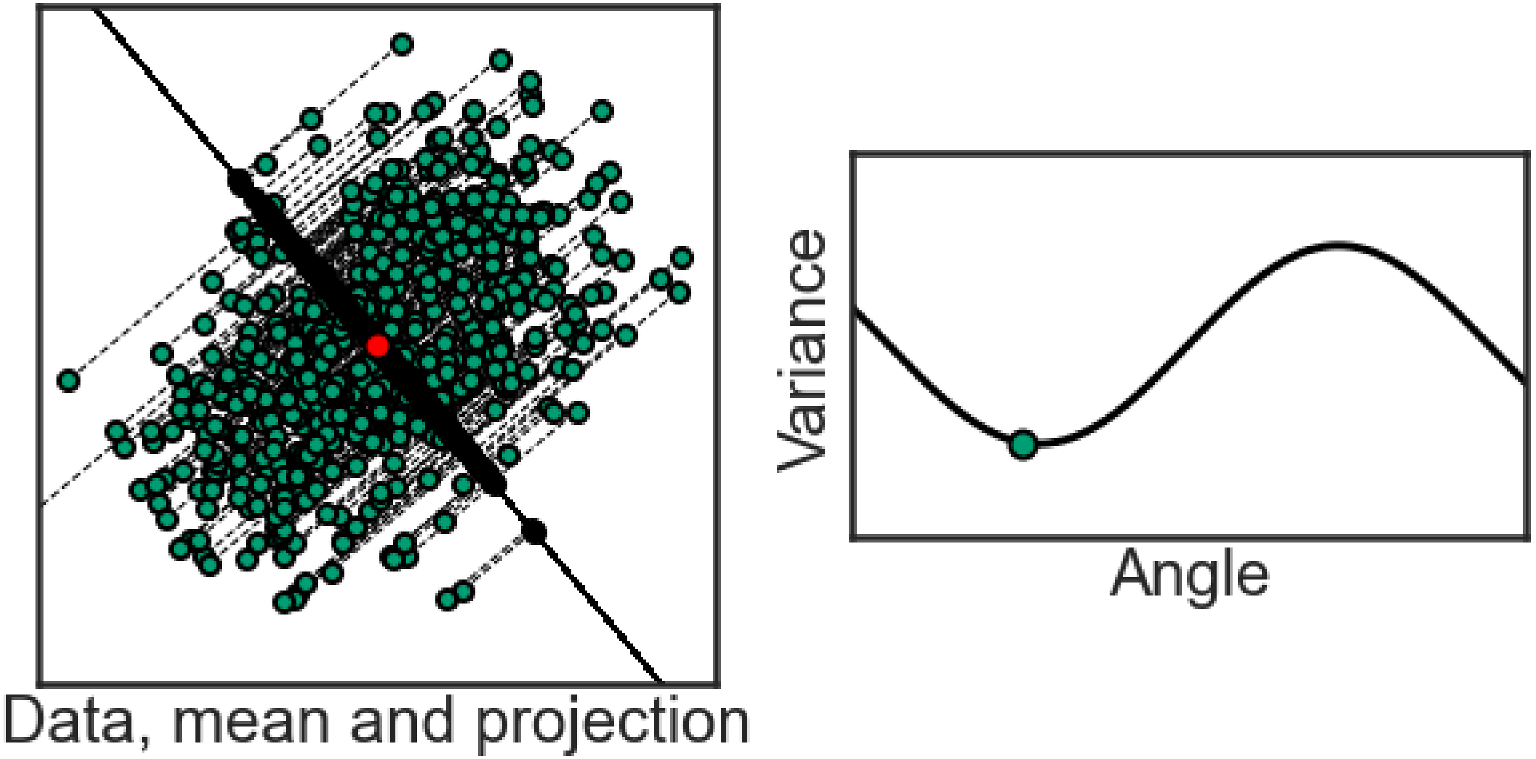

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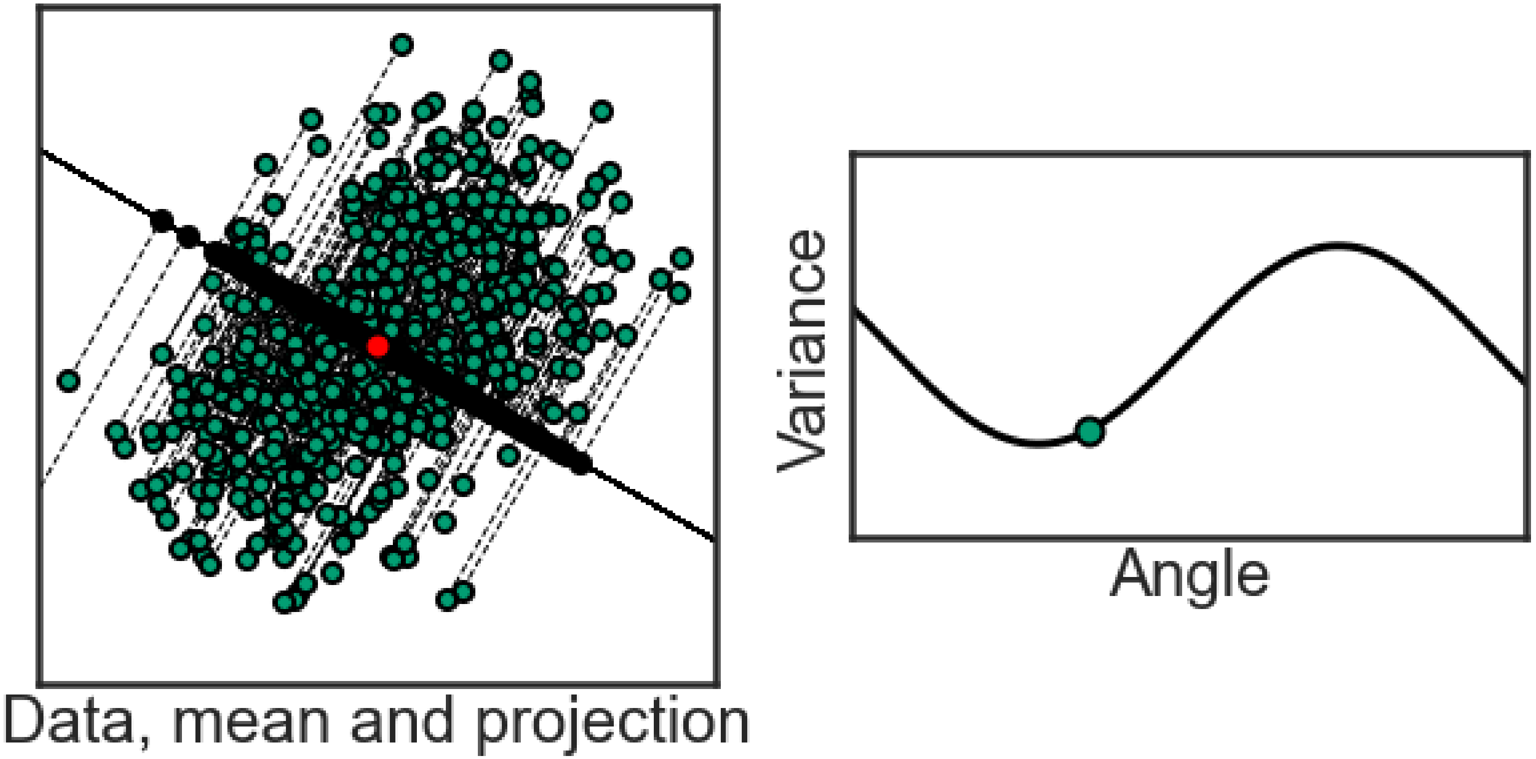
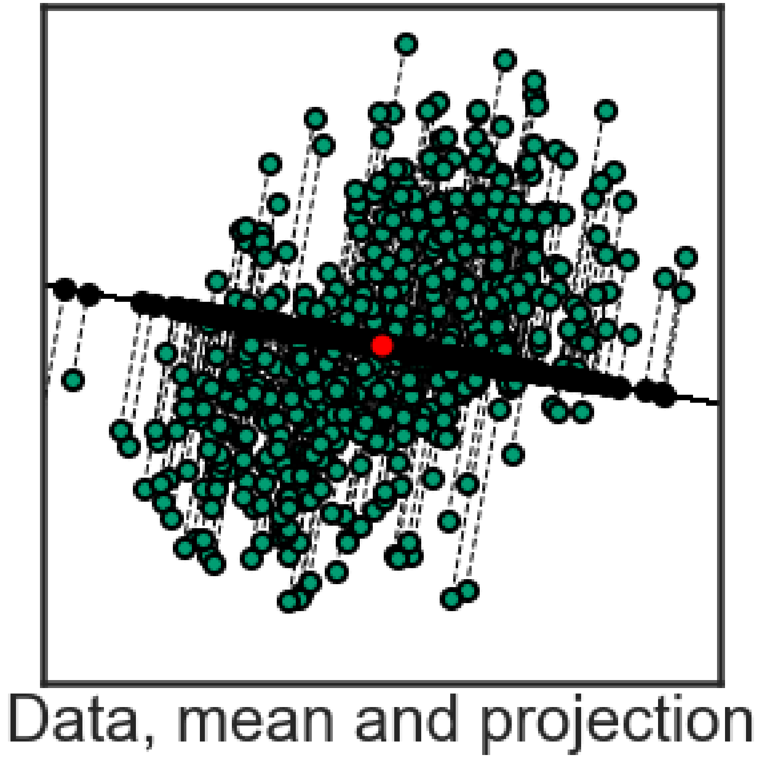
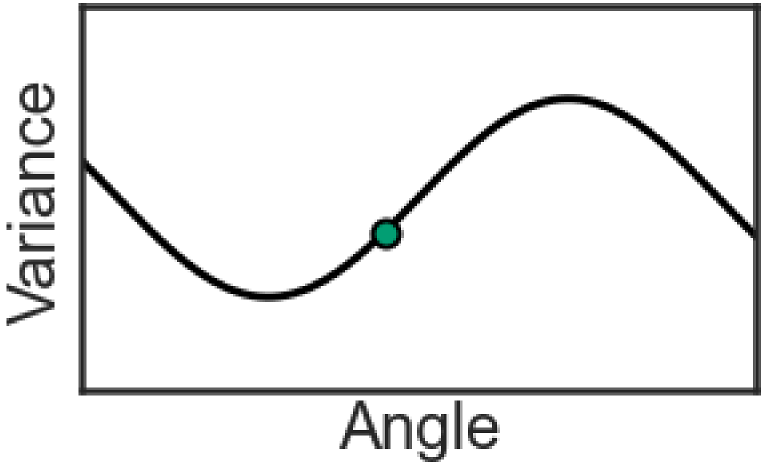
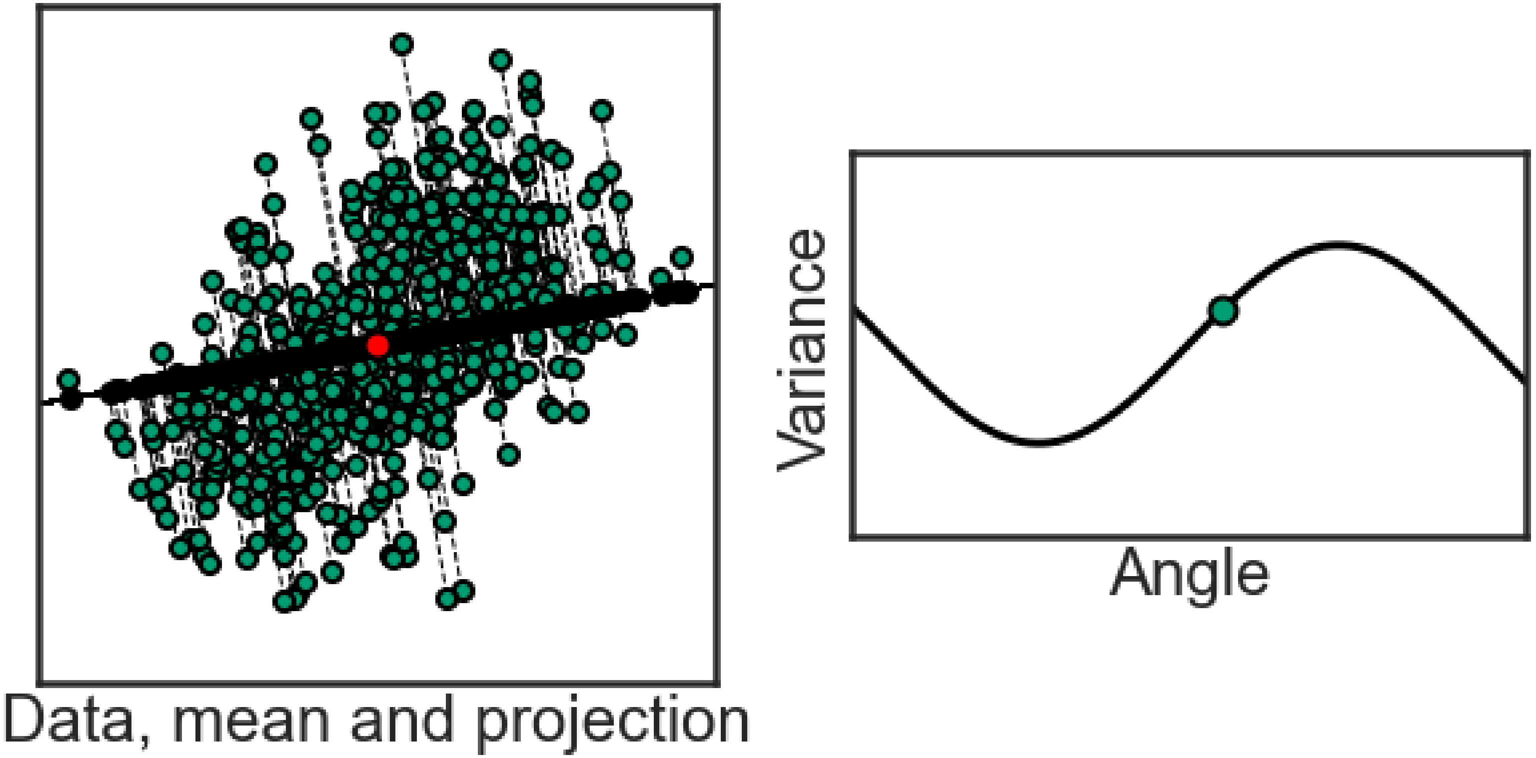


Principle of Principal Component Analysis (PCA)

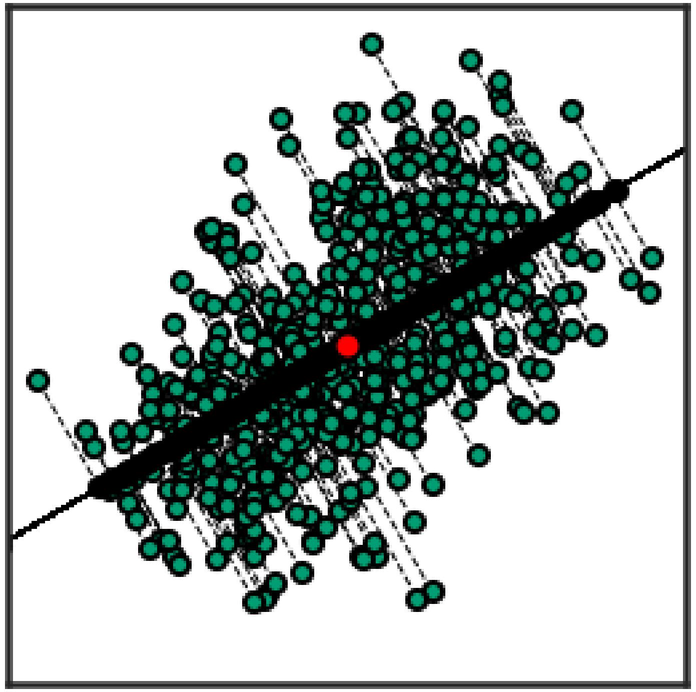




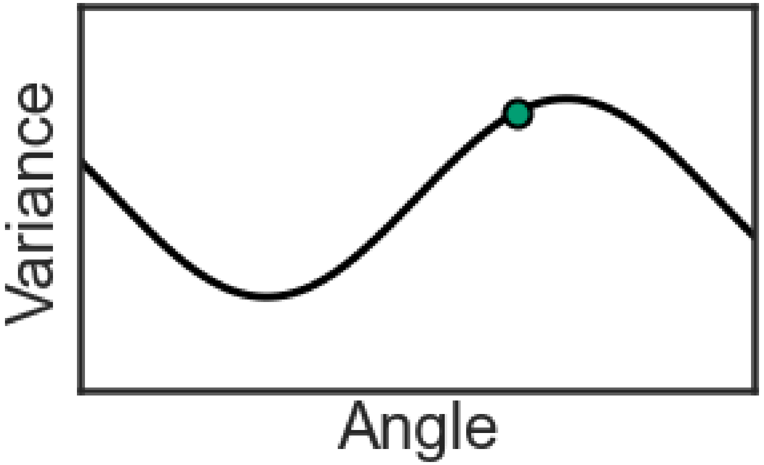
Principle of Principal Component Analysis (PCA)



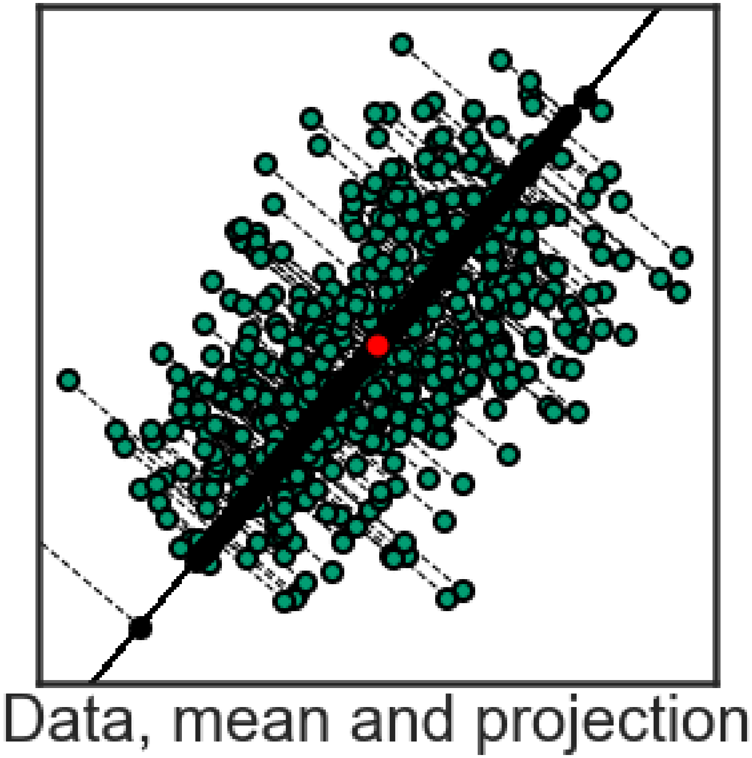
Principle of Principal Component Analysis (PCA)

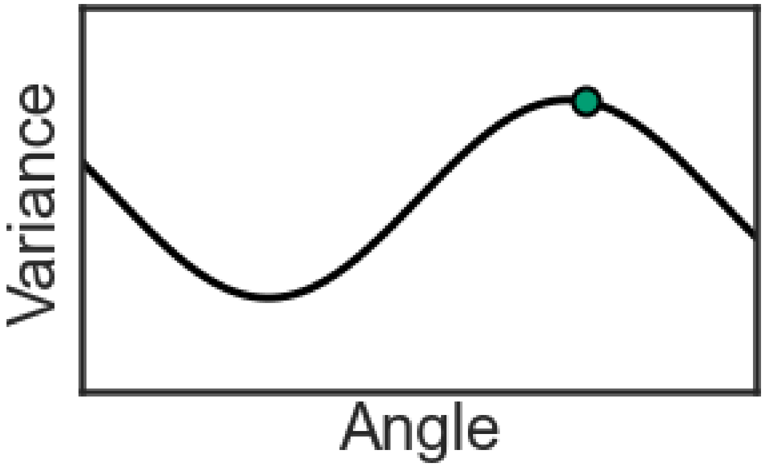


Data, mean and projection

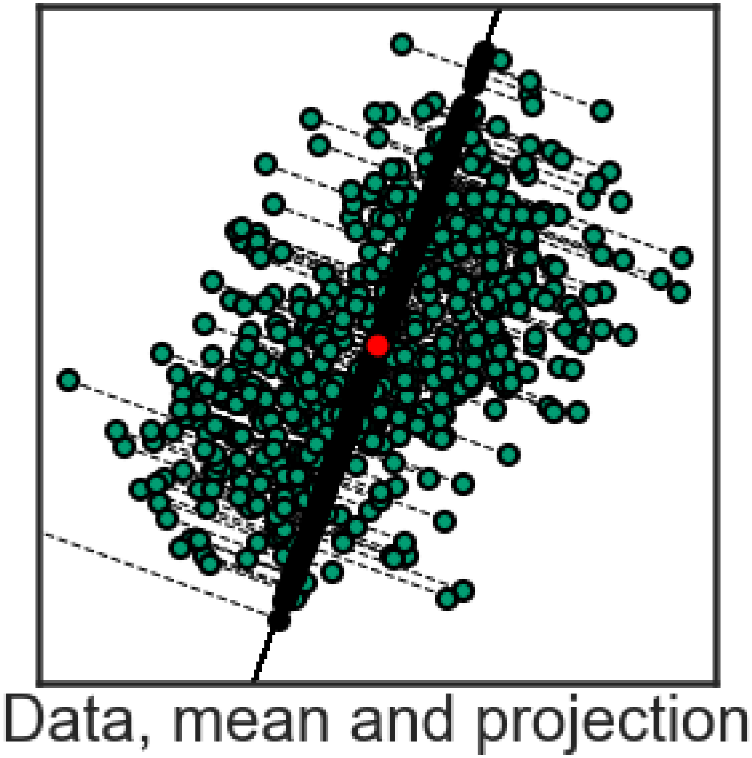


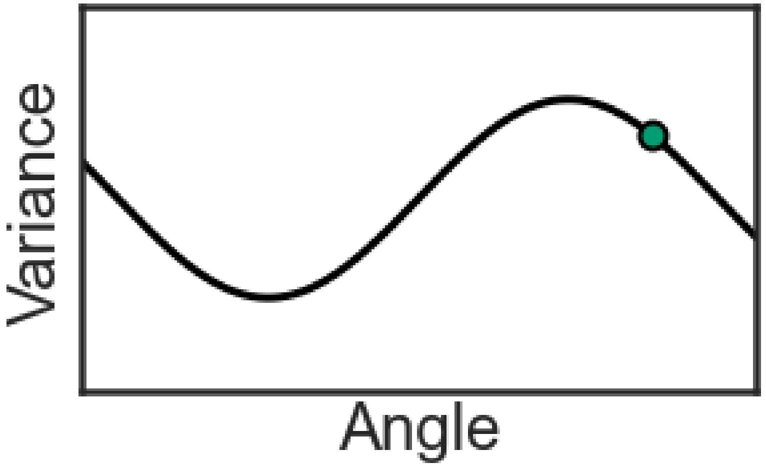
Principle of Principal Component Analysis (PCA)





Principle of Principal Component Analysis (PCA)





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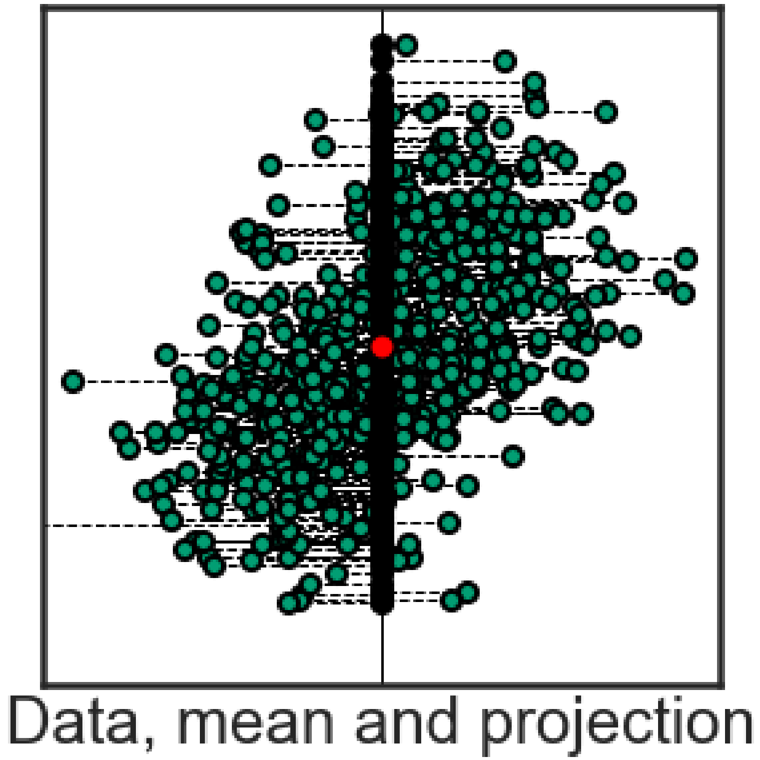

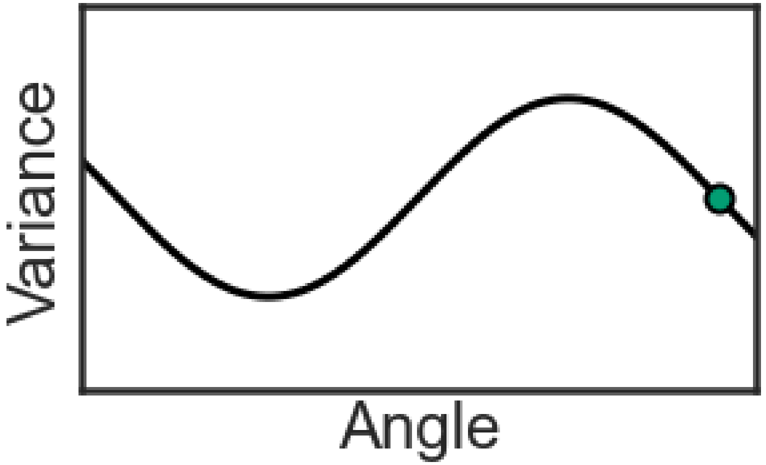

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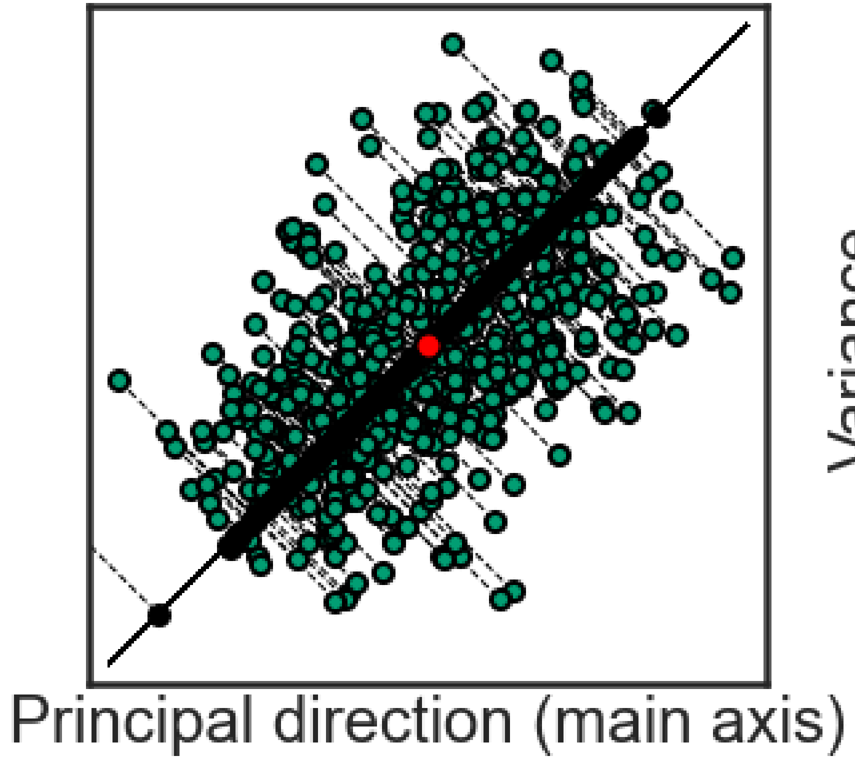

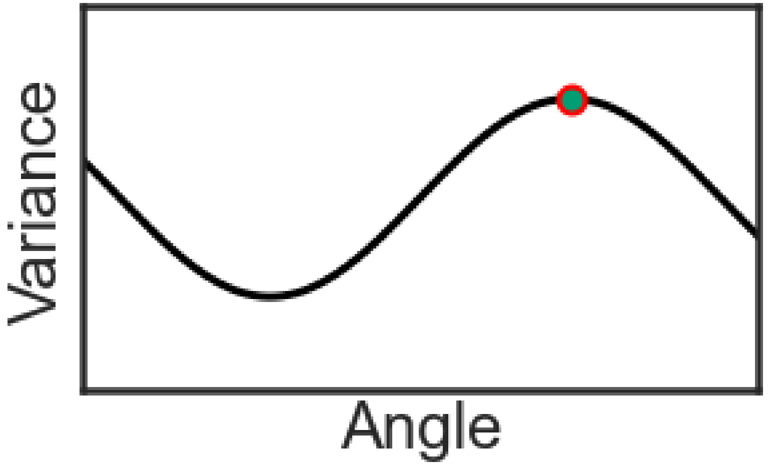

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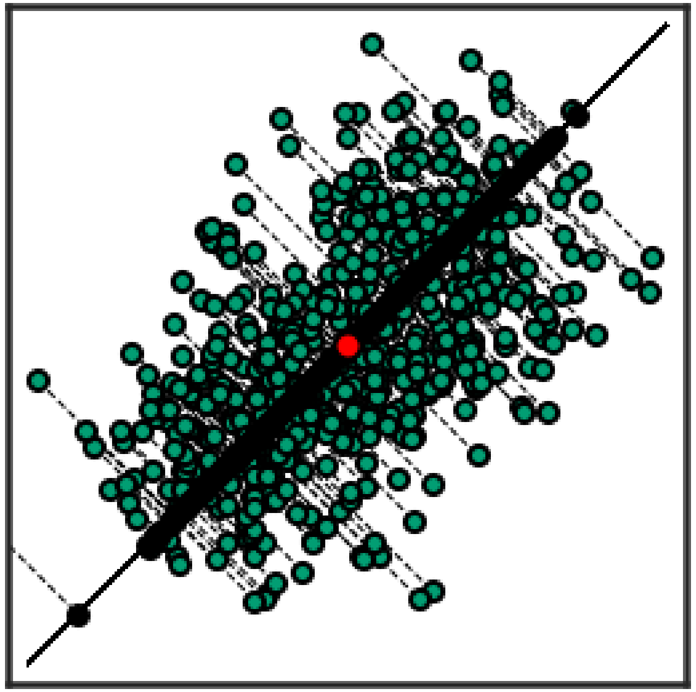
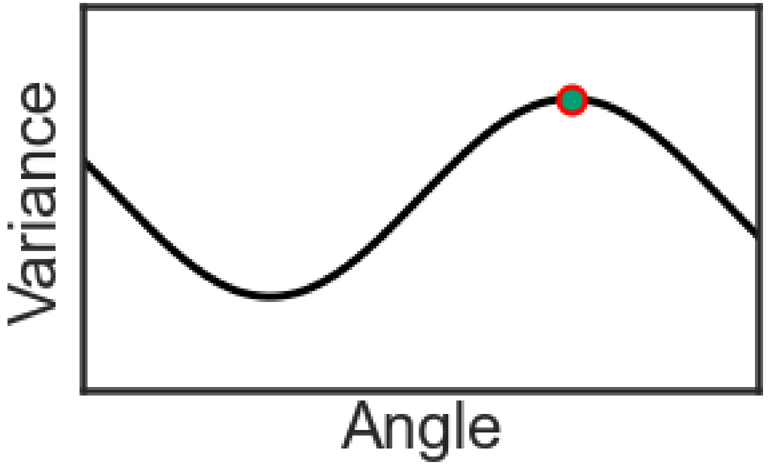


Principal direction (main axis)



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

$$\overset{p \text{ variables}}{\longleftrightarrow}$$

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

Total Variance

n individuals/subjects

p variables

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

Total Variance

n individuals/subjects

p variables

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

Total Variance

n individuals/subjects

p variables

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

Total Variance

n individuals/subjects

p variables

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

Total Variance (TV)

Total Variance

n individuals/subjects

p variables

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

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

Total Variance

n individuals/subjects

p variables

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

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

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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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

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

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

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

Total Variance

n individuals/subjects

p variables

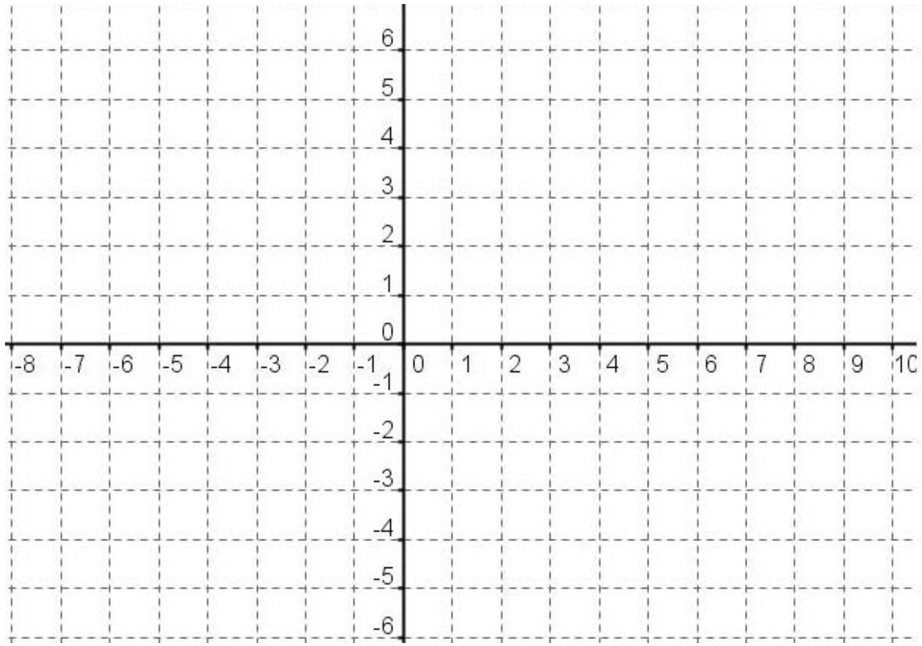
$$\mathbf{X} = \begin{pmatrix} x_{11} & \cdots & x_{1p} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{np} \end{pmatrix} = \begin{pmatrix} \mathbf{x}_1^\top \\ \mathbf{x}_2^\top \\ \vdots \\ \mathbf{x}_n^\top \end{pmatrix} \text{ where } \mathbf{x}_\mathrm{i} = \begin{pmatrix} x_{i1} \\ x_{i2} \\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

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

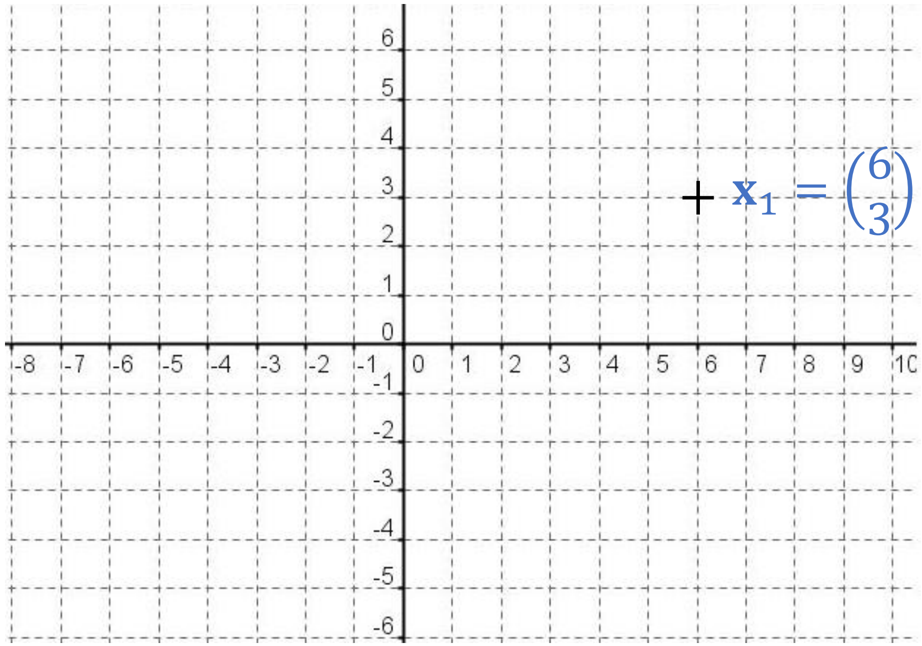
$$= \frac{1}{n}\sum_{i=1}^{n}\left\|\begin{pmatrix} x_{i1} \\ x_{i2} \\ \vdots \\ x_{ip} \end{pmatrix} - \begin{pmatrix} \overline{x_1} \\ \overline{x_2} \\ \vdots \\ \overline{x_p} \end{pmatrix}\right\|_2^2 = \frac{1}{n}\sum_{i=1}^{n}\|\mathbf{x}_\mathrm{i} - \bar{\mathbf{x}}\|_2^2$$

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

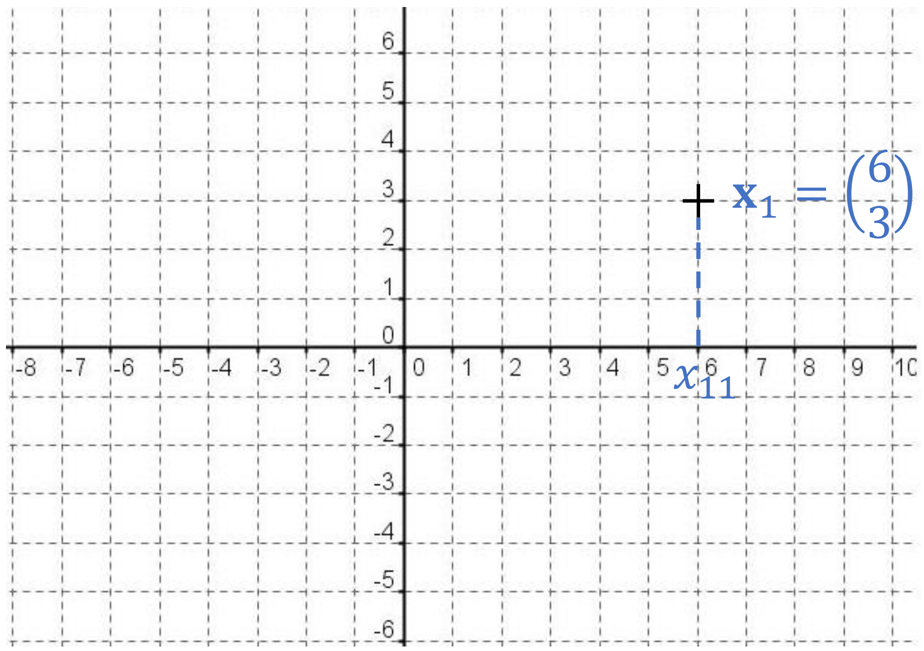
Total Variance – Example in 2D



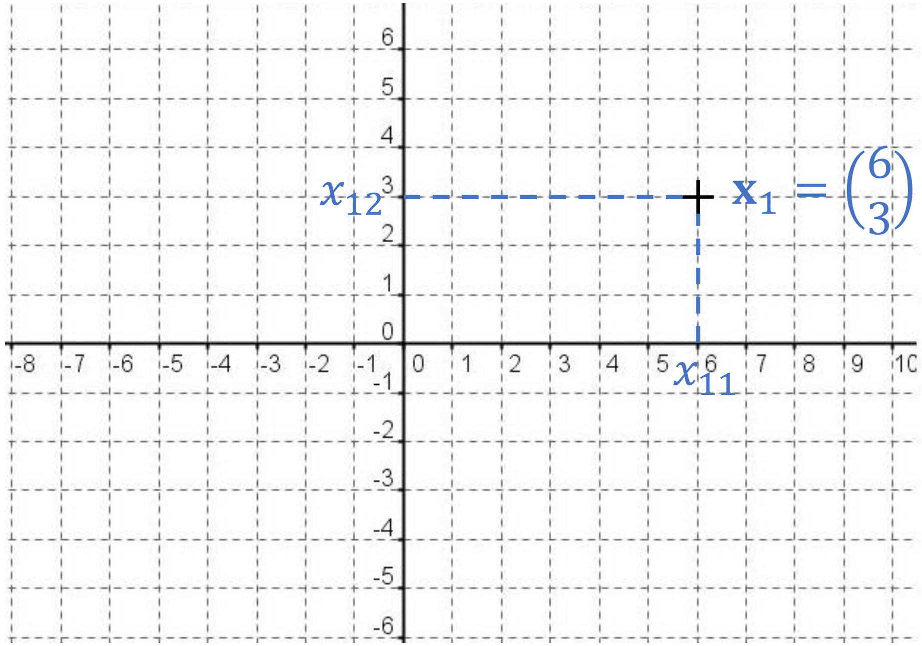
Total Variance – Example in 2D



Total Variance – Example in 2D

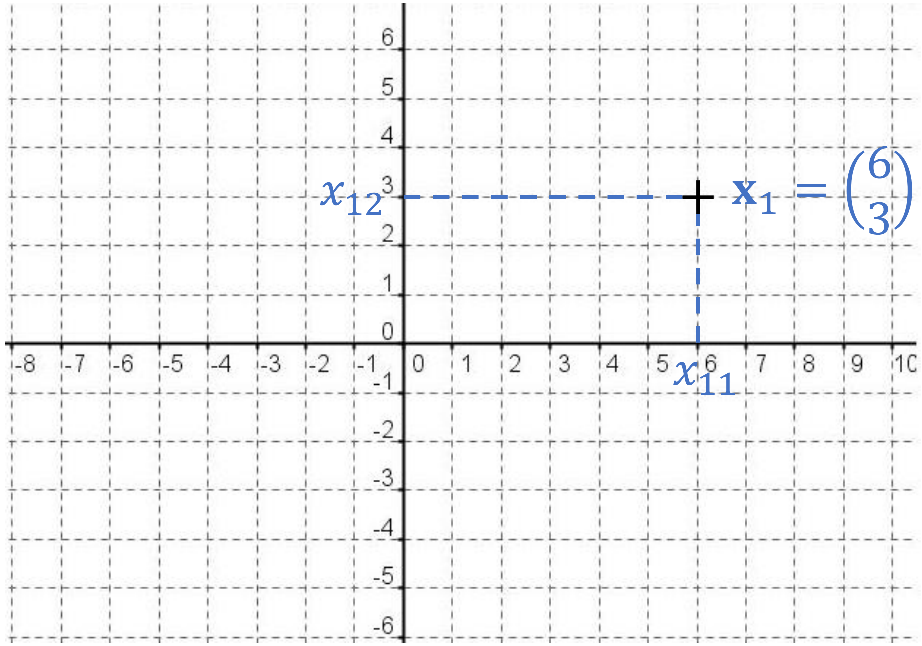


Total Variance – Example in 2D



Total Variance – Example in 2D

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



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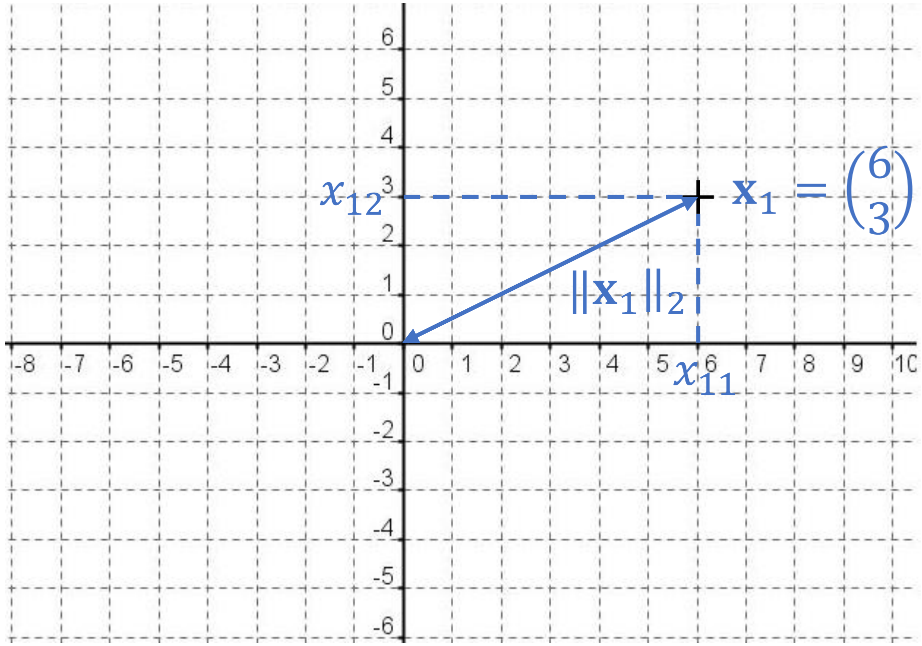

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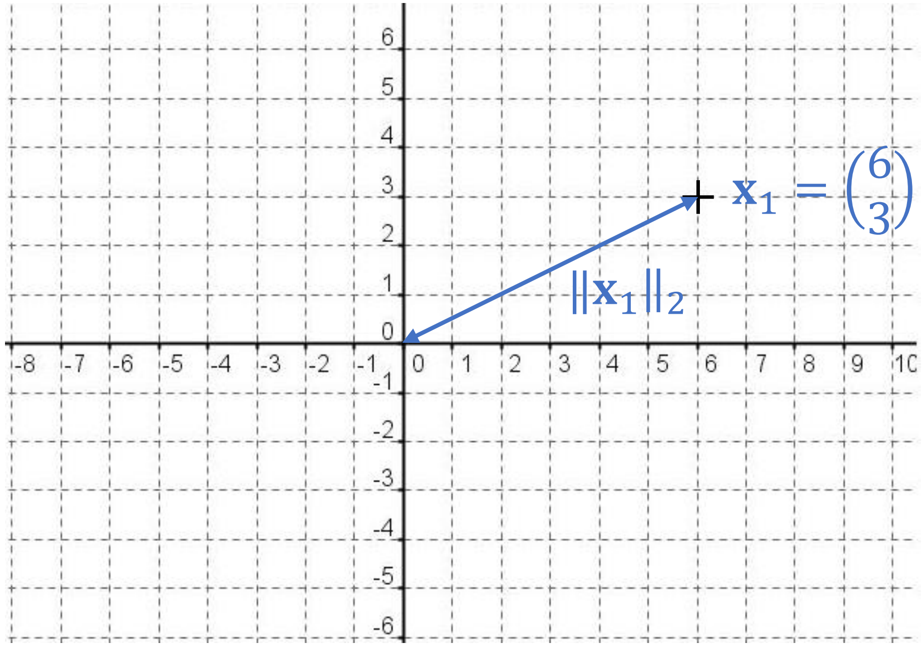
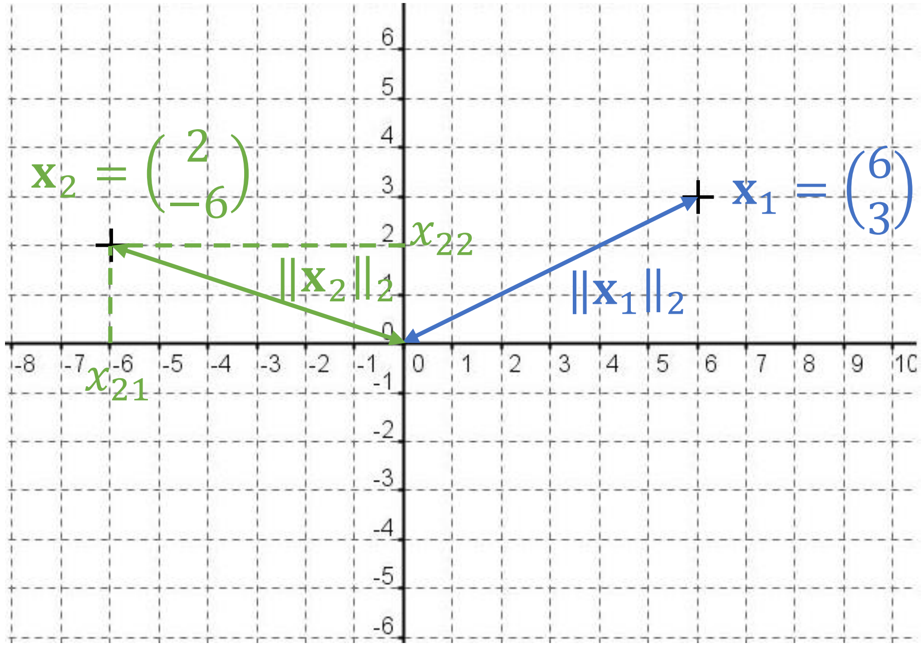


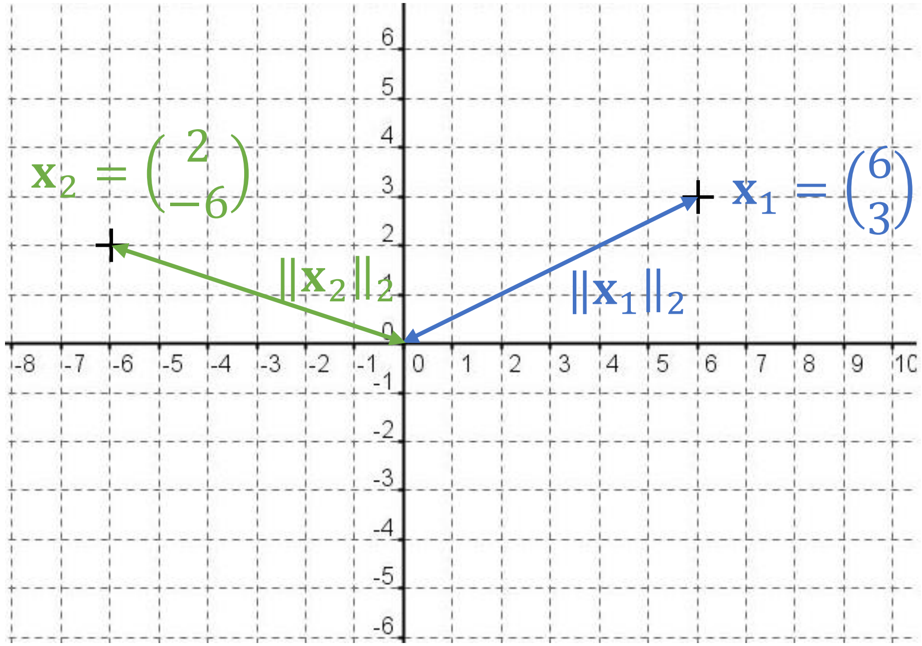
Total Variance – Example in 2D

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



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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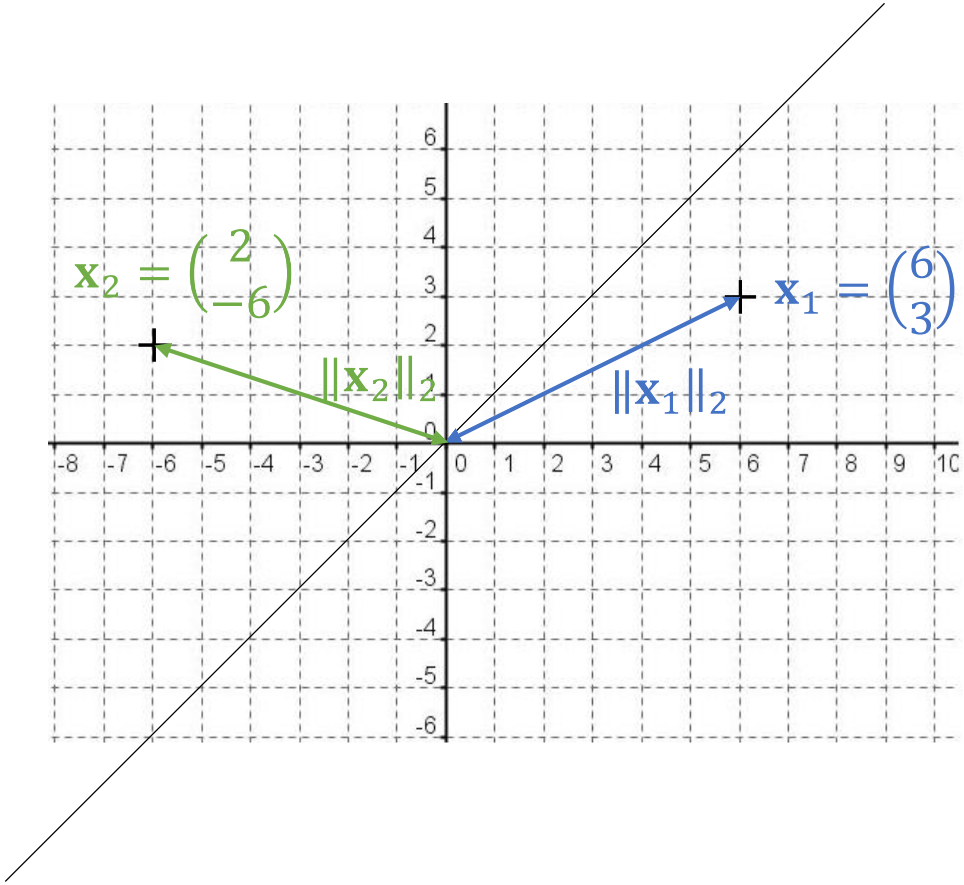

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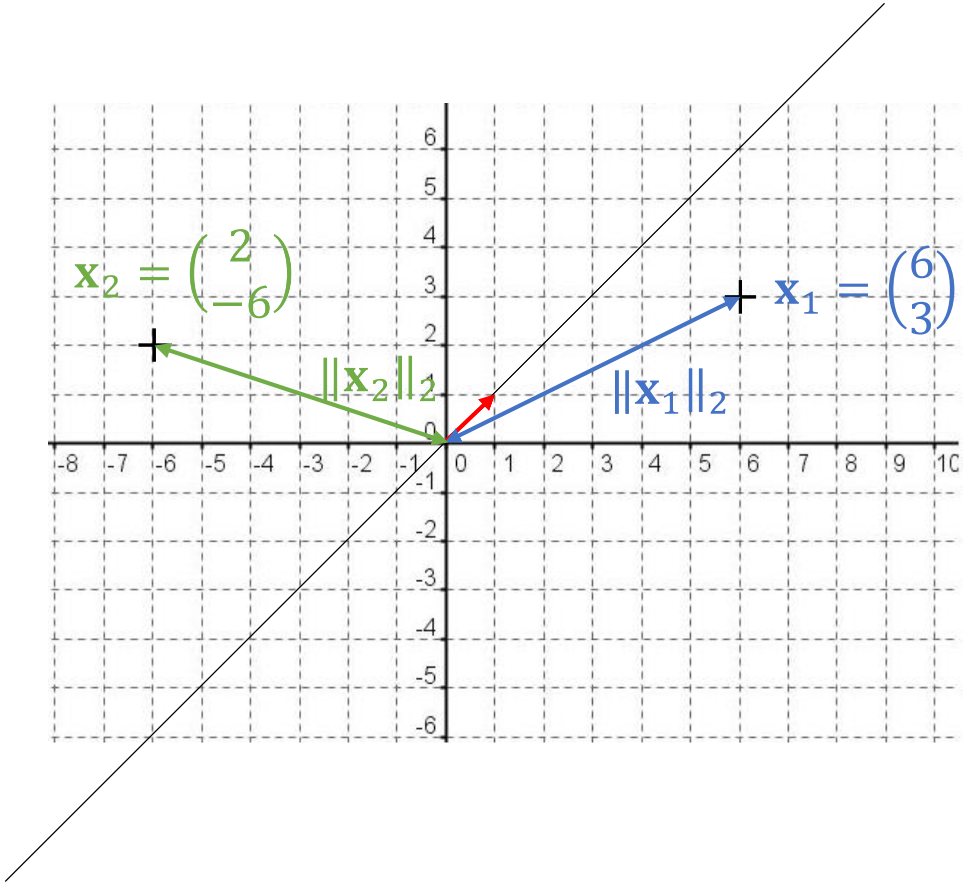
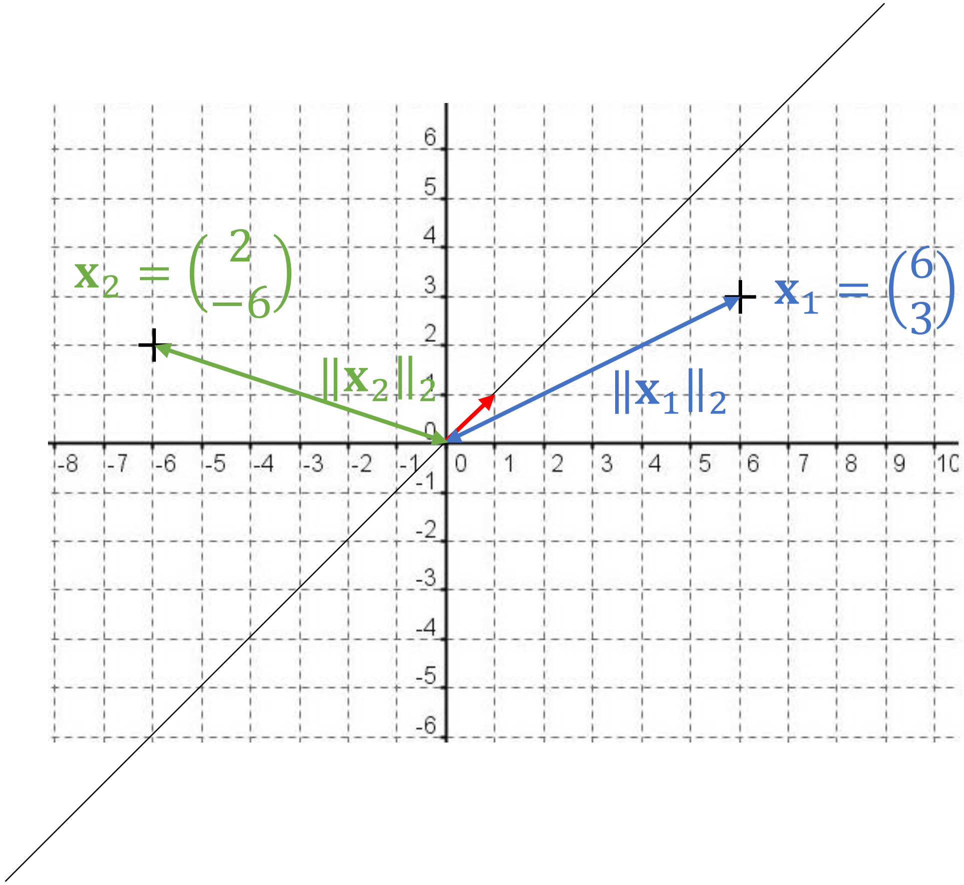


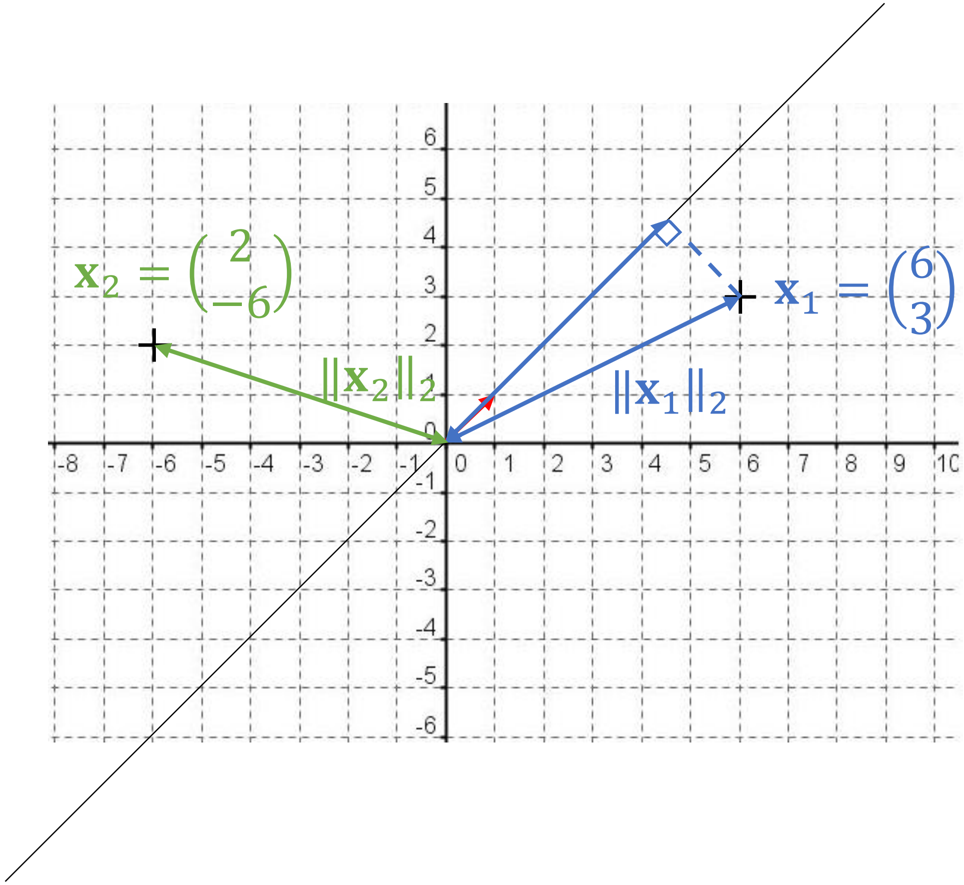
Total Variance – Example in 2D



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

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



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

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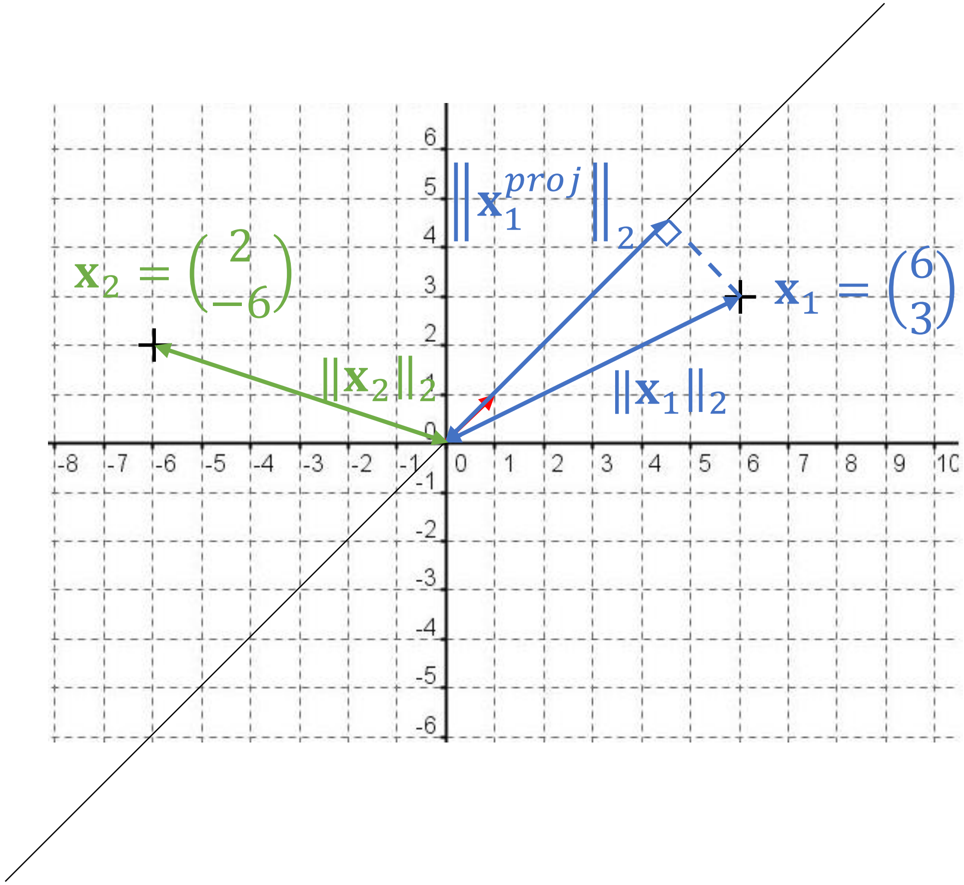
Total Variance – Example in 2D



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

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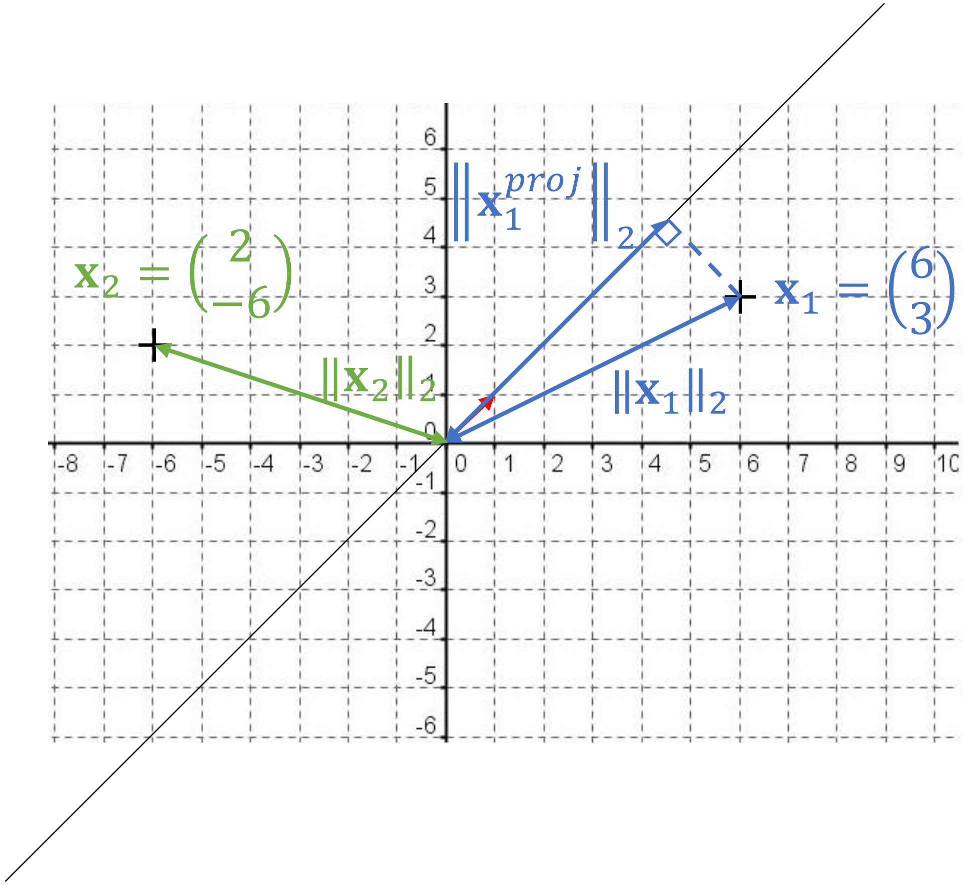

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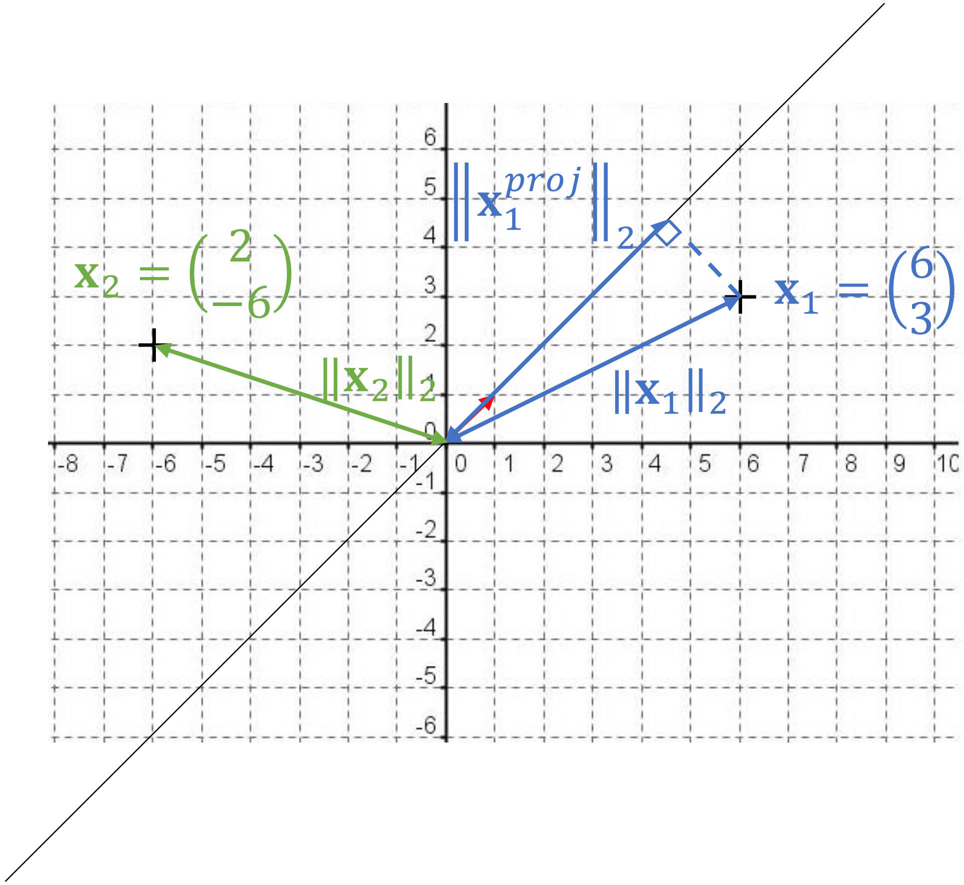
$\mathbf{x}_1^\top \mathbf{w}$

Total Variance – Example in 2D

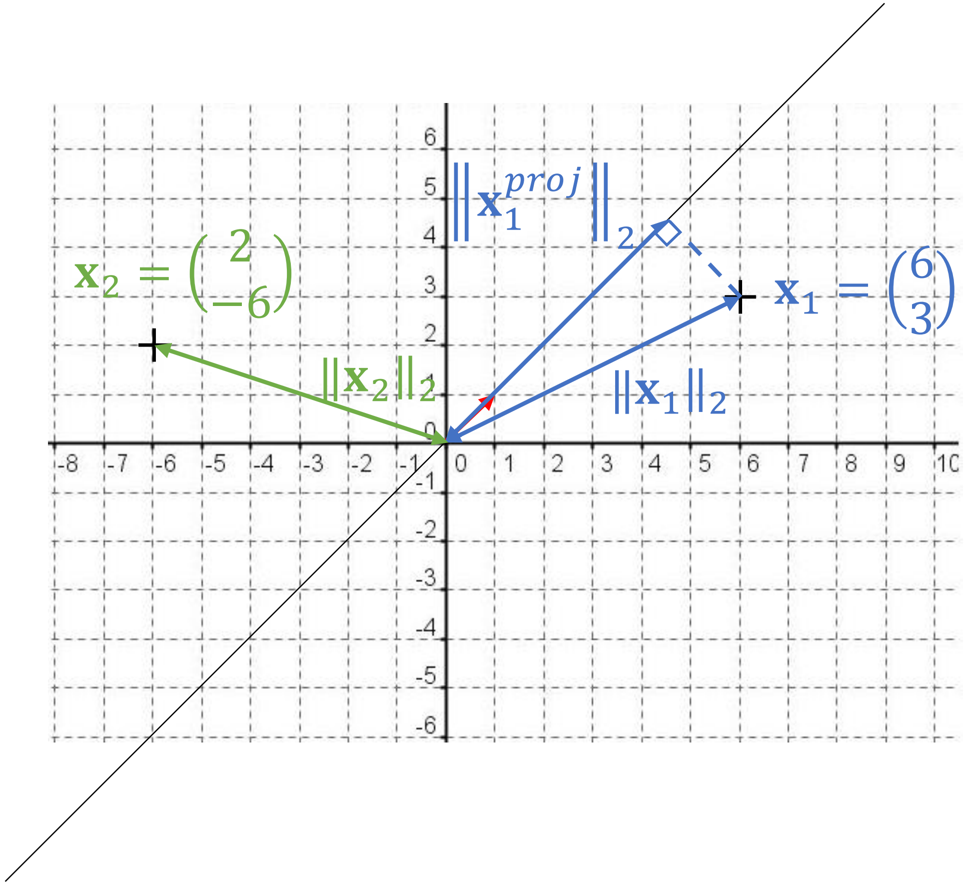


$\|\mathbf{x}_1\|_2 = \sqrt{x_{11}^2 + x_{12}^2}$ $\|\mathbf{x}_2\|_2 = \sqrt{x_{21}^2 + x_{22}^2}$

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

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

Total Variance – Example in 2D



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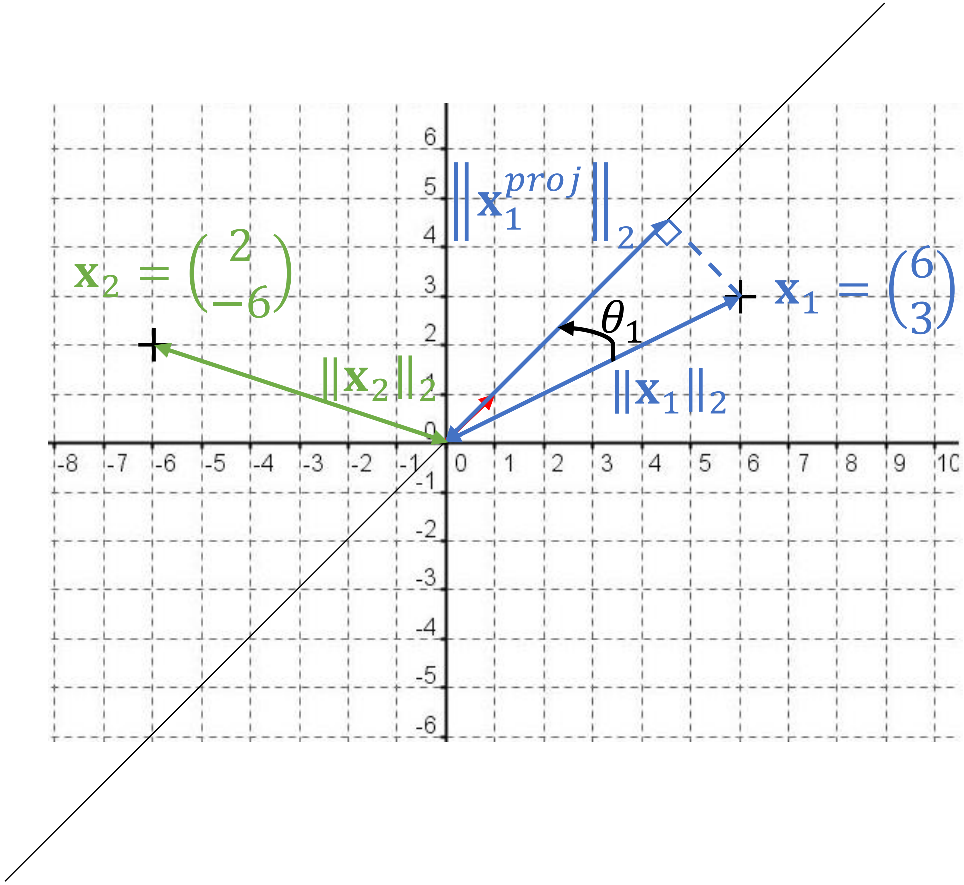
$$\mathbf{x}_1^\top \mathbf{w} = \begin{pmatrix} x_{11} & x_{12} \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} = \frac{x_{11}}{\sqrt{2}} + \frac{x_{12}}{\sqrt{2}}$$

Total Variance – Example in 2D



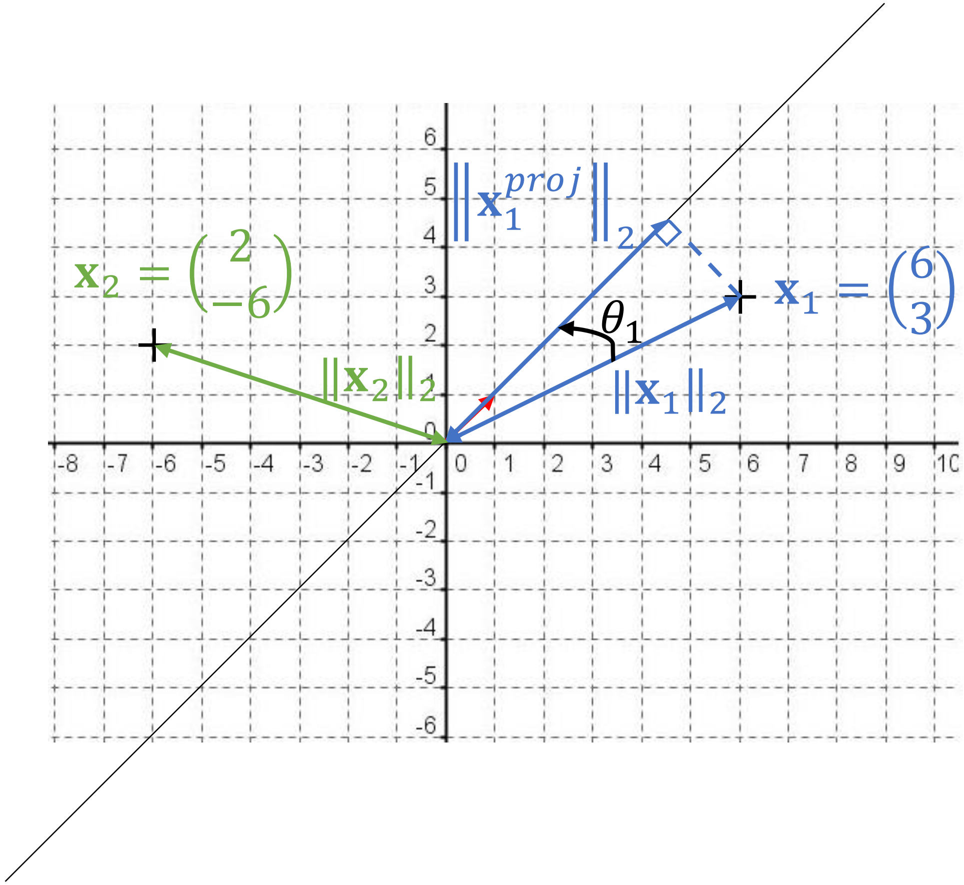
$\|\mathbf{x}_1\|_2 = \sqrt{x_{11}^2 + x_{12}^2}$ $\|\mathbf{x}_2\|_2 = \sqrt{x_{21}^2 + x_{22}^2}$

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

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

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

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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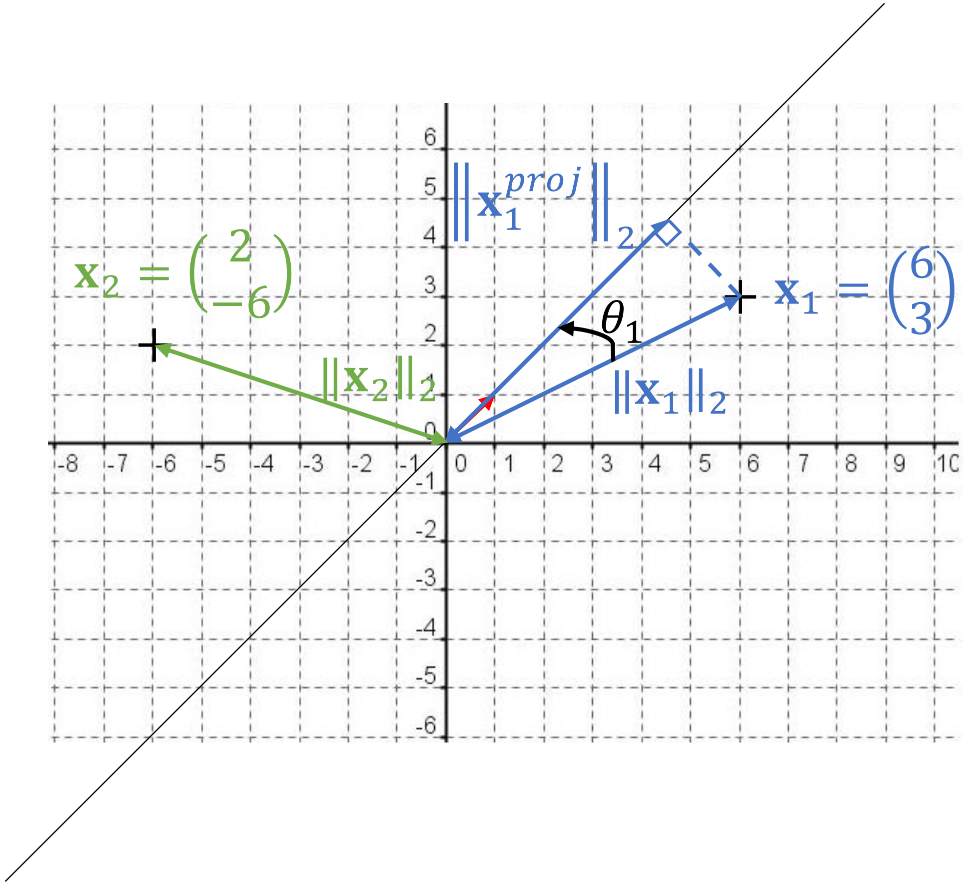
$$\mathbf{x}_1^\top \mathbf{w} = \begin{pmatrix} x_{11} & x_{12} \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} = \frac{x_{11}}{\sqrt{2}} + \frac{x_{12}}{\sqrt{2}}$$

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

Total Variance – Example in 2D



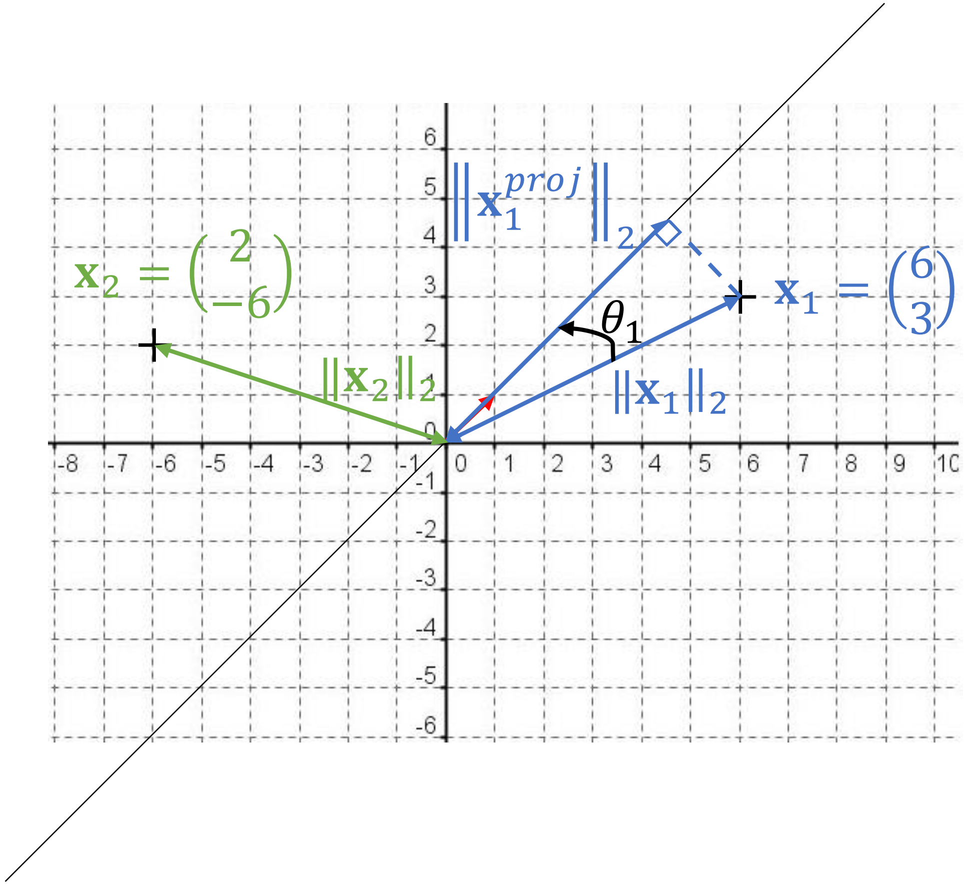
$$\|\mathbf{x}_1\|_2 = \sqrt{x_{11}^2 + x_{12}^2} \qquad \|\mathbf{x}_2\|_2 = \sqrt{x_{21}^2 + x_{22}^2}$$

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

$$\mathbf{x}_1^\top \mathbf{w} = \begin{pmatrix} x_{11} & x_{12} \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} = \frac{x_{11}}{\sqrt{2}} + \frac{x_{12}}{\sqrt{2}}$$

$$= \|\mathbf{x}_1\|_2 \|\mathbf{w}\|_2 \cos(\theta_1) = \|\mathbf{x}_1\|_2 \cos(\theta_1) = \left\| \mathbf{x}_1^{proj} \right\|_2$$

Total Variance – Example in 2D



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

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

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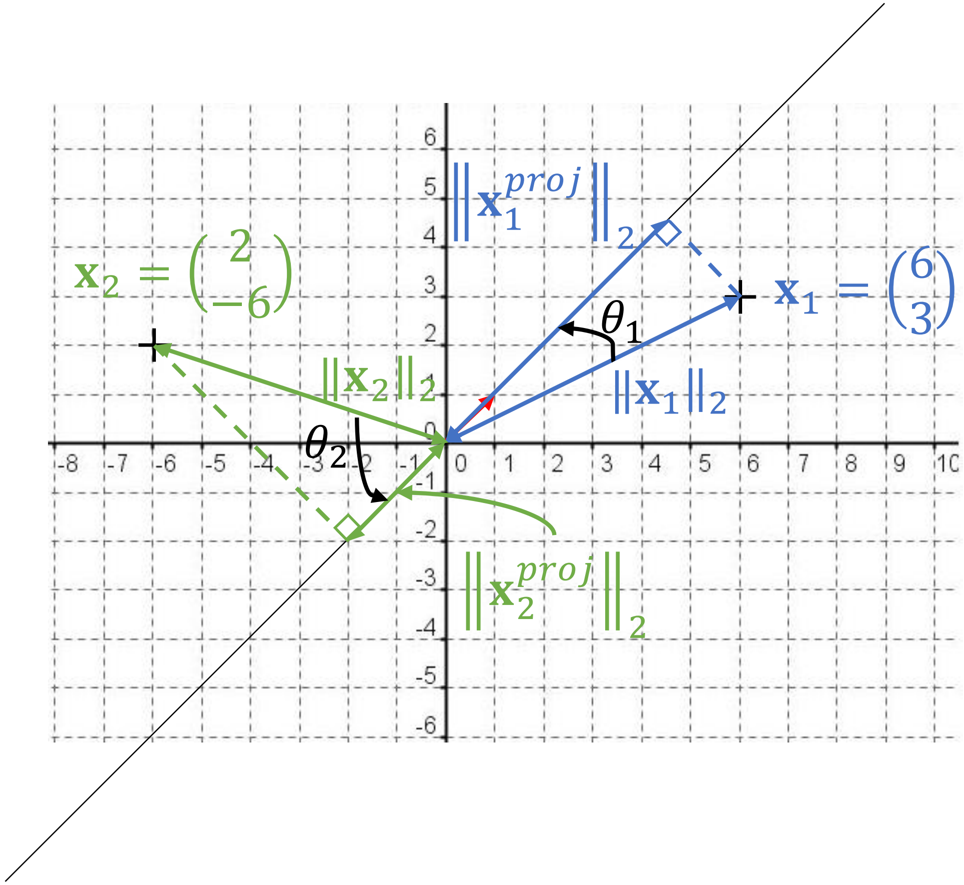
$$= \|\mathbf{x}_1\|_2 \|\mathbf{w}\|_2 \cos(\theta_1) = \|\mathbf{x}_1\|_2 \cos(\theta_1) = \left\|\mathbf{x}_1^{proj}\right\|_2$$

Similarly:

Total Variance – Example in 2D



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

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

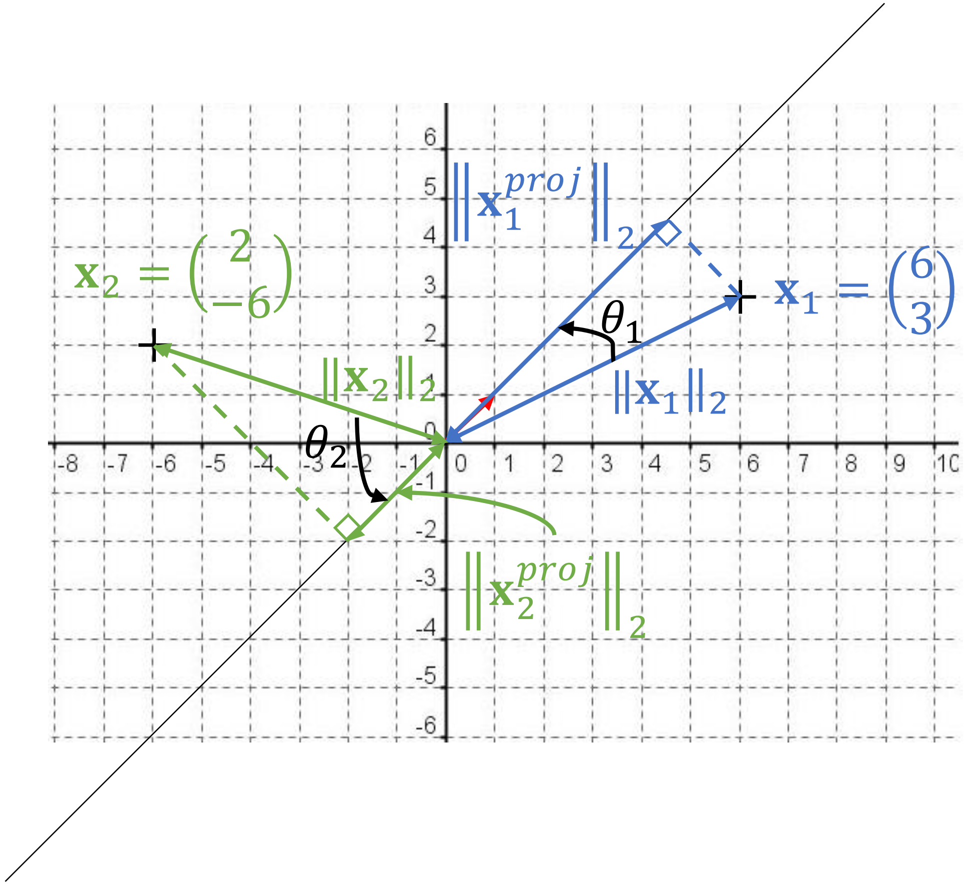
$$\mathbf{x}_1^\top \mathbf{w} = \begin{pmatrix} x_{11} & x_{12} \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} = \frac{x_{11}}{\sqrt{2}} + \frac{x_{12}}{\sqrt{2}}$$

$$= \|\mathbf{x}_1\|_2 \|\mathbf{w}\|_2 \cos(\theta_1) = \|\mathbf{x}_1\|_2 \cos(\theta_1) = \left\| \mathbf{x}_1^{proj} \right\|_2$$

Similarly:

$$\mathbf{x}_2^\top \mathbf{w} = \frac{x_{21}}{\sqrt{2}} + \frac{x_{22}}{\sqrt{2}} = \left\| \mathbf{x}_2^{proj} \right\|_2$$

Total Variance – Example in 2D



$$\Vert \mathbf{x}_1 \Vert_2 = \sqrt{x_{11}^2 + x_{12}^2} \qquad \Vert \mathbf{x}_2 \Vert_2 = \sqrt{x_{21}^2 + x_{22}^2}$$

Director vector $\mathbf{w} = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$. We can see that $\Vert \mathbf{w} \Vert_2 = 1$.

$$\mathbf{x}_1^\top \mathbf{w} = \begin{pmatrix} x_{11} & x_{12} \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} = \frac{x_{11}}{\sqrt{2}} + \frac{x_{12}}{\sqrt{2}}$$

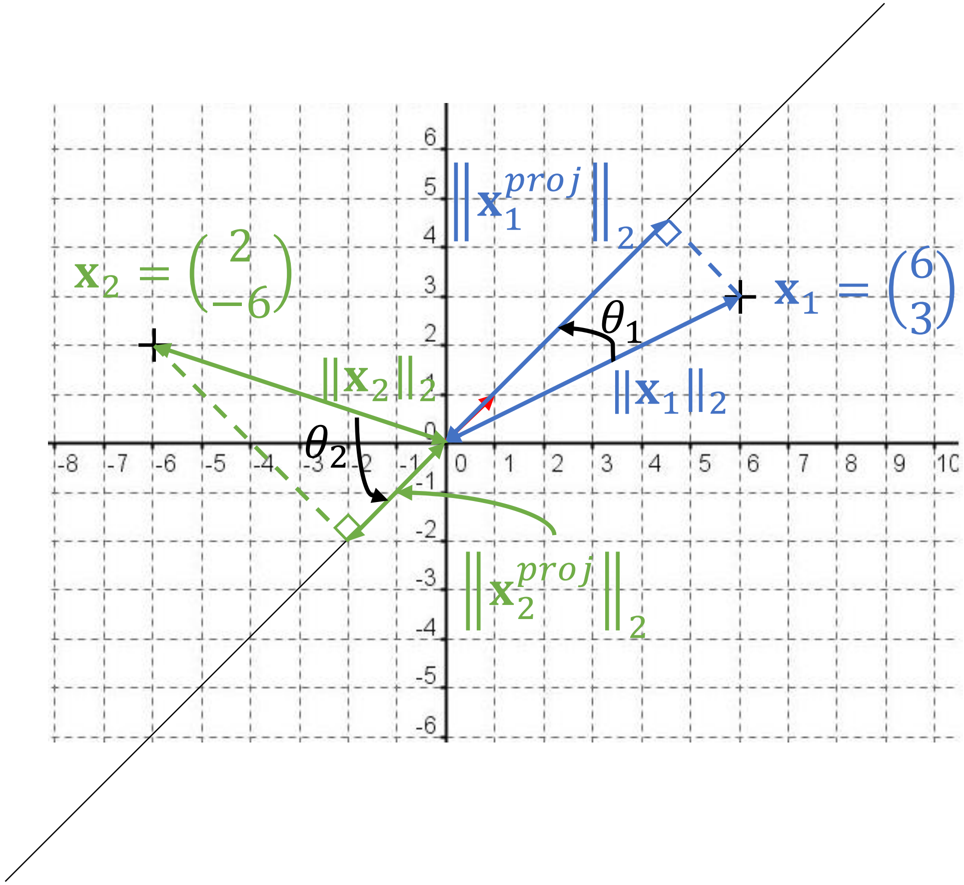
$$= \Vert \mathbf{x}_1 \Vert_2 \Vert \mathbf{w} \Vert_2 \cos(\theta_1) = \Vert \mathbf{x}_1 \Vert_2 \cos(\theta_1) = \left\Vert \mathbf{x}_1^{proj} \right\Vert_2$$

Similarly:

$$\mathbf{x}_2^\top \mathbf{w} = \frac{x_{21}}{\sqrt{2}} + \frac{x_{22}}{\sqrt{2}} = \left\Vert \mathbf{x}_2^{proj} \right\Vert_2$$

In the end:

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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Similarly:

$$\mathbf{x}_2^\top \mathbf{w} = \frac{x_{21}}{\sqrt{2}} + \frac{x_{22}}{\sqrt{2}} = \left\|\mathbf{x}_2^{proj}\right\|_2$$

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

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

PCA optimization criterion

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

By the way:

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: $\begin{pmatrix}\mathbf{x}_1^\top \mathbf{w} \\ \mathbf{x}_2^\top \mathbf{w}\end{pmatrix}$

PCA optimization criterion

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

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

PCA optimization criterion

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

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

PCA optimization criterion

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

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:

PCA optimization criterion

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

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:

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

PCA optimization criterion

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

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:

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

PCA optimization criterion

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

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

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

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:

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

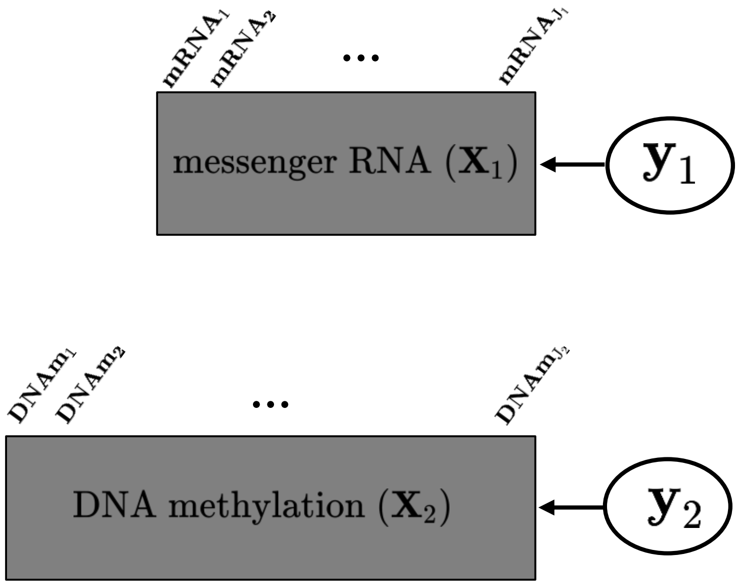
It is possible to show in the general case that: $\mathrm{TV}^{\mathrm{proj}} = \frac{1}{n} \mathbf{w}^\top \mathbf{X}^\top \mathbf{X} \mathbf{w} = \mathrm{Var}(\mathbf{X}\mathbf{w})$

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

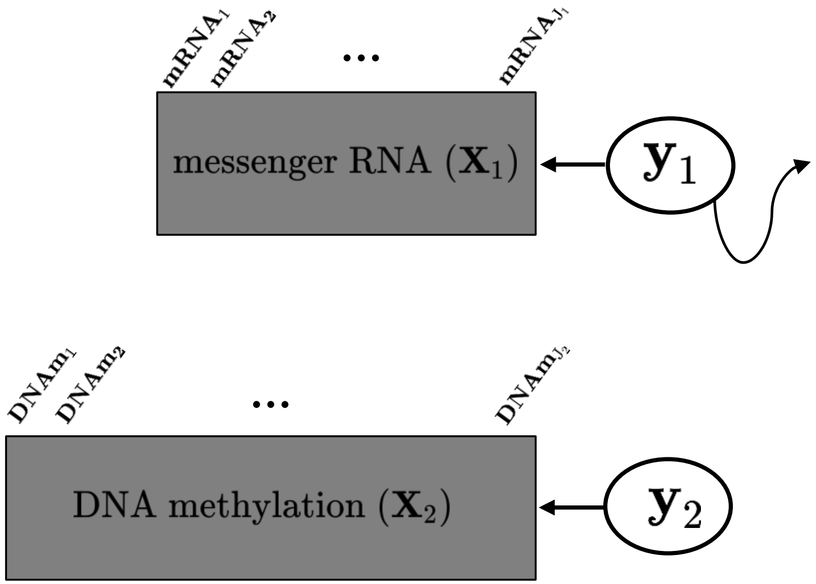
$$\max_{\substack{\mathbf{w} \\ \|\mathbf{w}\|_2^2 = 1}} \mathrm{Var}(\mathbf{X}\mathbf{w})$$

3. Unsupervised analysis with two-blocks

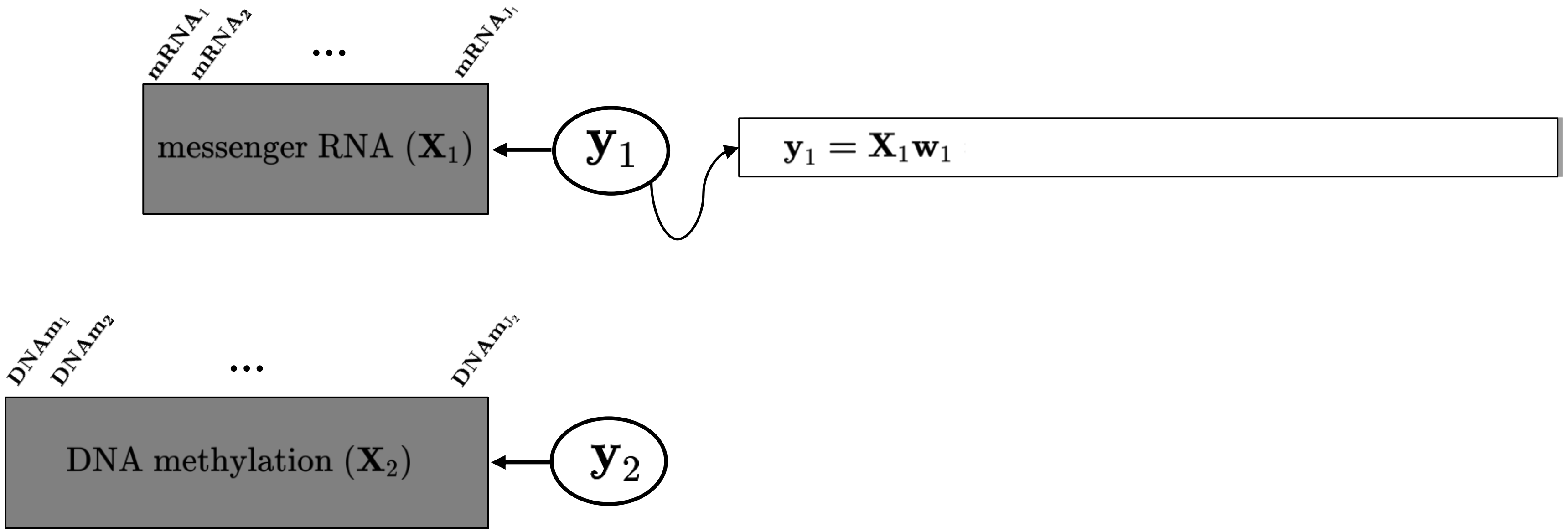
The philosophy of multiblock component methods



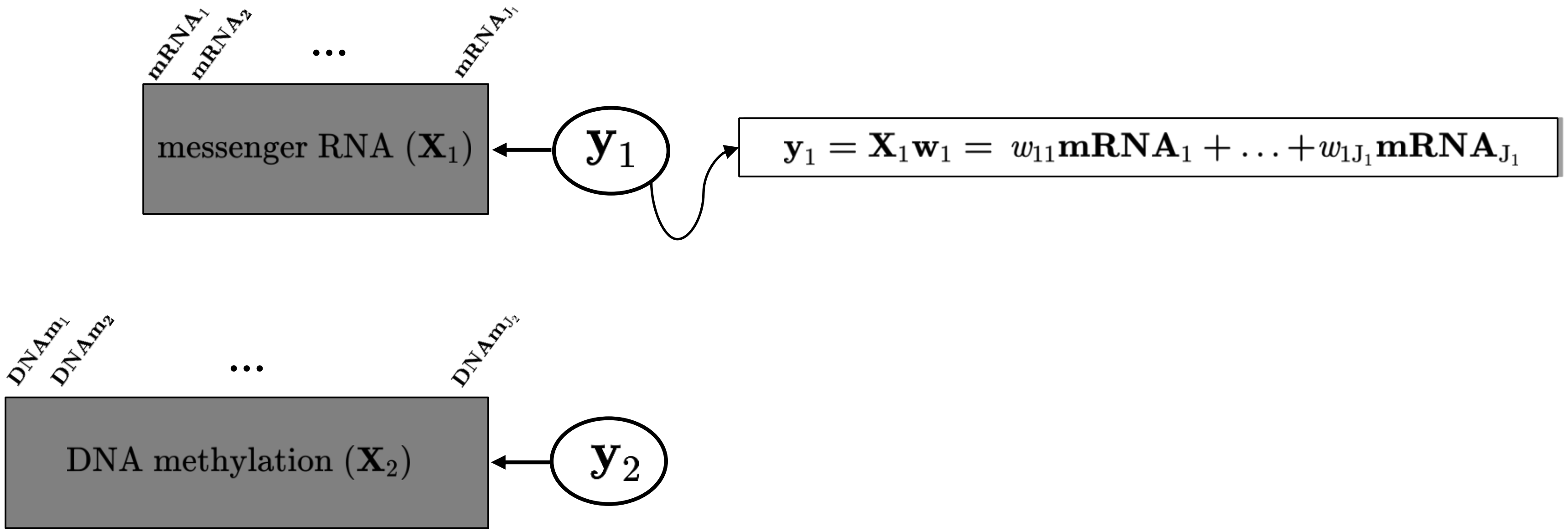
The philosophy of multiblock component methods



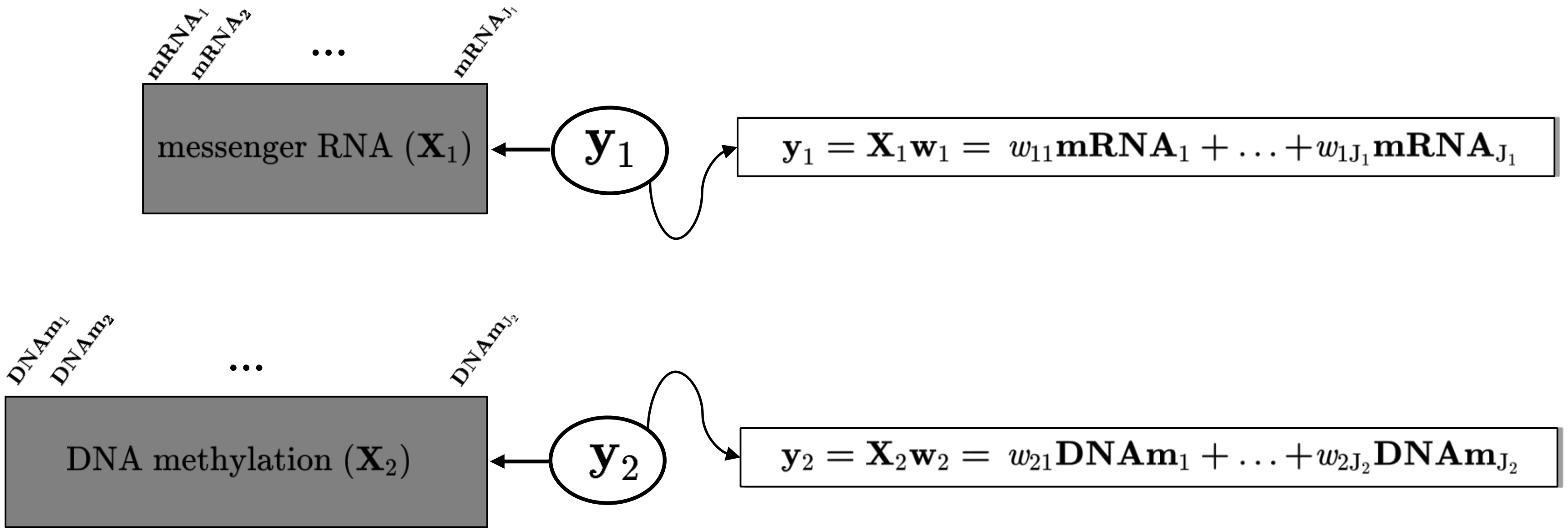
The philosophy of multiblock component methods



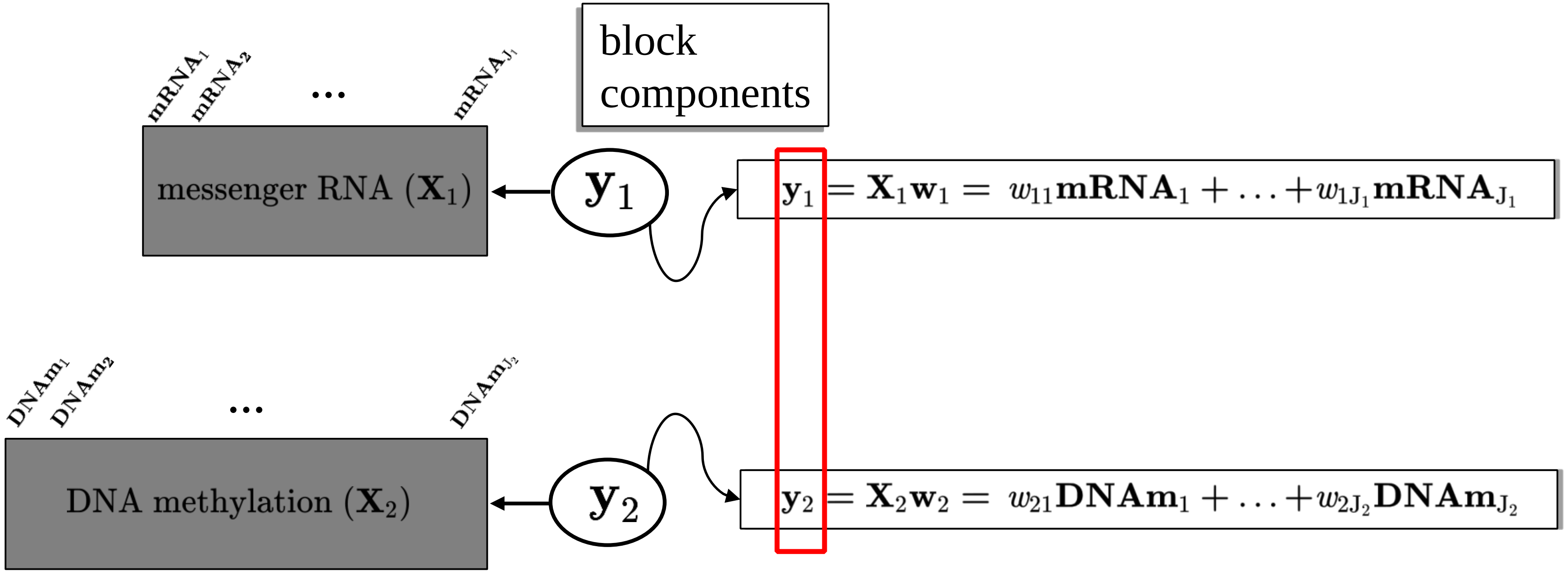
The philosophy of multiblock component methods



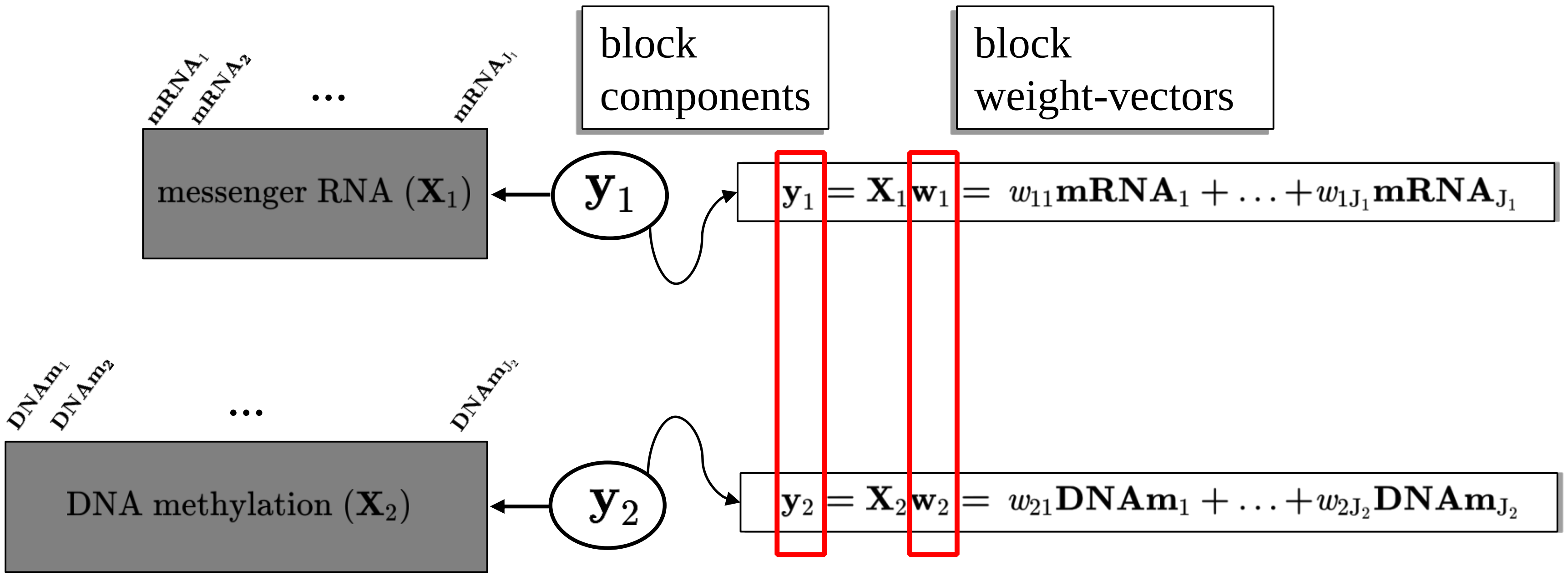
The philosophy of multiblock component methods



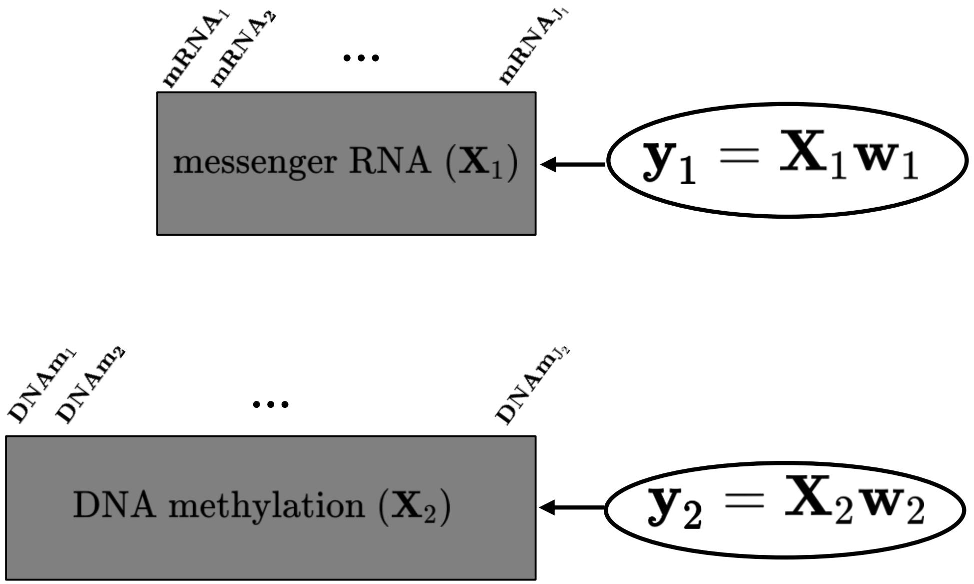
The philosophy of multiblock component methods



The philosophy of multiblock component methods



The philosophy of multiblock component methods

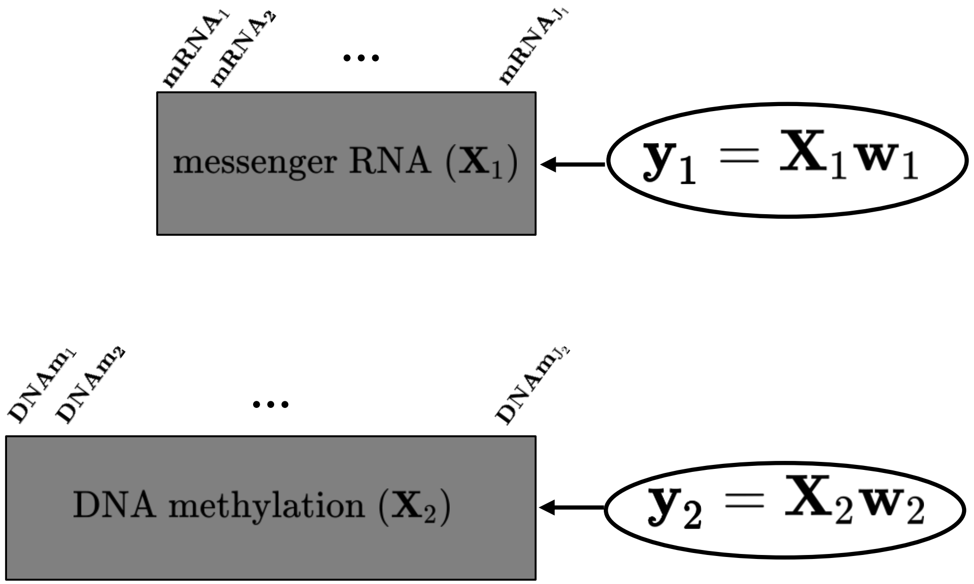


Block components should verified two properties at the same time:

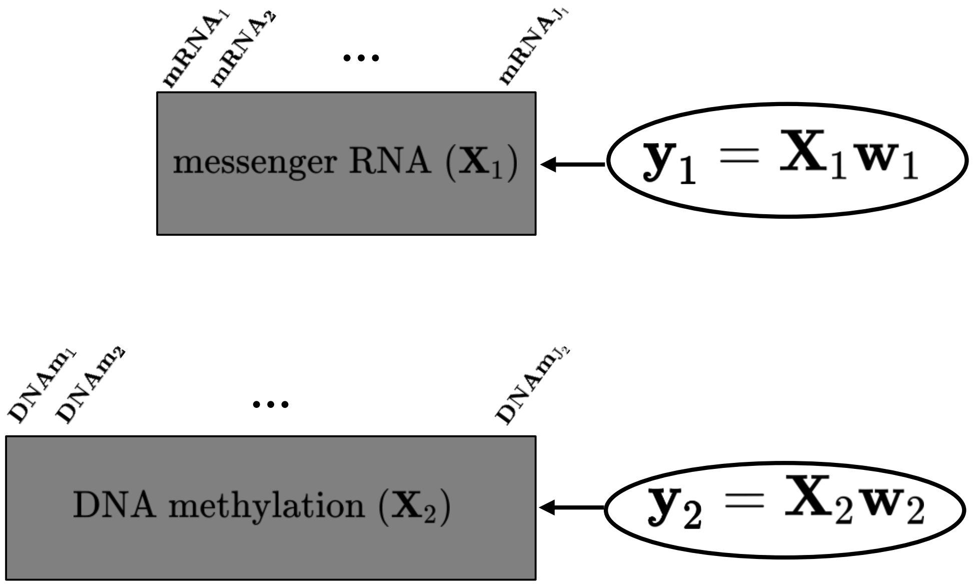
1. Block components well explain their own block.

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

The philosophy of multiblock component methods



The philosophy of multiblock component methods



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

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

Courtesy to Arthur Tenenhaus.

From PCA to PLS/CCA

Principal Component Analysis (PCA)

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

From PCA to PLS/CCA

Principal Component Analysis (PCA)

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

From PCA to PLS/CCA

Principal Component Analysis (PCA)

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

From PCA to PLS/CCA

Principal Component Analysis (PCA)

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

From PCA to PLS/CCA

Principal Component Analysis (PCA)

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

From PCA to PLS/CCA

Principal Component Analysis (PCA)

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

From PCA to PLS/CCA

Principal Component Analysis (PCA)

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

From PCA to PLS/CCA

Principal Component Analysis (PCA)

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

From PCA to PLS/CCA

Principal Component Analysis (PCA)

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

From PCA to PLS/CCA

From PCA to PLS/CCA

Partial Least Squares (PLS2)

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

From PCA to PLS/CCA

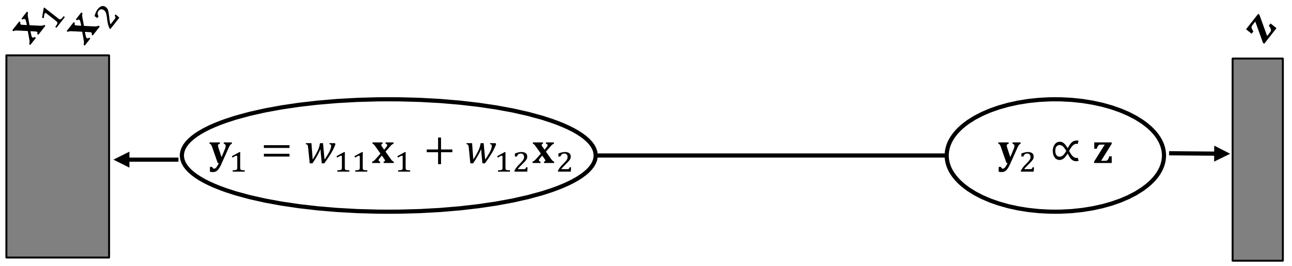
Canonical Correlation Analysis (CCA)

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

Partial Least Squares (PLS2)

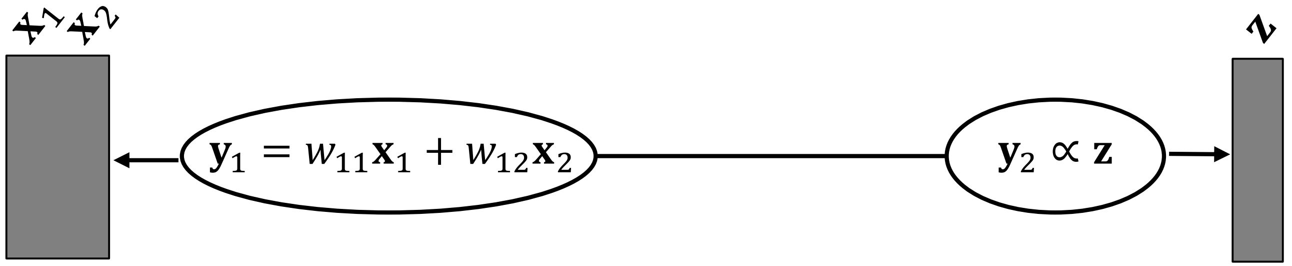
$$\max_{\substack{\mathbf{w}_1,\mathbf{w}_2 \\ \|\mathbf{w}_i\|_2^2=1}} \mathrm{Cov}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)$$

PLS & CCA with a figure



PLS & CCA with a figure

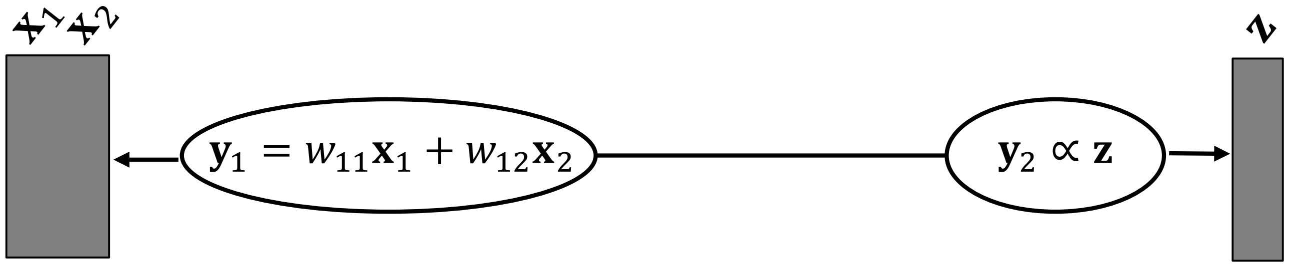
$$[\mathbf{x}_1\ \mathbf{x}_2] \sim \mathcal{N}\left((0,0), \begin{pmatrix} 1 & 0.5 \\ 0.5 & 1 \end{pmatrix}\right)$$



PLS & CCA with a figure

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

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



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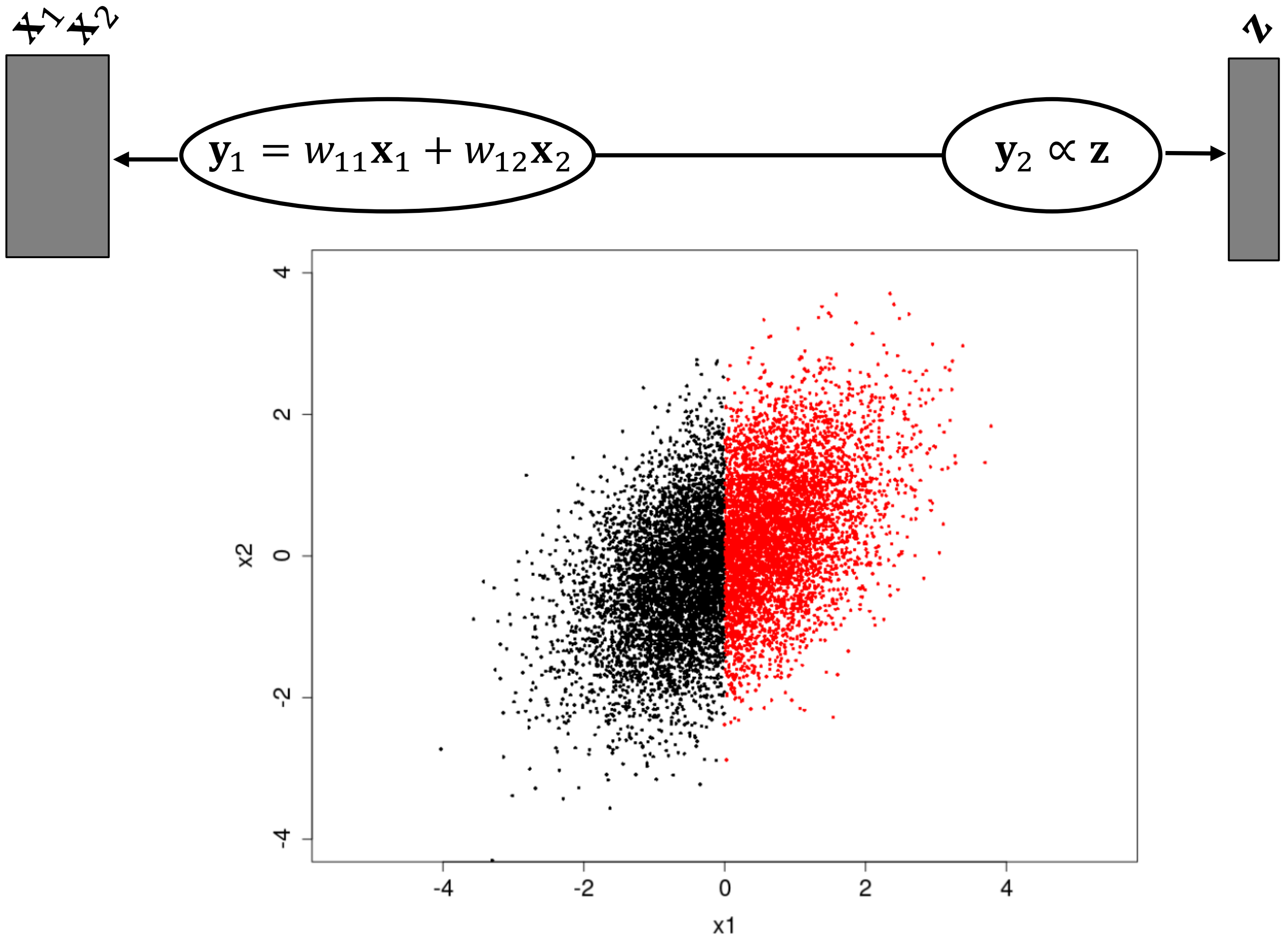

PLS & CCA with a figure

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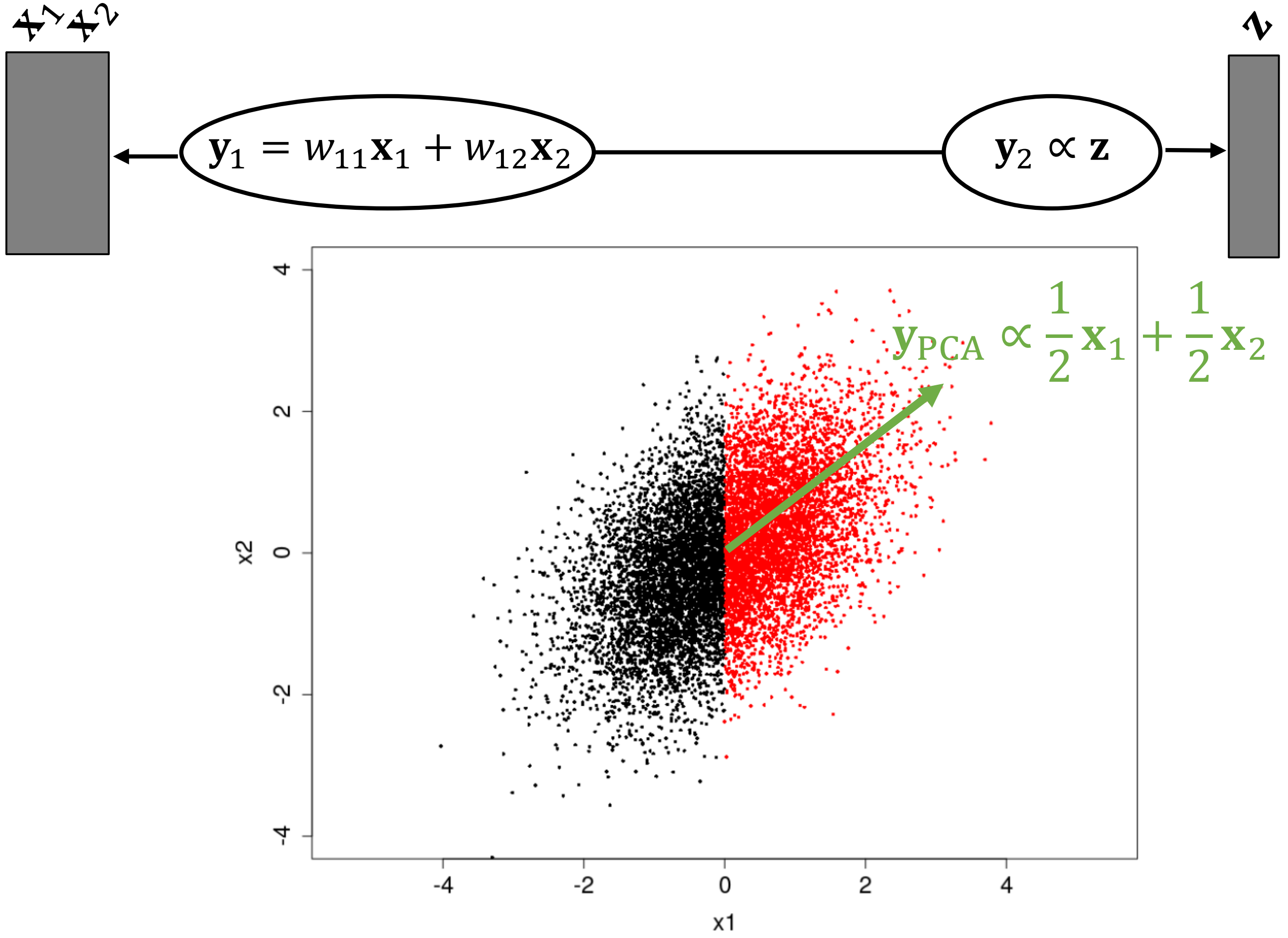

PLS & CCA with a figure

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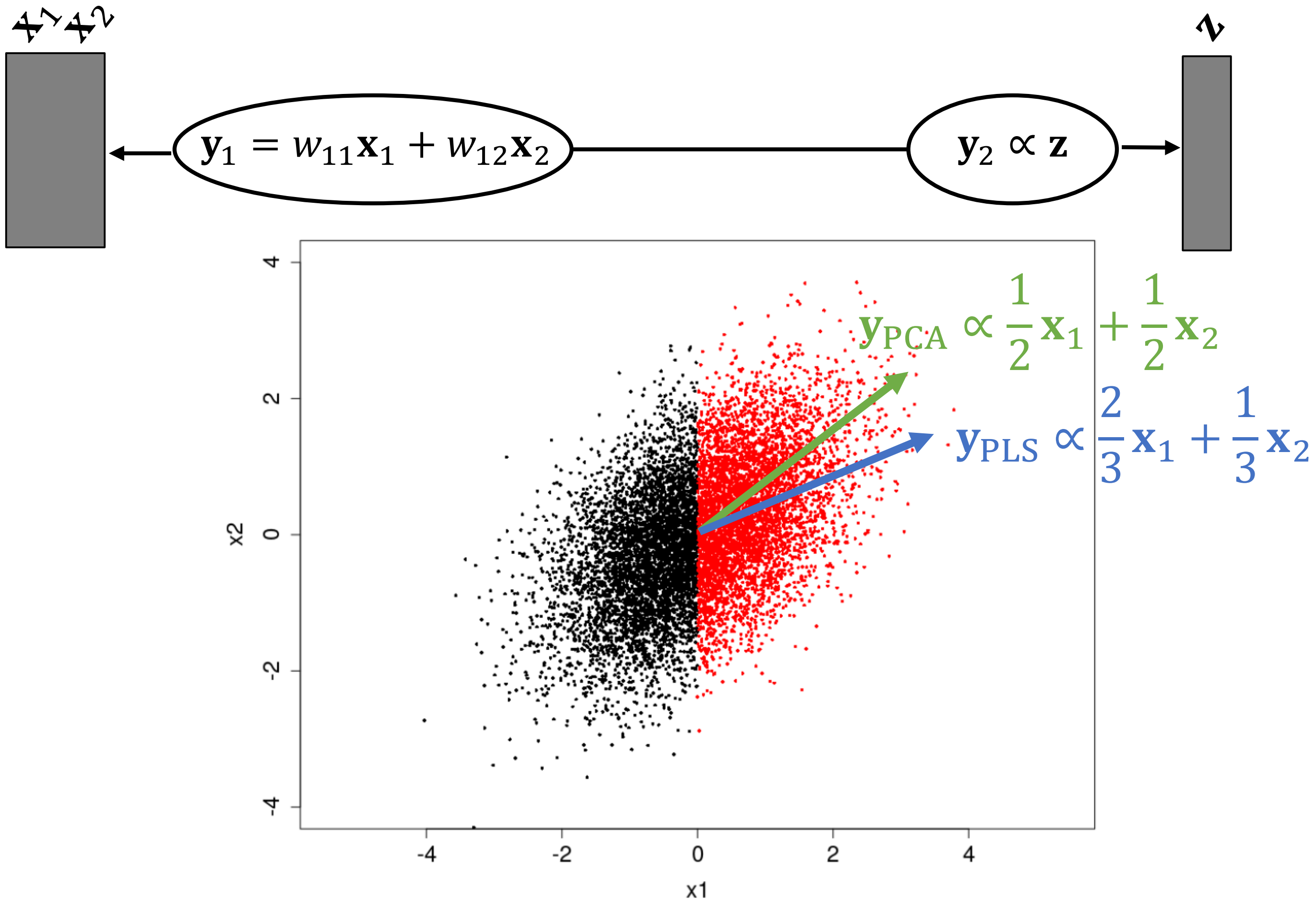

PLS & CCA with a figure

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

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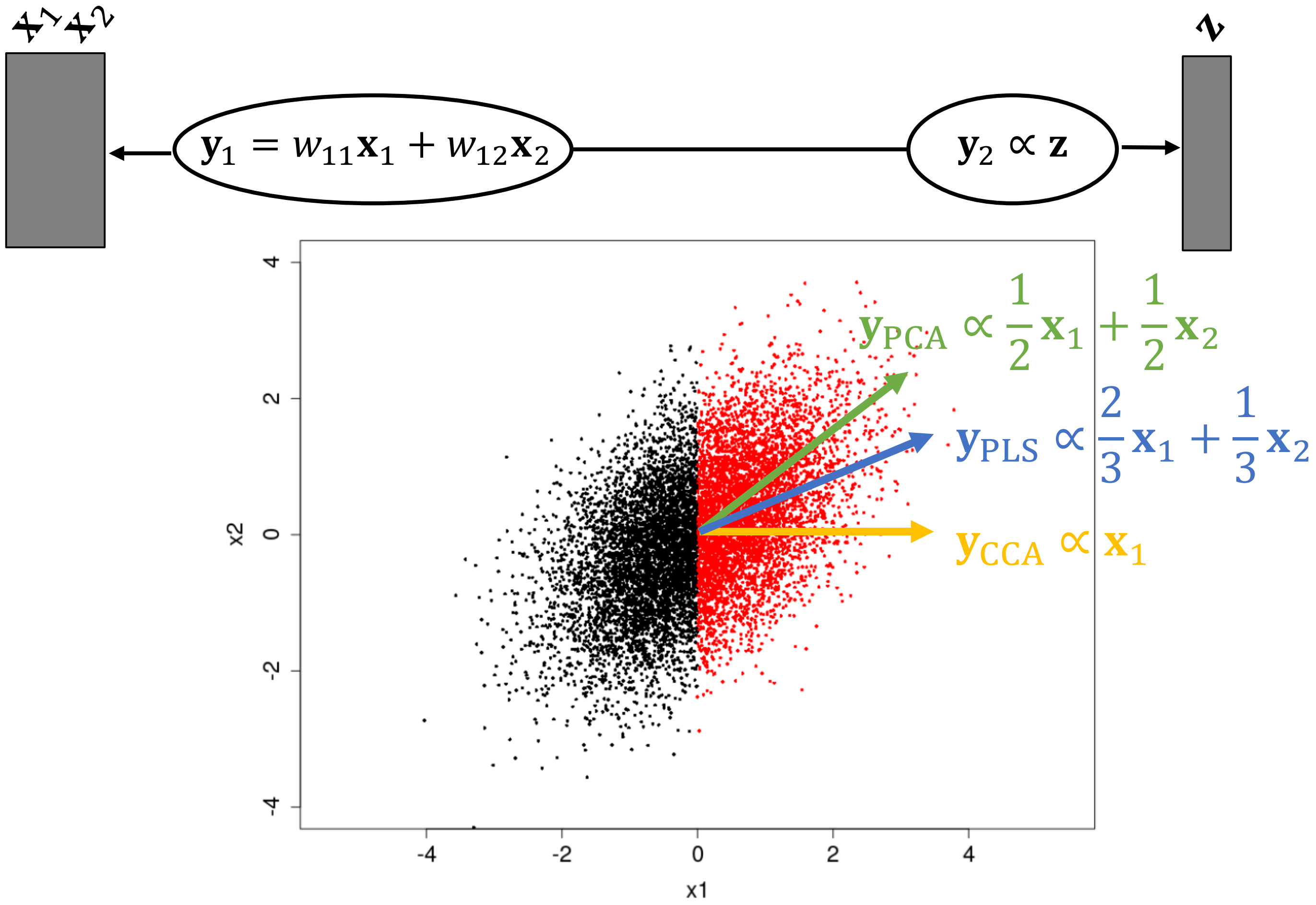


Two-blocks special cases: PLS & CCA

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

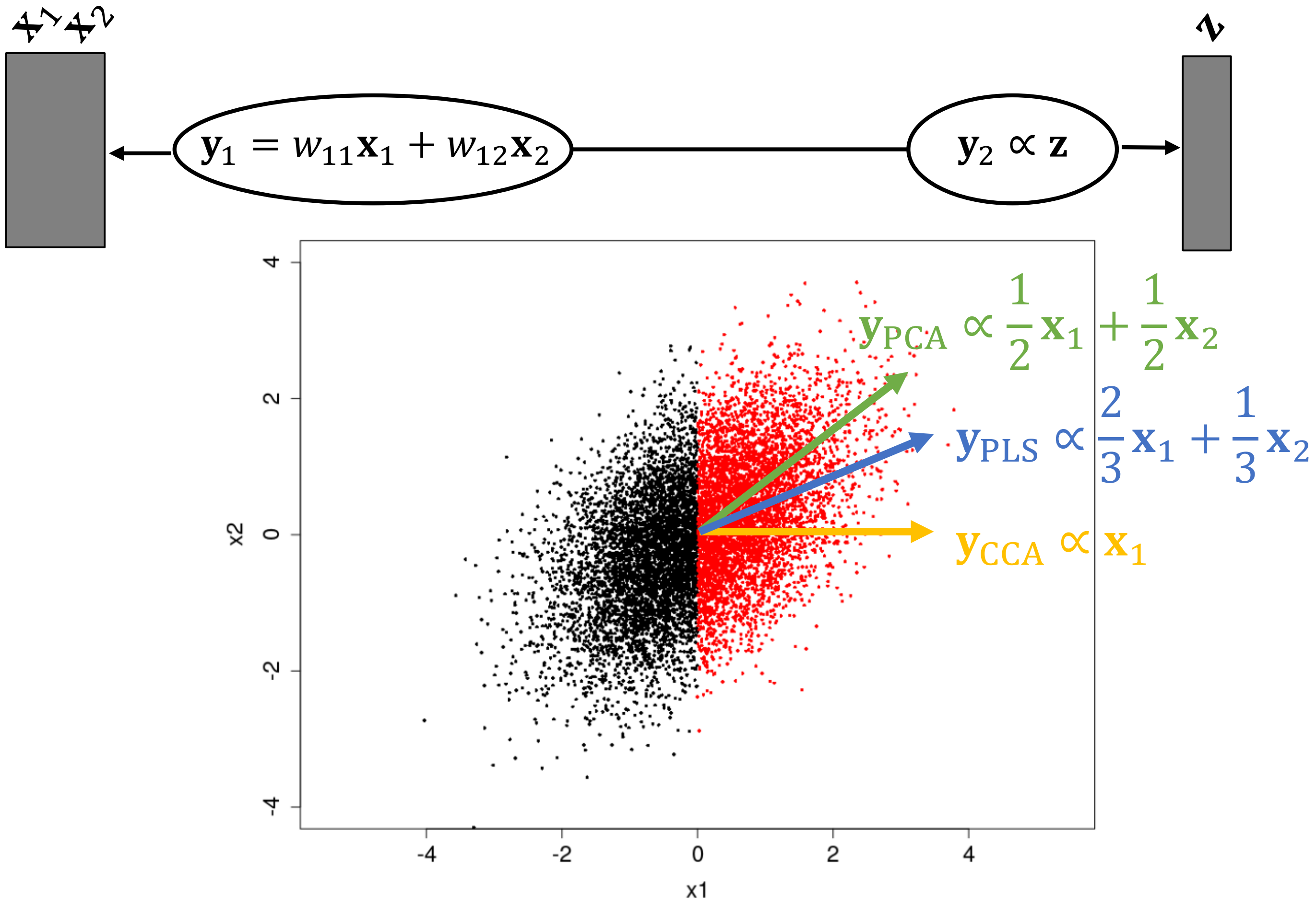
$$\max_{\mathbf{w}_1,\mathbf{w}_2} \mathrm{Cov}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)$$

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

PLS & CCA with a figure

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

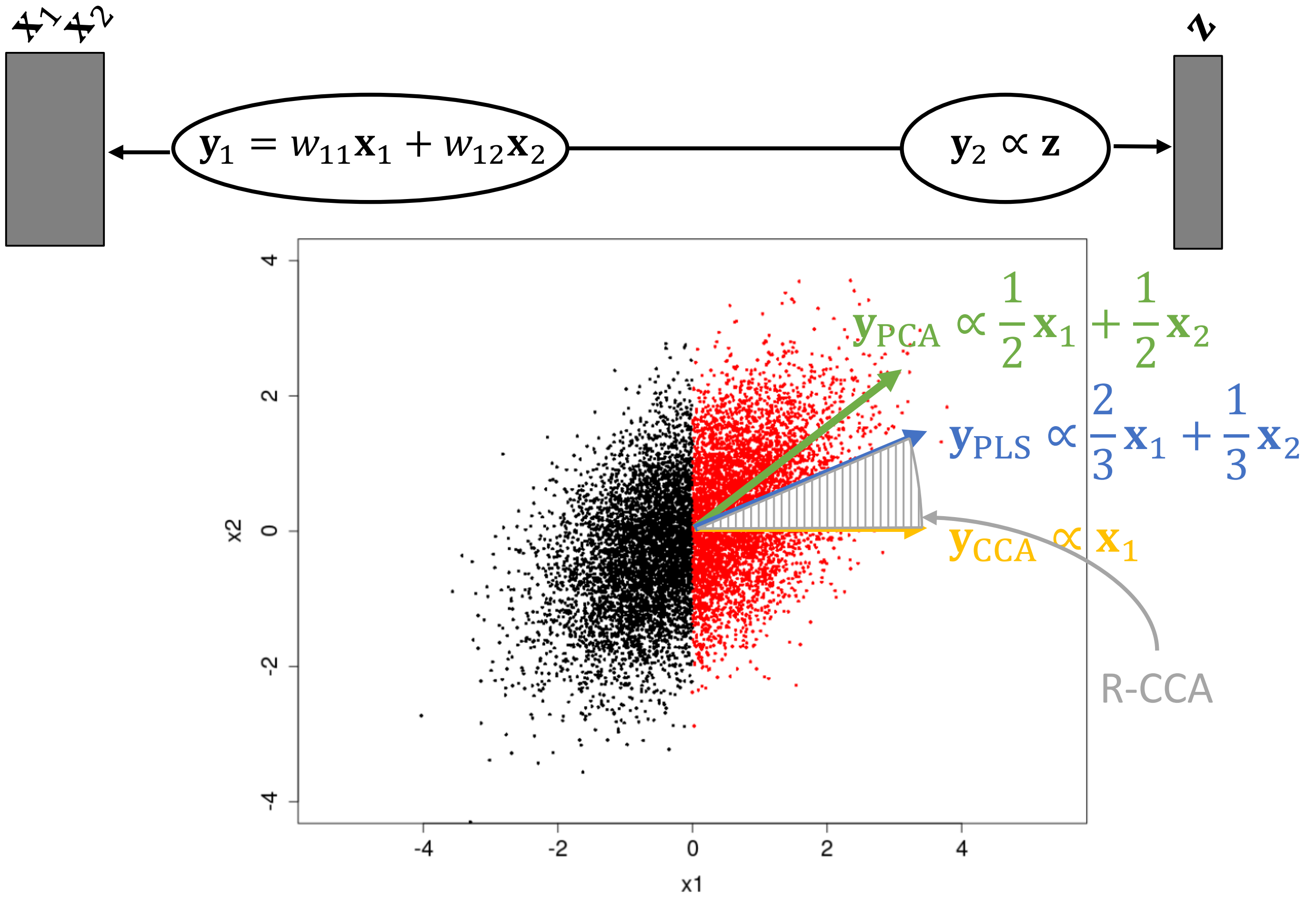
$(\boldsymbol{z})_i = \begin{cases} 0 \text{ if } (\mathbf{x})_i < 0 \\ 1 \text{ otherwise} \end{cases}$



PLS & CCA with a figure

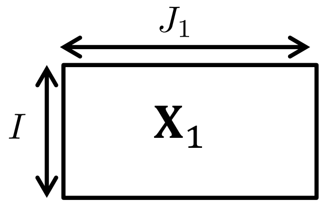
$$[\mathbf{x}_1\ \mathbf{x}_2] \sim \mathcal{N}\left((0,0), \begin{pmatrix} 1 & 0.5 \\ 0.5 & 1 \end{pmatrix}\right)$$

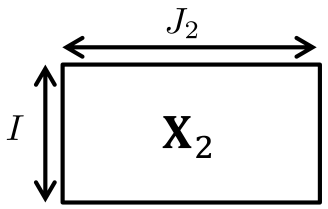
$$(\mathbf{z})_i = \begin{cases} 0 \text{ if } (\mathbf{x})_i < 0 \\ 1 \text{ otherwise} \end{cases}$$



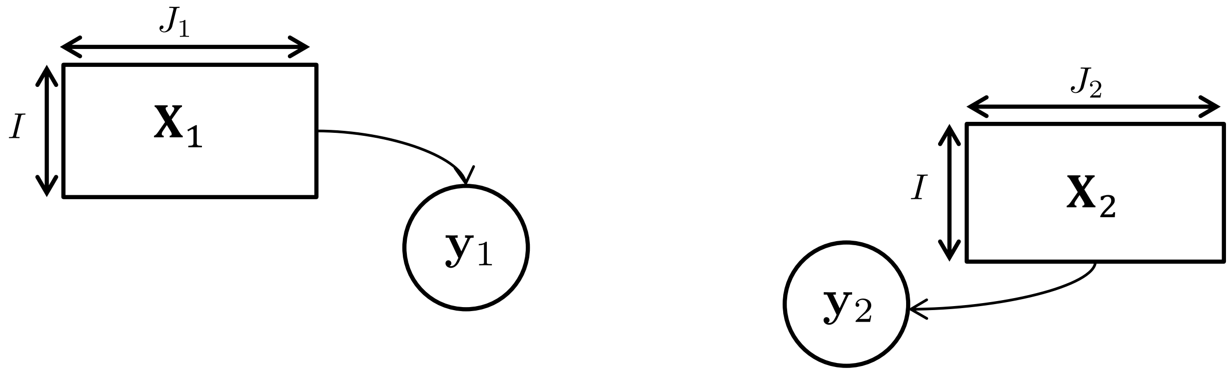
4. Unsupervised analysis with L-blocks

Regularized Generalized Canonical Correlation Analysis (RGCCA)





Regularized Generalized Canonical Correlation Analysis (RGCCA)



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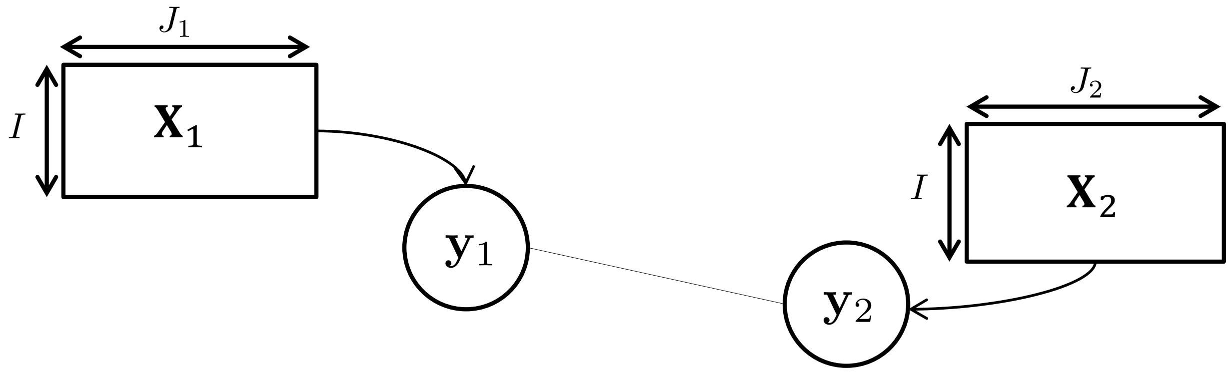

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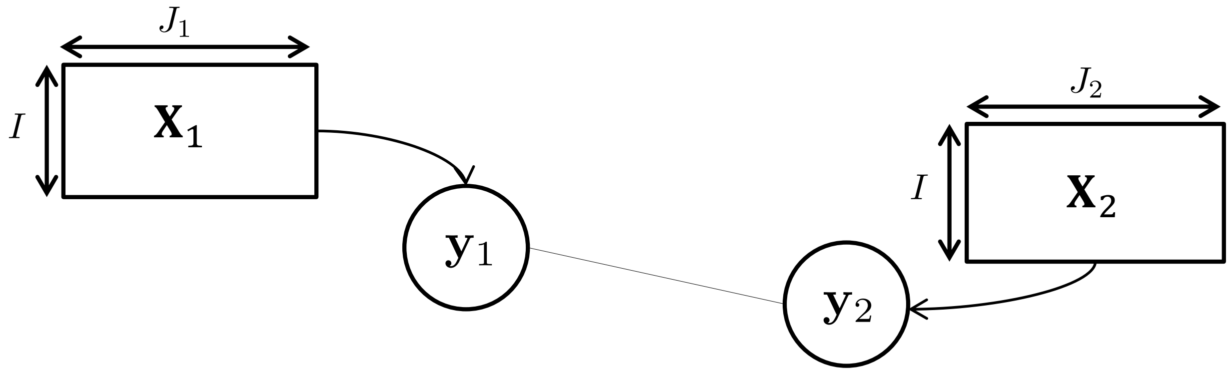
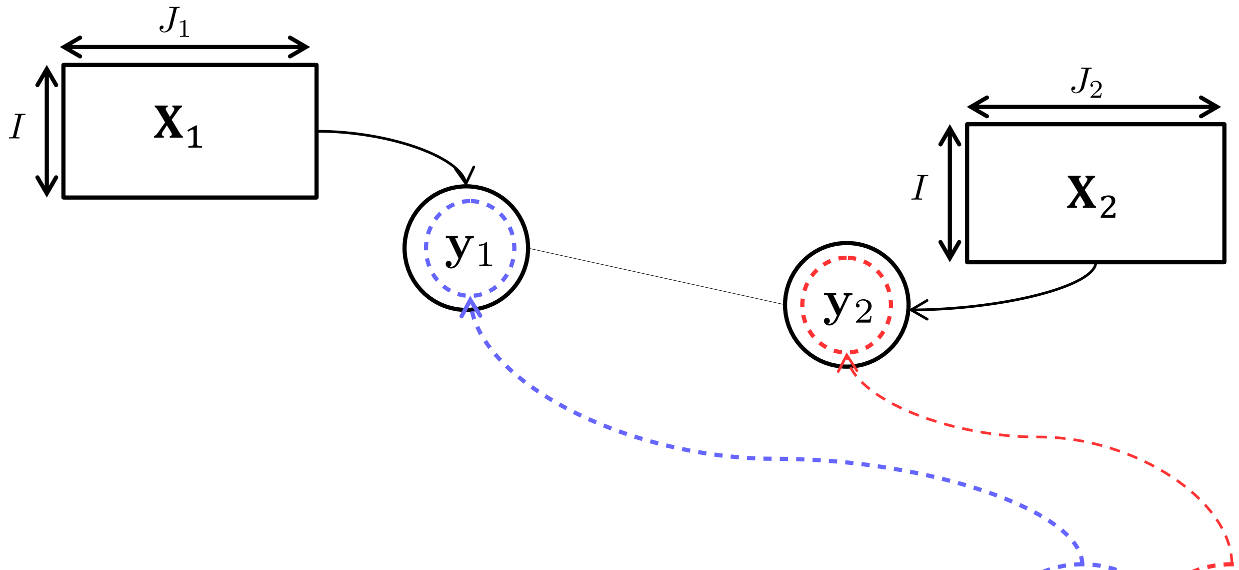


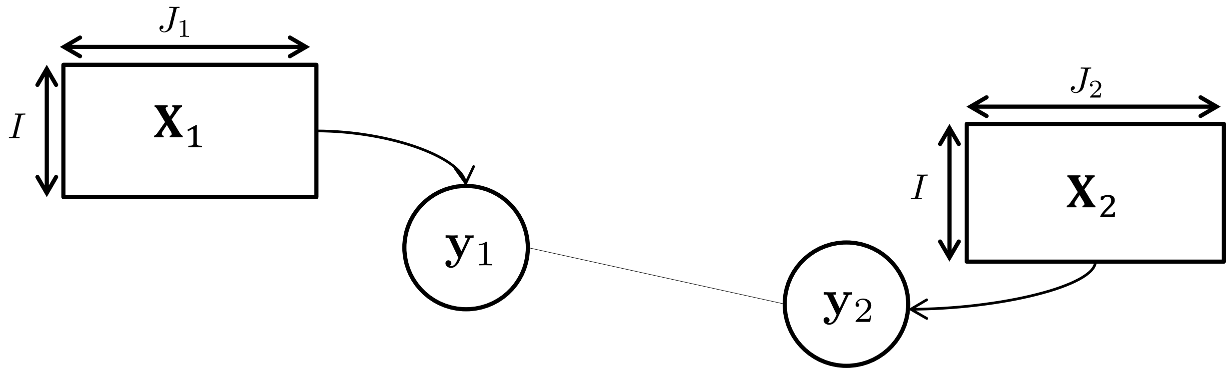
$$\max_{\mathbf{w}_1,\mathbf{w}_2} \mathrm{Cov}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)$$

Regularized Generalized Canonical Correlation Analysis (RGCCA)



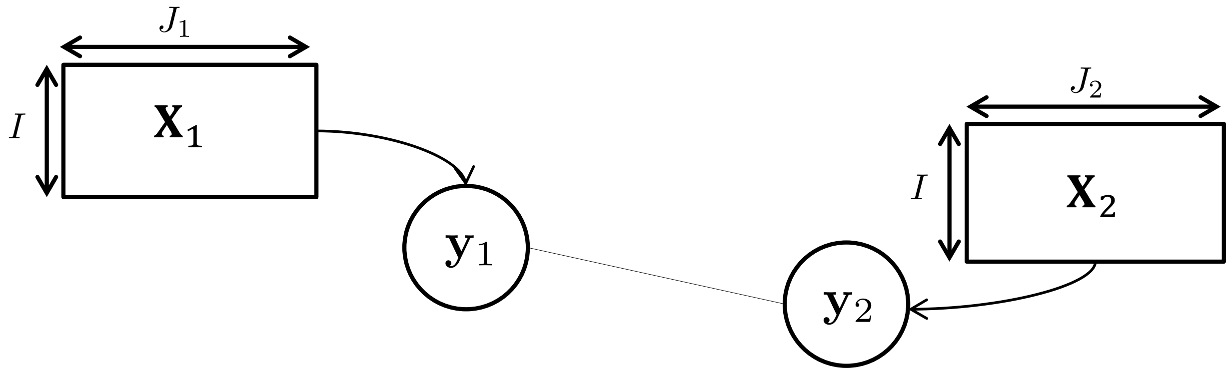
$$\max_{\mathbf{w}_1,\mathbf{w}_2} \text{Cov}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)$$

Regularized Generalized Canonical Correlation Analysis (RGCCA)



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

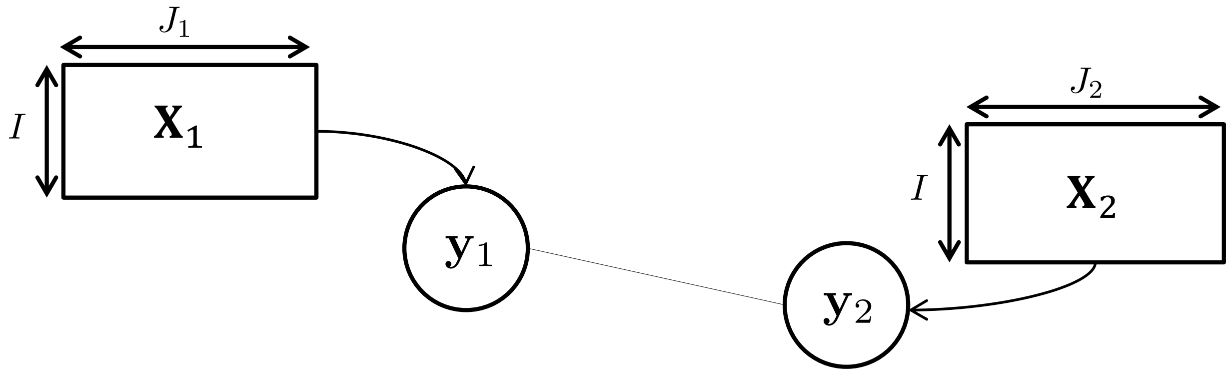
Regularized Generalized Canonical Correlation Analysis (RGCCA)



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

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

Regularized Generalized Canonical Correlation Analysis (RGCCA)

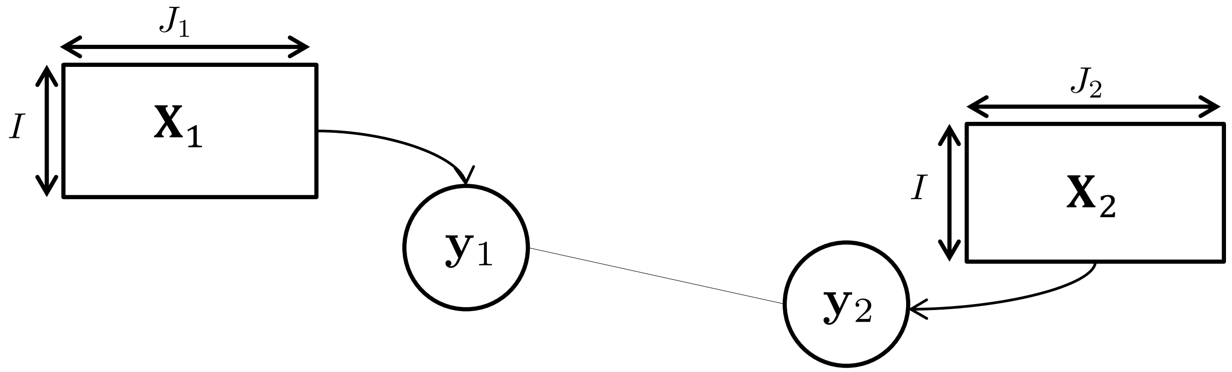


$$\max_{\mathbf{w}_1,\mathbf{w}_2} \mathrm{Cov}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)$$

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

→ Canonical Correlation Analysis

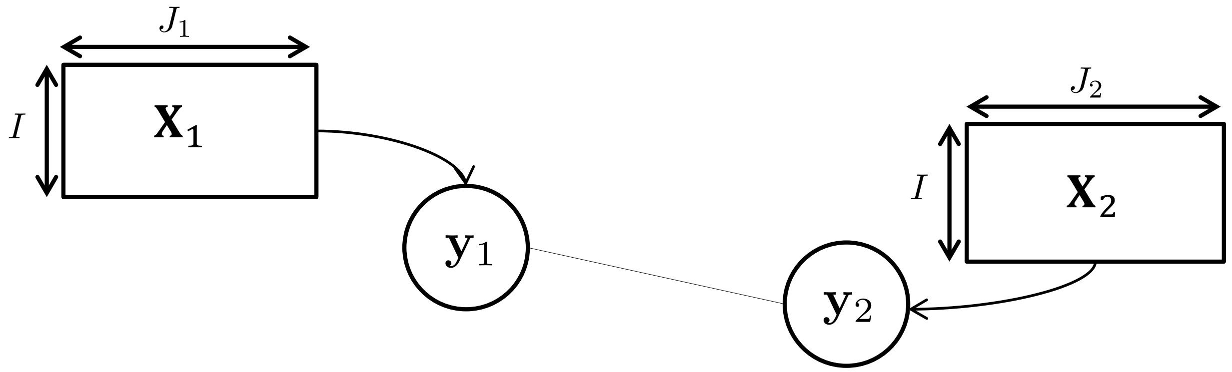
Regularized Generalized Canonical Correlation Analysis (RGCCA)



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

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

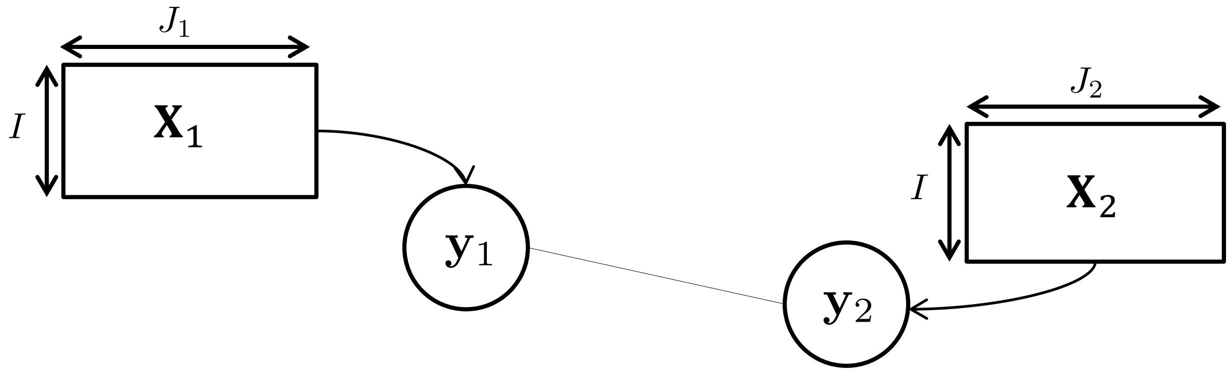
Regularized Generalized Canonical Correlation Analysis (RGCCA)



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

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

Regularized Generalized Canonical Correlation Analysis (RGCCA)

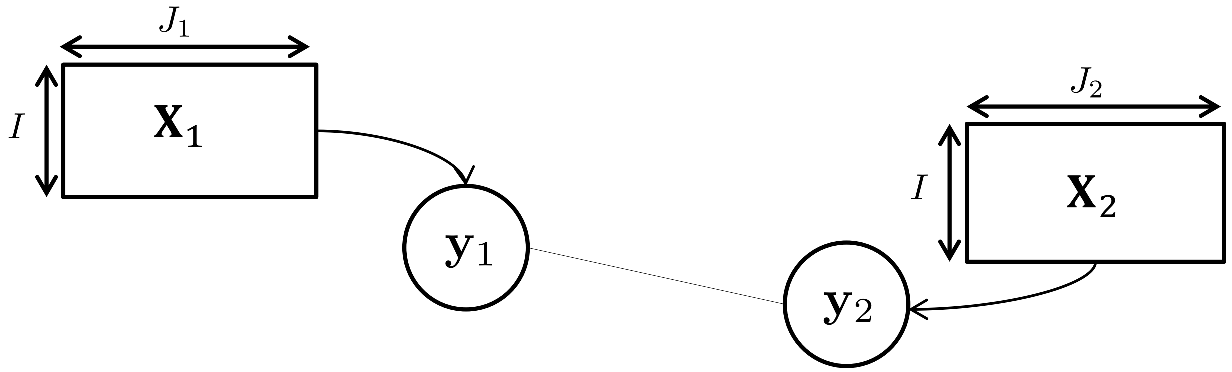


$$\max_{\mathbf{w}_1,\mathbf{w}_2} \mathrm{Cov}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)$$

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

➡ Partial Least Squares 2

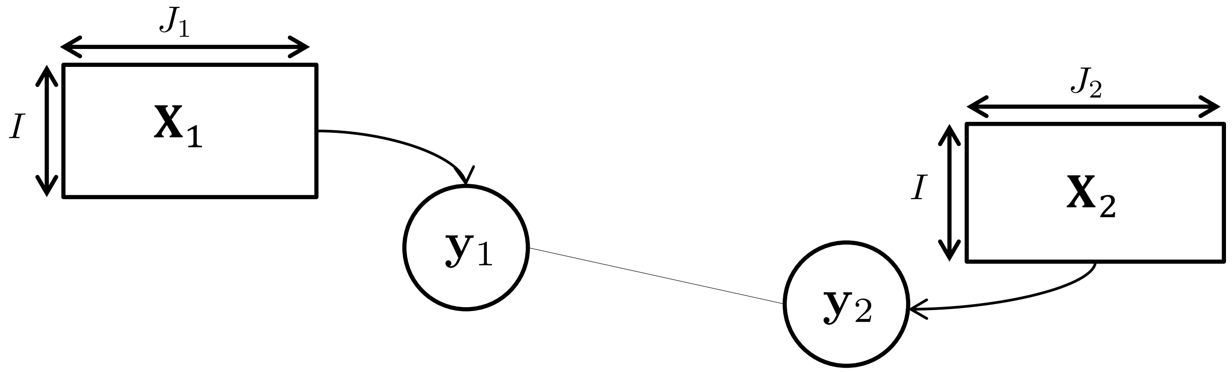
Regularized Generalized Canonical Correlation Analysis (RGCCA)



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

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

Regularized Generalized Canonical Correlation Analysis (RGCCA)



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

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

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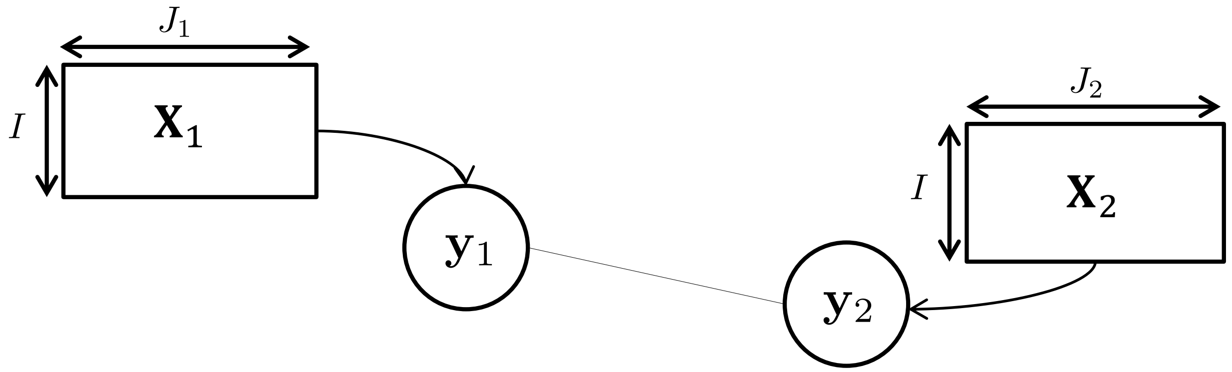
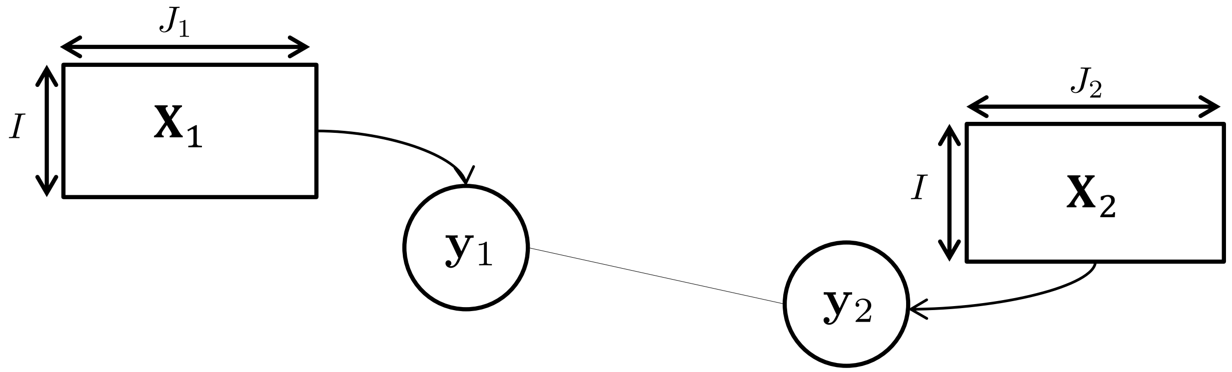


$$\max_{\mathbf{w}_1,\mathbf{w}_2} \text{Cov}(\mathbf{X}_1\mathbf{w}_1, \mathbf{X}_2\mathbf{w}_2)$$

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

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

Regularized Generalized Canonical Correlation Analysis (RGCCA)



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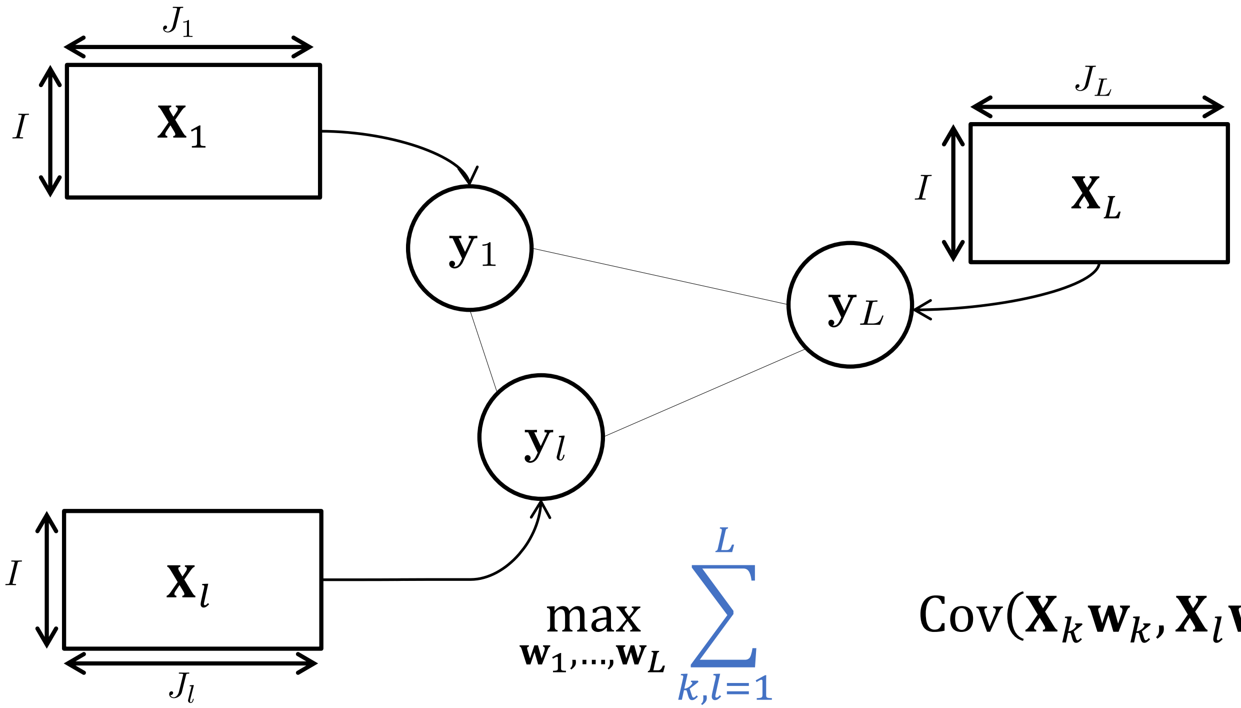
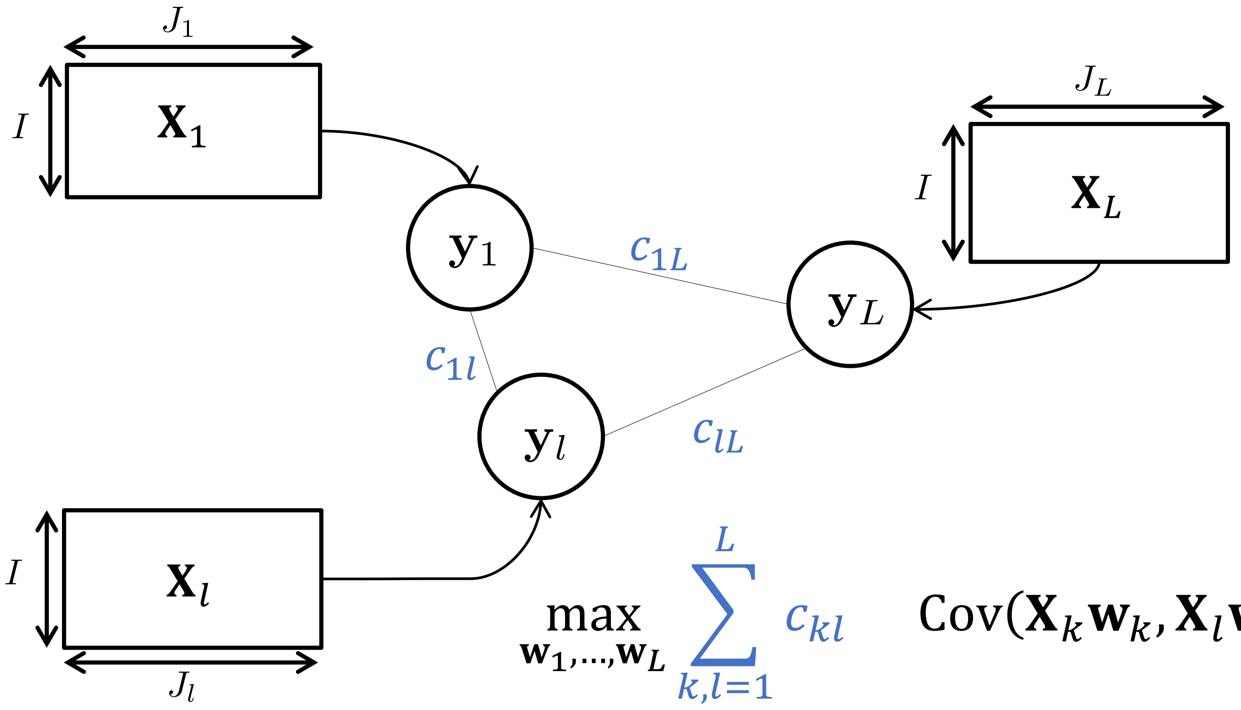


$$\max_{\mathbf{w}_1,\ldots,\mathbf{w}_L} \sum_{k,l=1}^{L} \mathrm{Cov}(\mathbf{X}_k\mathbf{w}_k, \mathbf{X}_l\mathbf{w}_l)$$

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

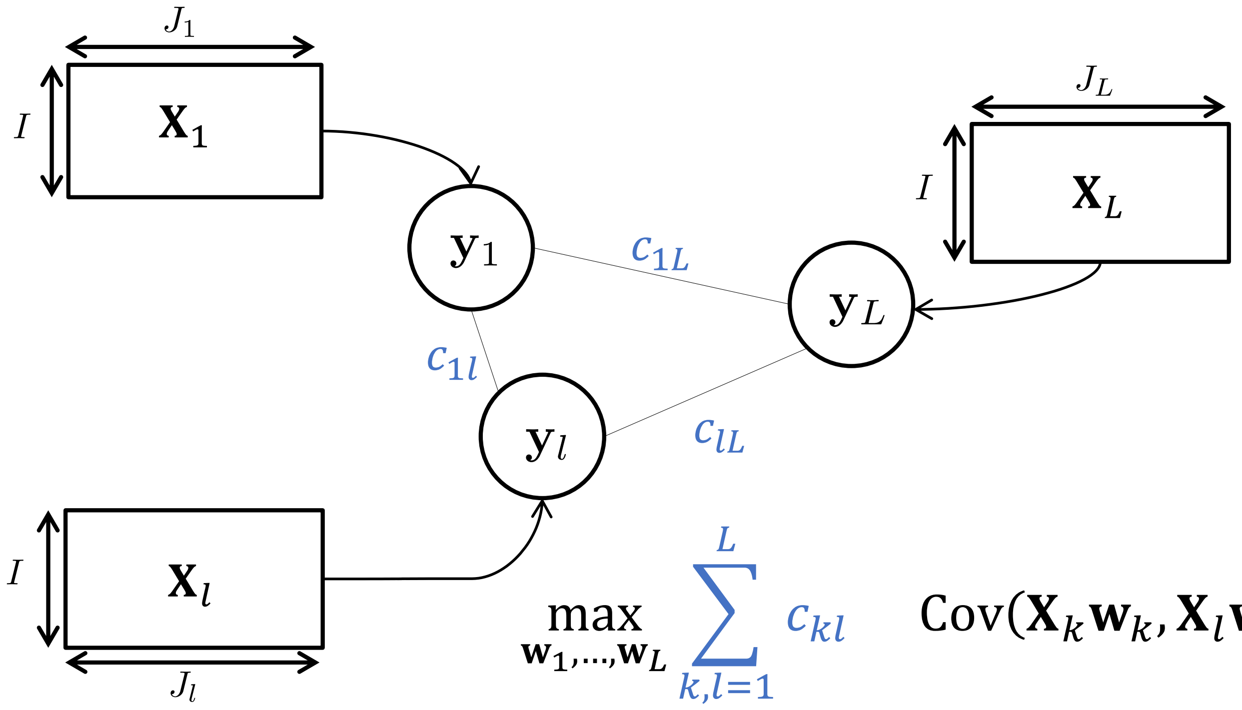
Regularized Generalized Canonical Correlation Analysis (RGCCA)



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

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

Regularized Generalized Canonical Correlation Analysis (RGCCA)

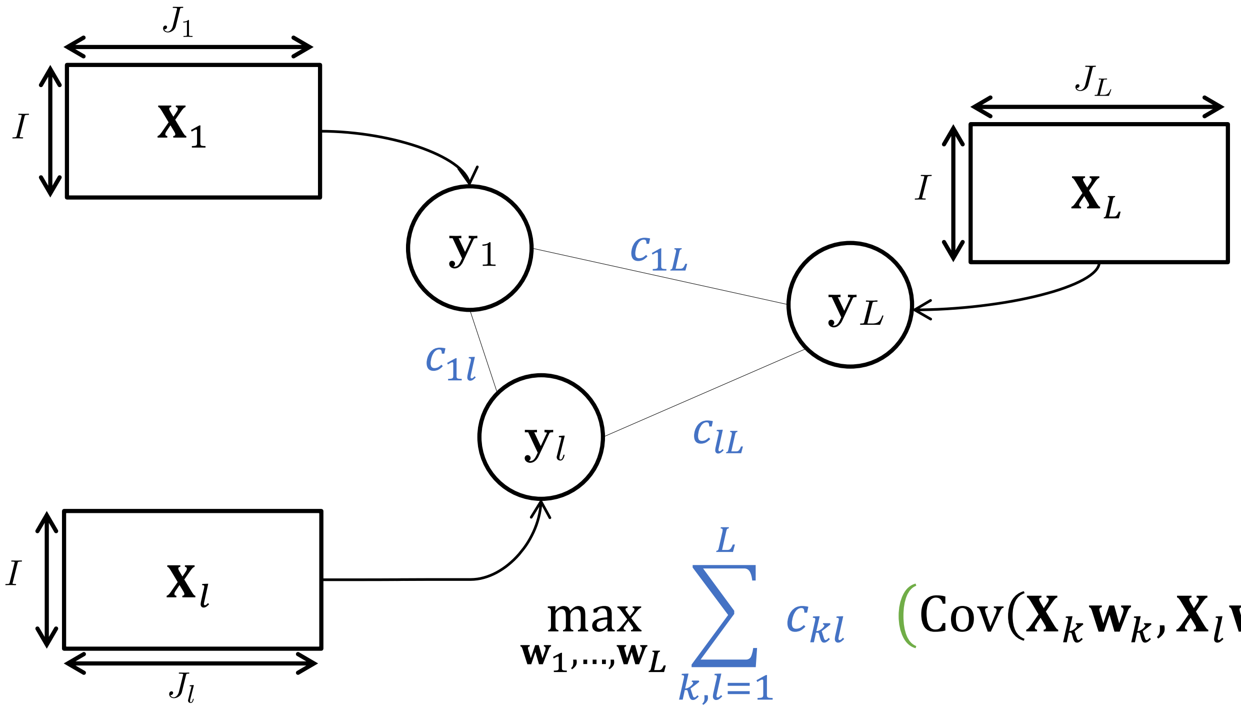


$$\max_{\mathbf{w}_1,\ldots,\mathbf{w}_L} \sum_{k,l=1}^{L} c_{kl} \quad \mathrm{Cov}(\mathbf{X}_k\mathbf{w}_k, \mathbf{X}_l\mathbf{w}_l)$$

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

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

Regularized Generalized Canonical Correlation Analysis (RGCCA)

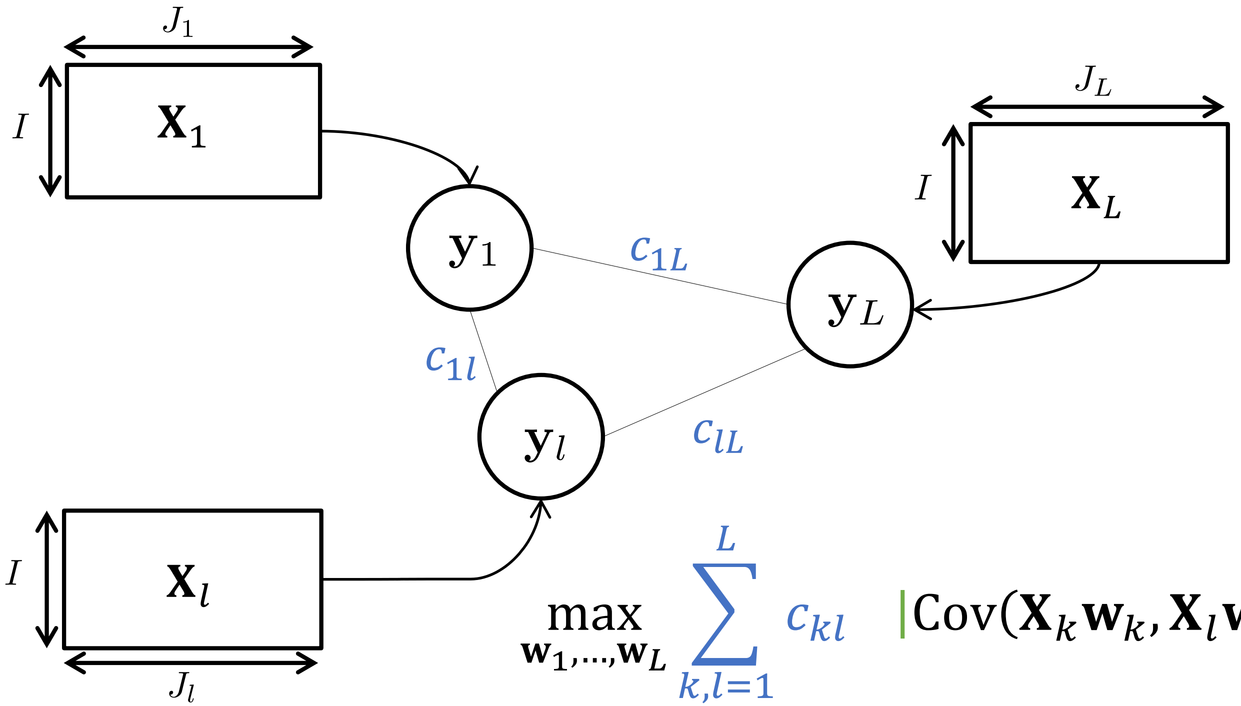


$$\max_{\mathbf{w}_1,\ldots,\mathbf{w}_L} \sum_{k,l=1}^{L} c_{kl} \left(\mathrm{Cov}(\mathbf{X}_k\mathbf{w}_k, \mathbf{X}_l\mathbf{w}_l)\right)^2$$

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

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

Regularized Generalized Canonical Correlation Analysis (RGCCA)

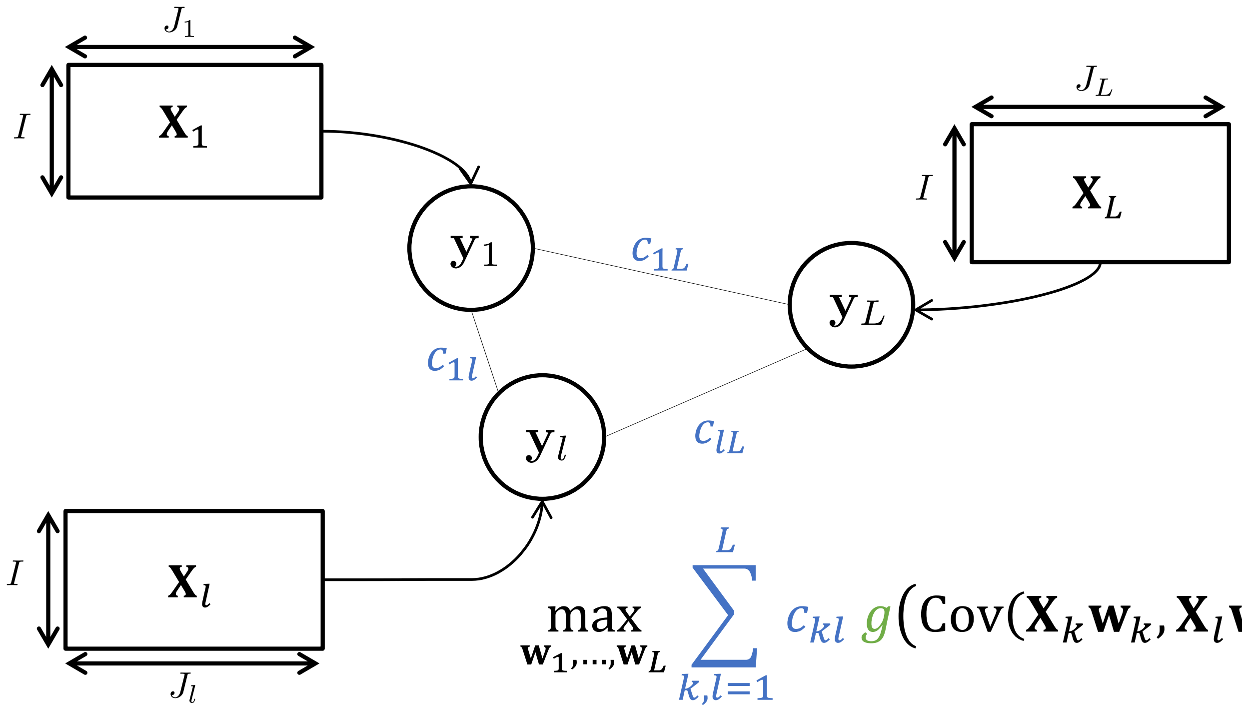


$$\max_{\mathbf{w}_1,\ldots,\mathbf{w}_L} \sum_{k,l=1}^{L} c_{kl} \, |\mathrm{Cov}(\mathbf{X}_k\mathbf{w}_k, \mathbf{X}_l\mathbf{w}_l)|$$

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

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

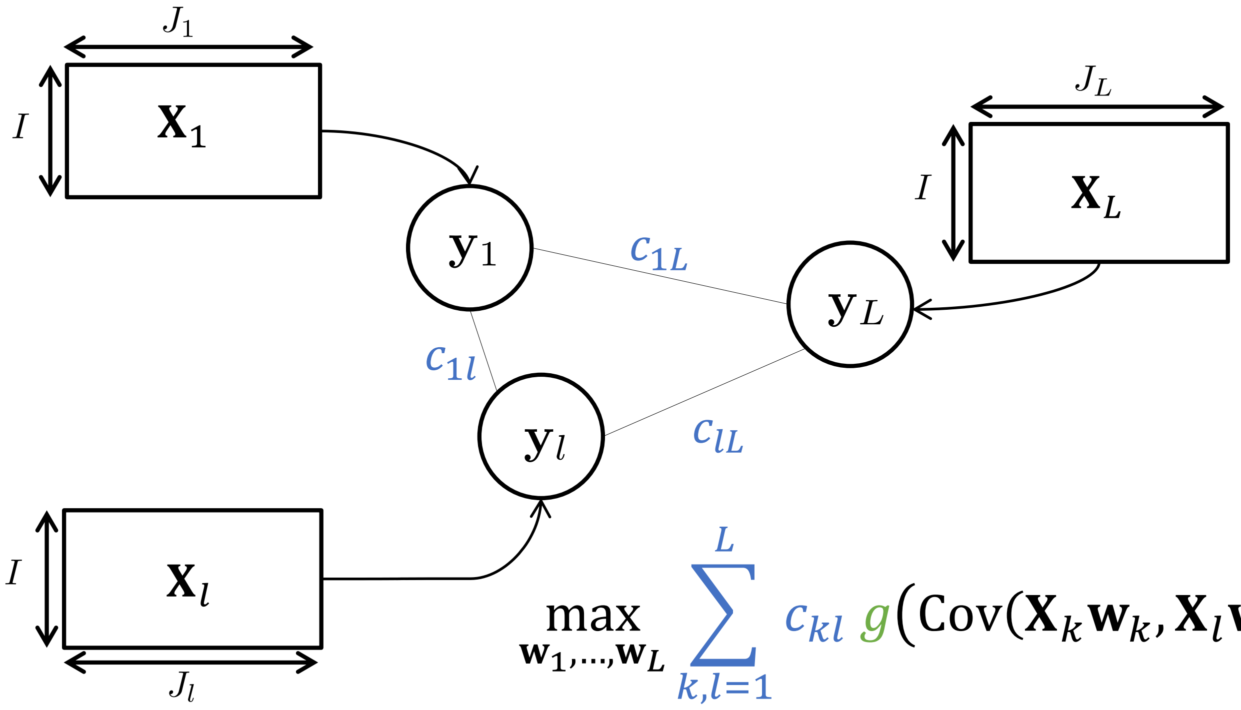
Regularized Generalized Canonical Correlation Analysis (RGCCA)



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

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

Regularized Generalized Canonical Correlation Analysis (RGCCA)



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

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

➡ with g a continuous, convex and derivable function.

Summary of RGCCA

The Regularized Generalized Canonical Correlation Analysis (RGCCA) Optimization criterion :

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

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

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- With "g" a continuous, convex and derivable function.
- $c_{lk} = 1$ for two connected blocks and 0 otherwise.

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- With "g" a continuous, convex and derivable function.
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$$\max_{\mathbf{w}_1,\dots,\mathbf{w}_L} \sum_{k,l=1}^{L} c_{kl}\, g\big(\mathrm{Cov}(\mathbf{X}_k\mathbf{w}_k, \mathbf{X}_l\mathbf{w}_l)\big)$$

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

- With "g" a continuous, convex and derivable function.
- $c_{lk} = 1$ for two connected blocks and 0 otherwise.
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Most of the time (this is the case today !) $\mathbf{M}_l$ is chosen such that:

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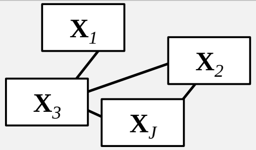
Overview of the Multi-Block litterature

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



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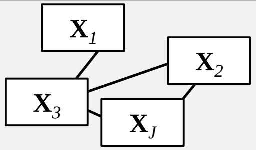

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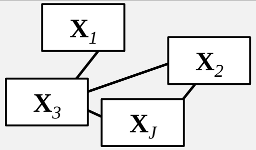

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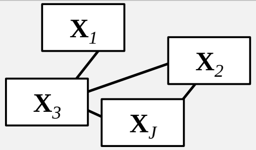

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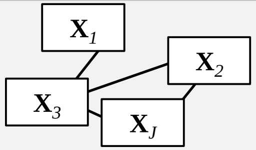
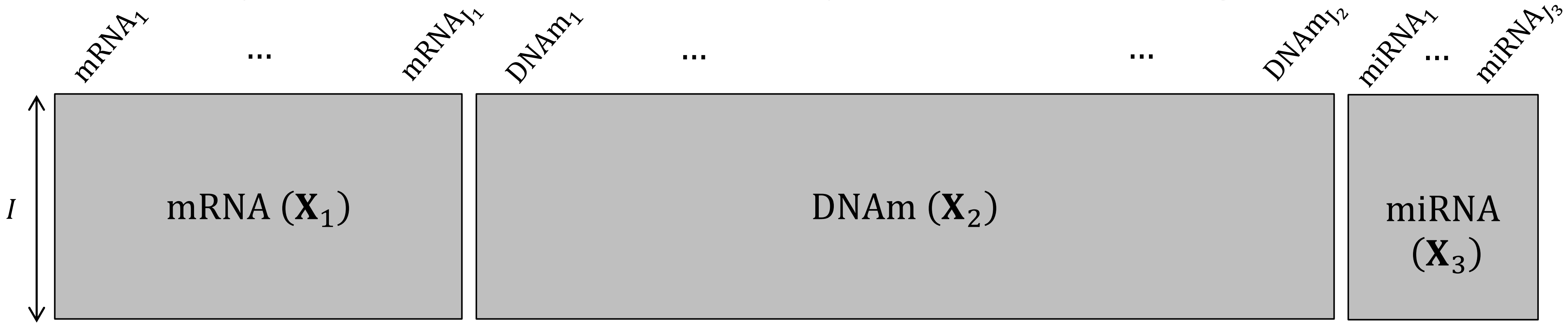


Courtesy to Arthur Tenenhaus.

Tune parameters in an unsupervised setting



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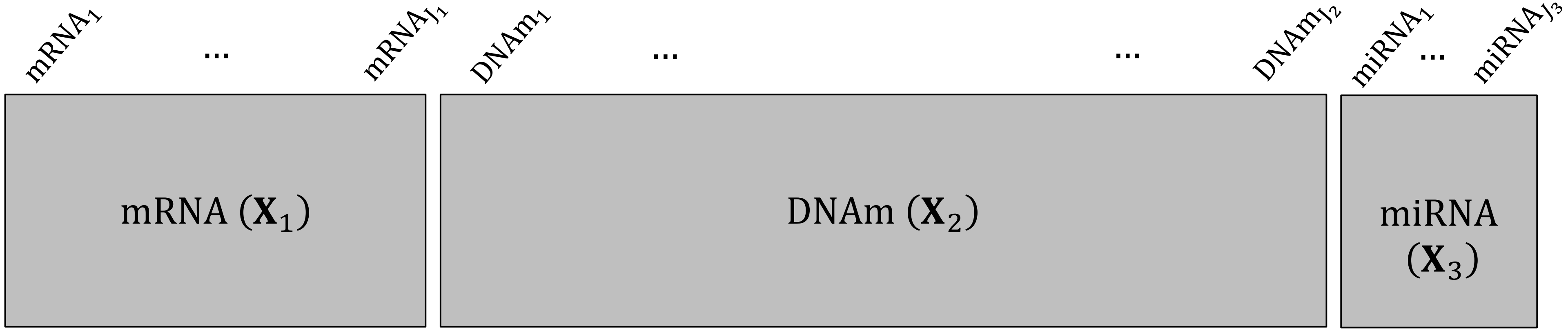

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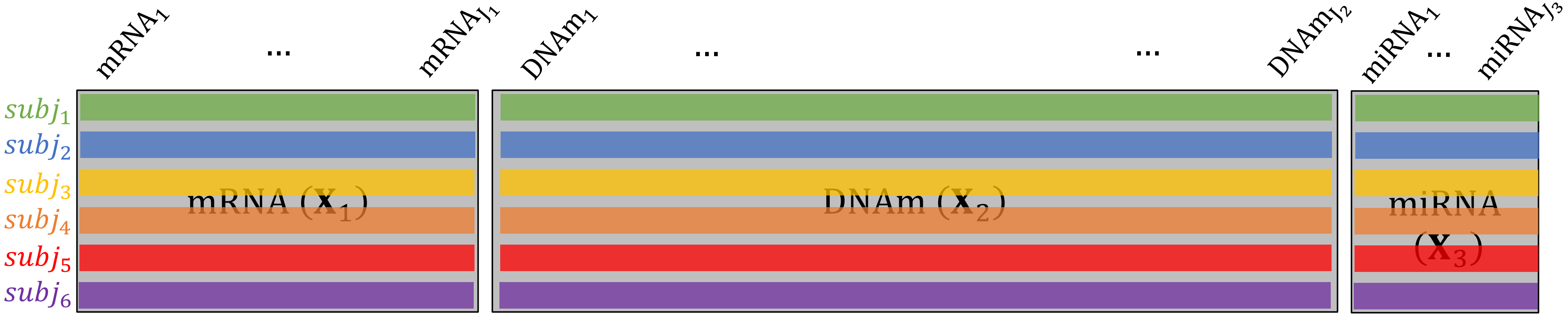

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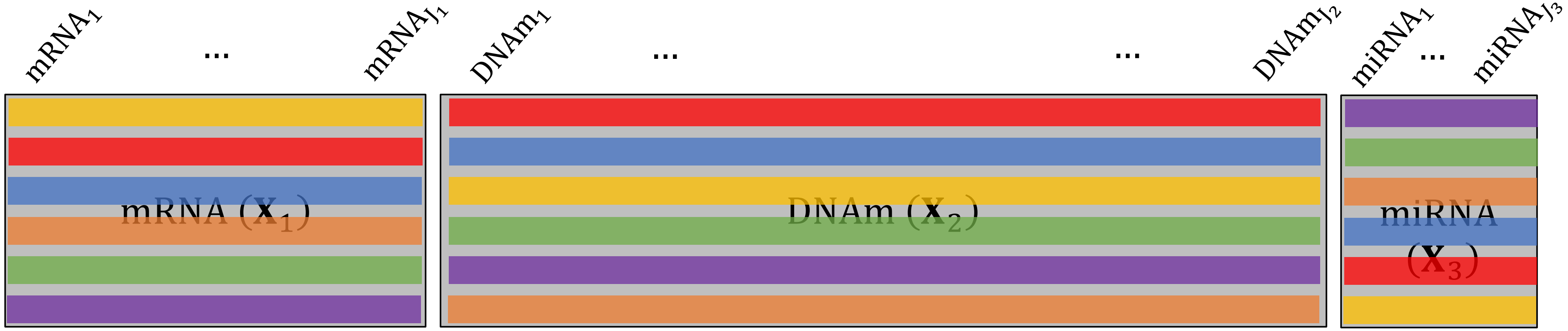
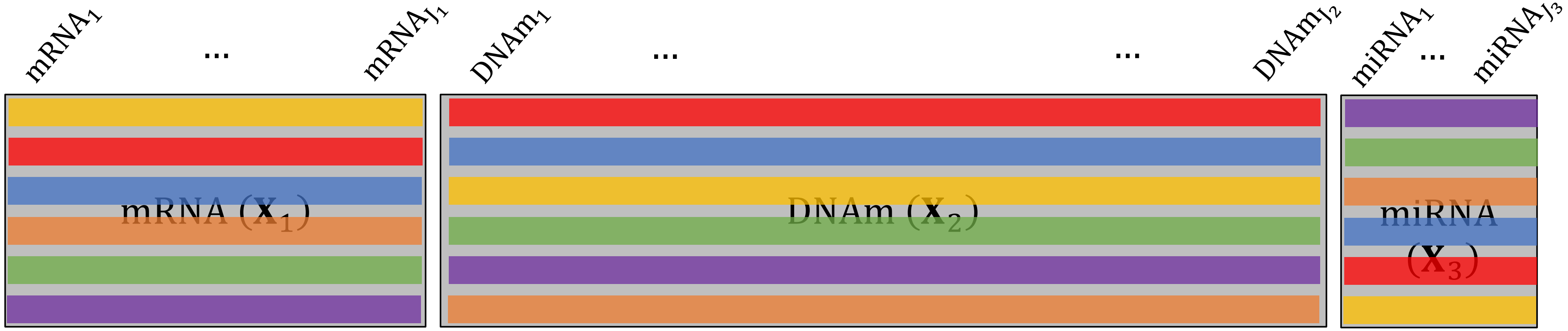


Permutation n°1

Tune parameters in an unsupervised setting



Permutation n°1

Parameter set n°1

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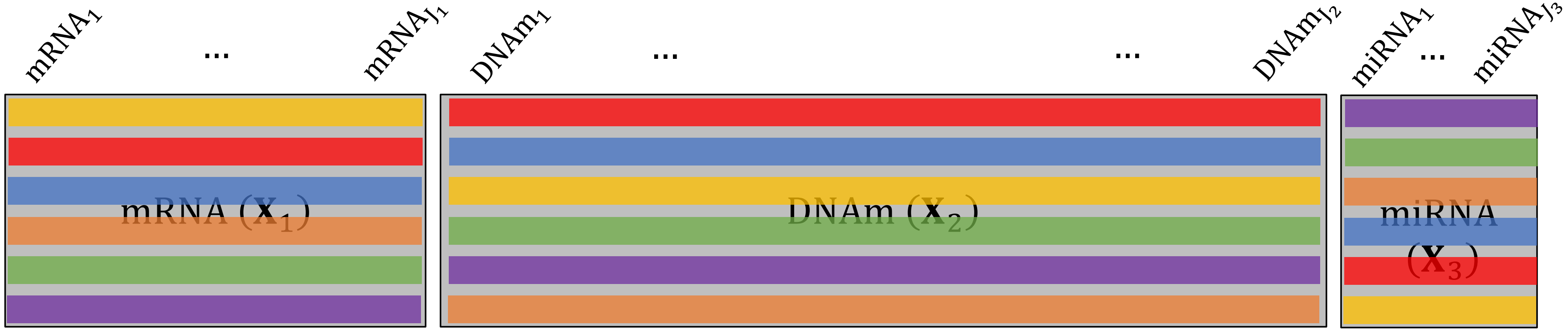

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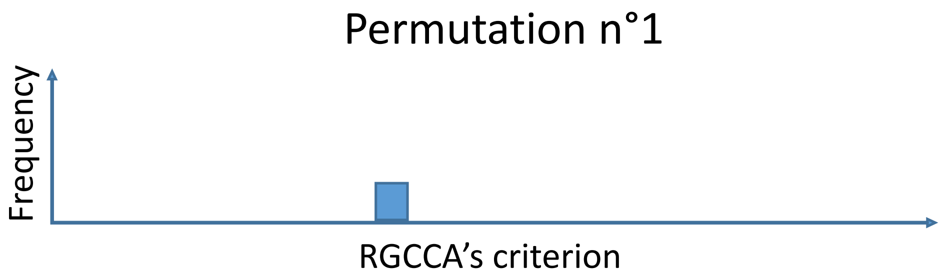

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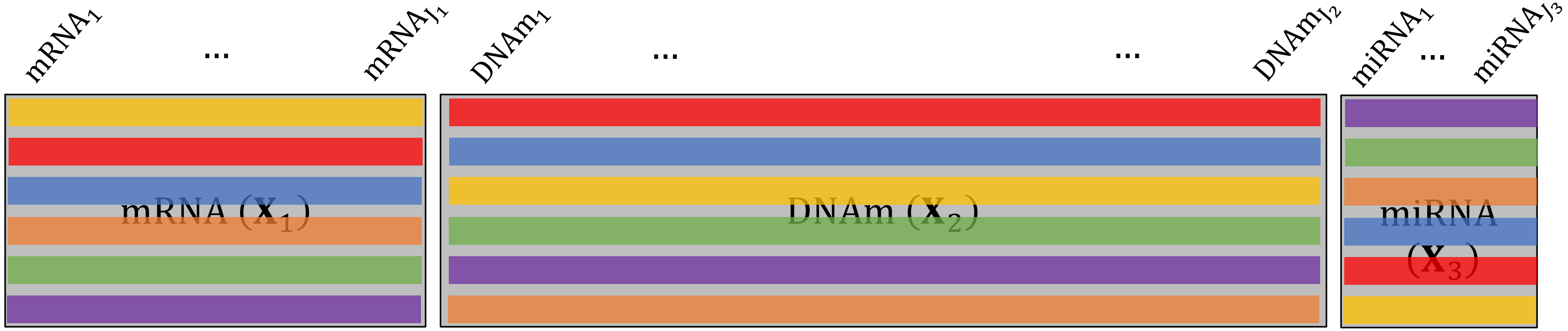

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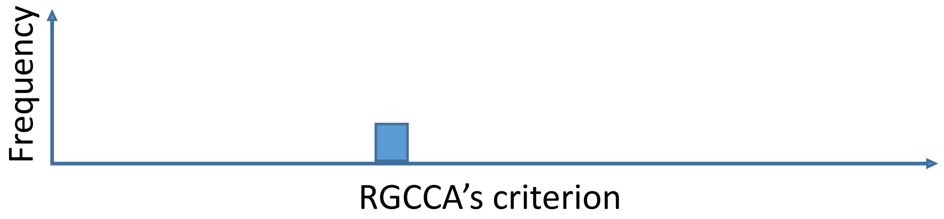
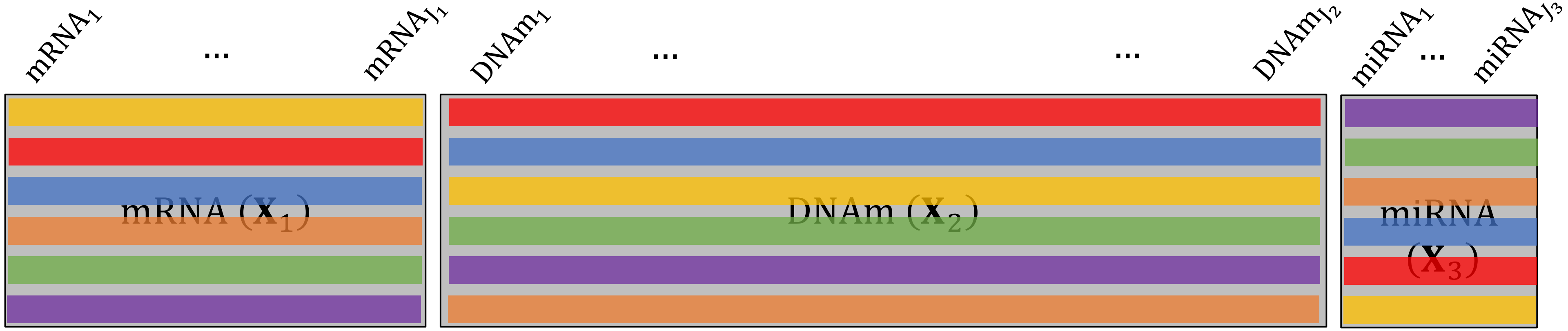


⋮

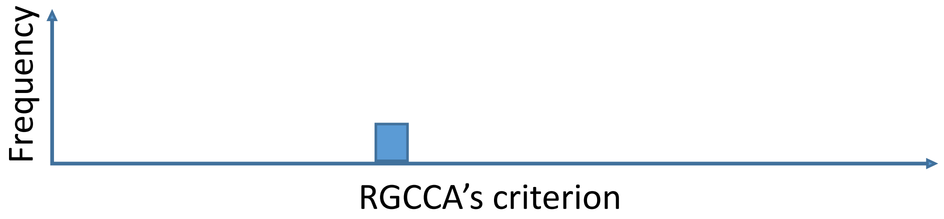
Parameter set n°K

Tune parameters in an unsupervised setting



Permutation n°1

Parameter set n°1



⋮ ⋮

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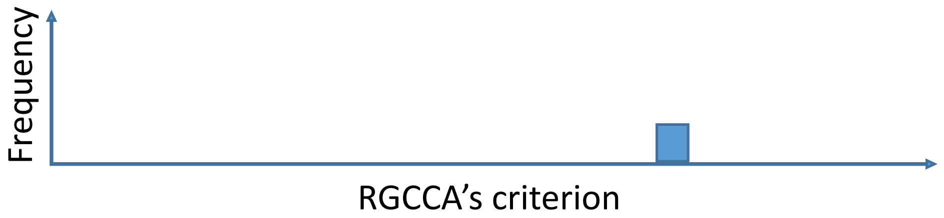
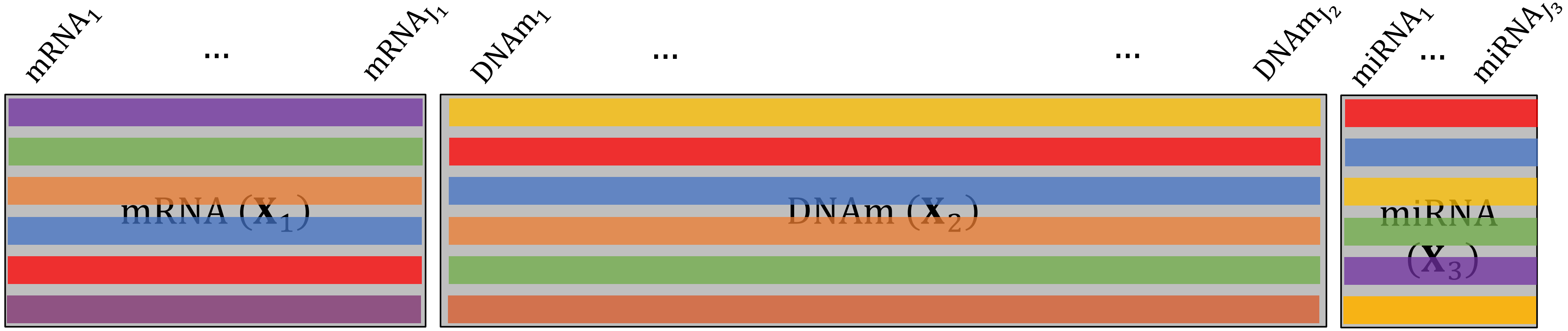
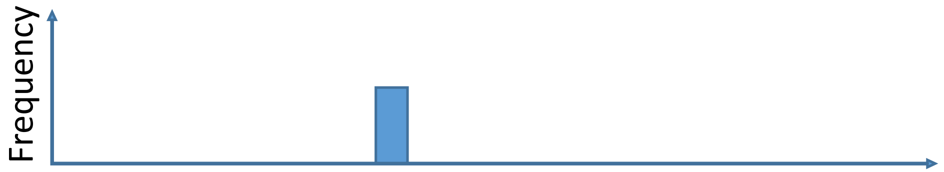


Tune parameters in an unsupervised setting



Permutation n°2

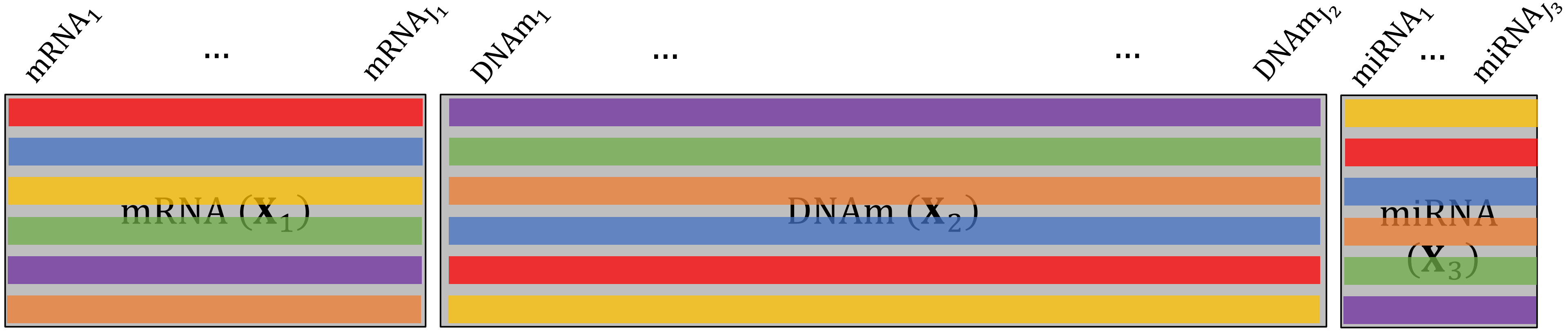
Parameter set n°1



⋮ ⋮

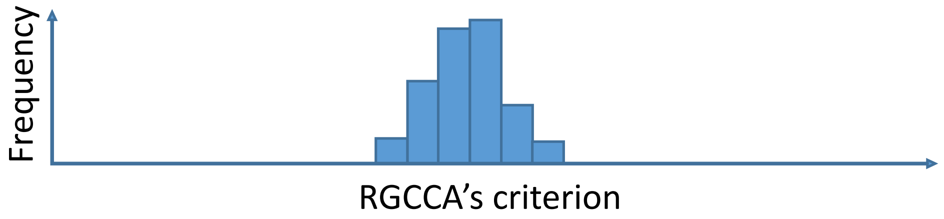
Parameter set n°K

Tune parameters in an unsupervised setting



Permutation n°N

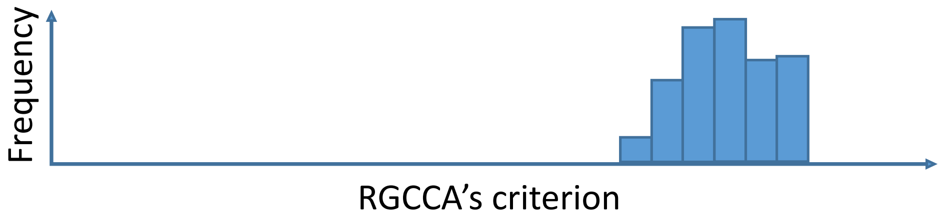
Parameter set n°1



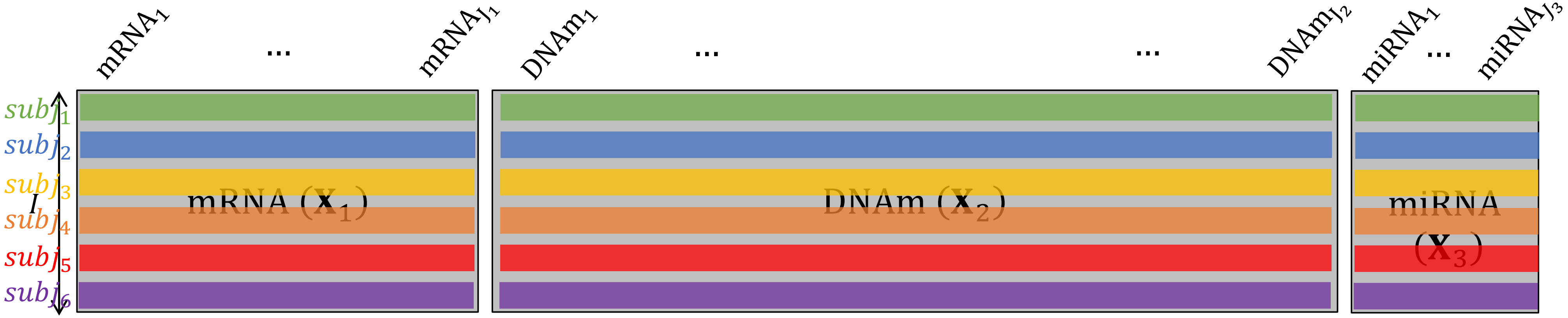
⋮

⋮

Parameter set n°K

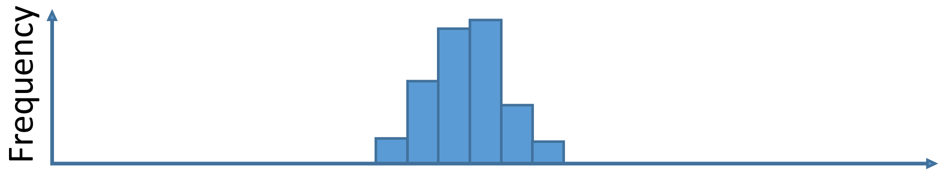


Tune parameters in an unsupervised setting



No Permutation

Parameter set n°1



⋮ ⋮

Parameter set n°K

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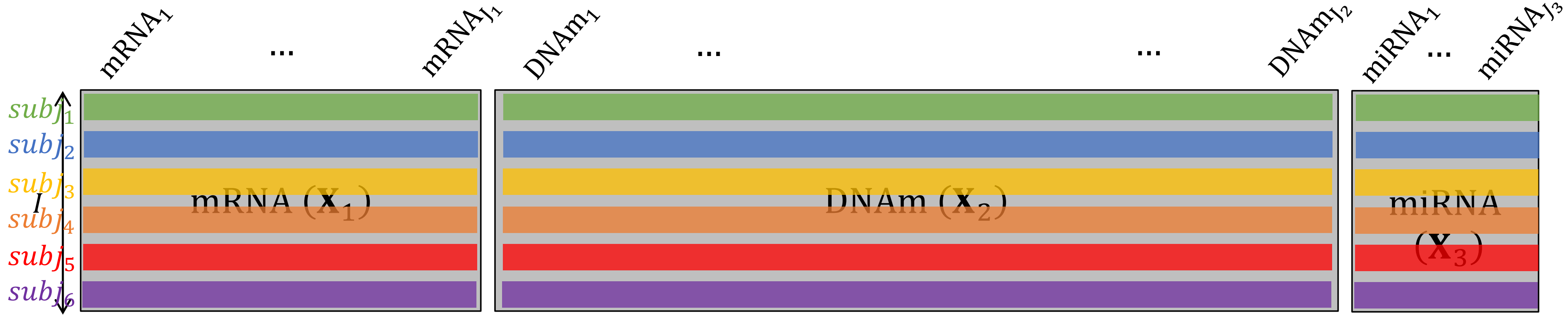

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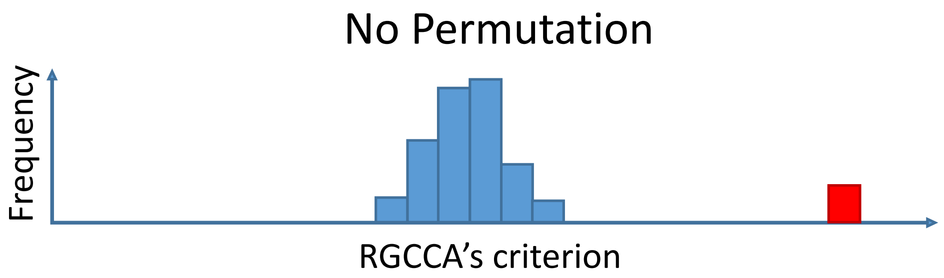

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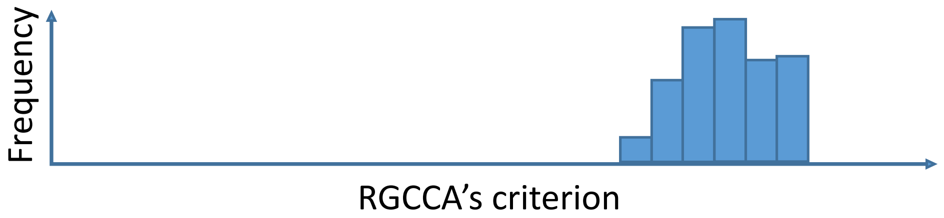
Parameter set n°K



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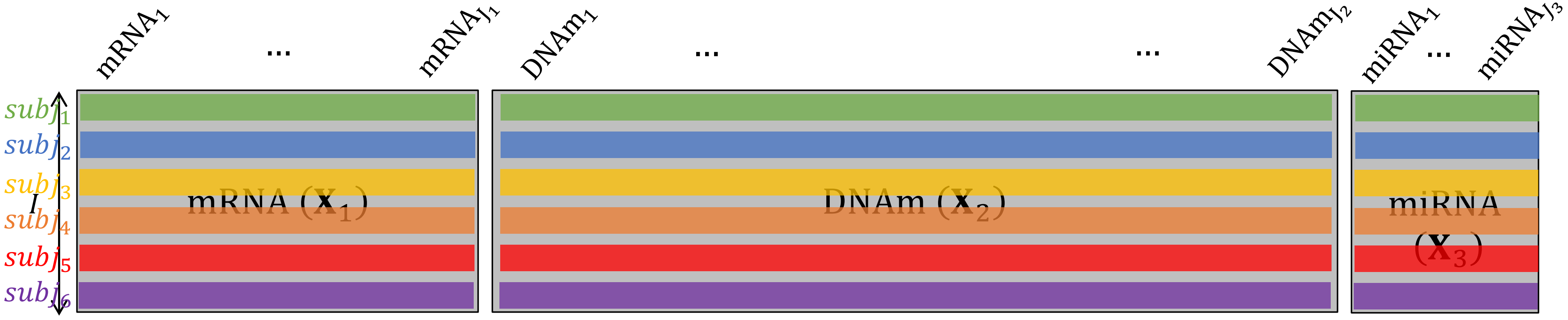

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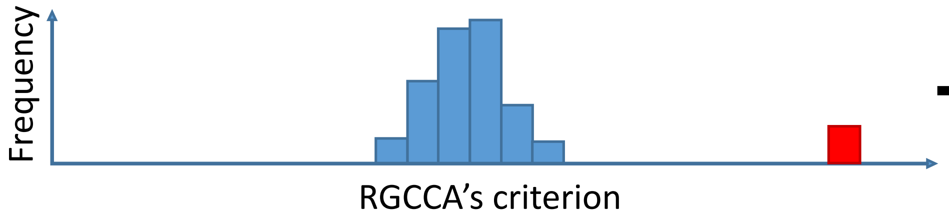
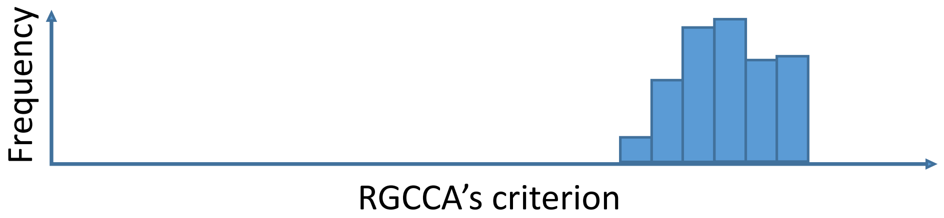


➔ The set of parameters is likely to be selected.

⋮ ⋮

Parameter set n°K



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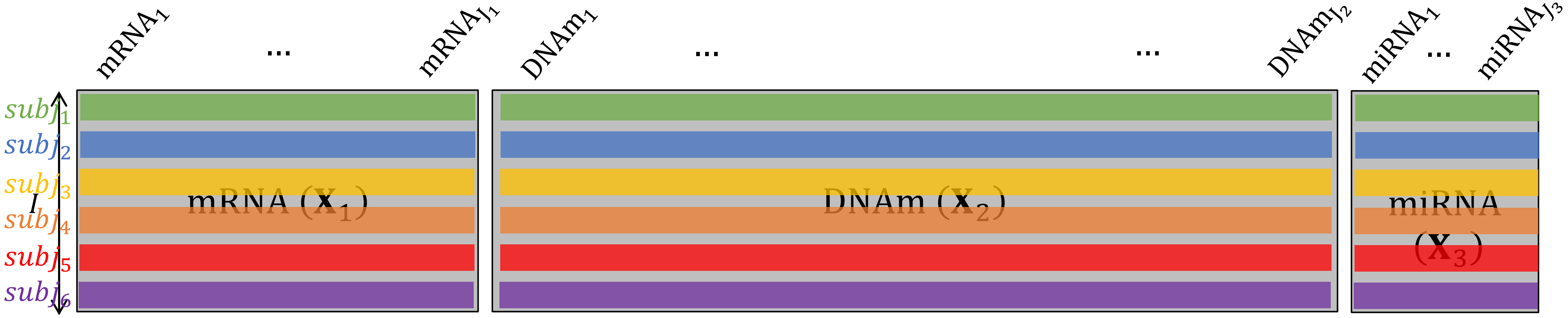

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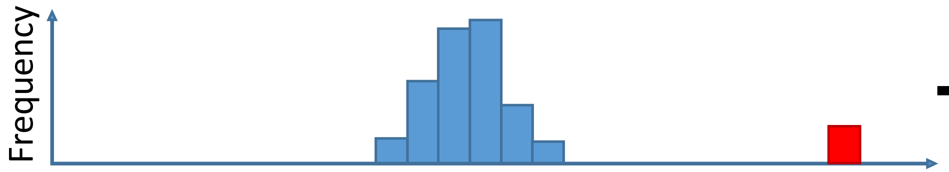

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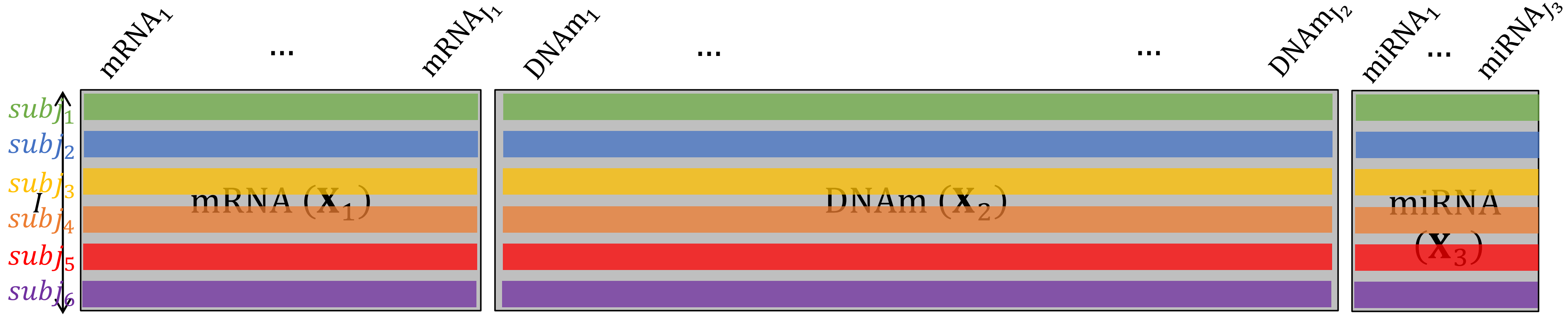

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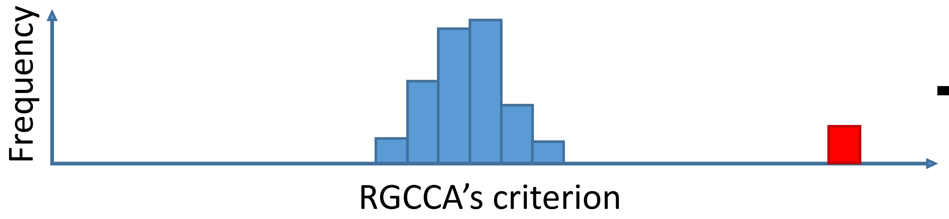

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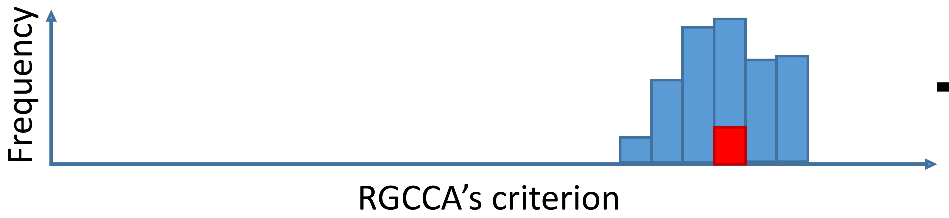

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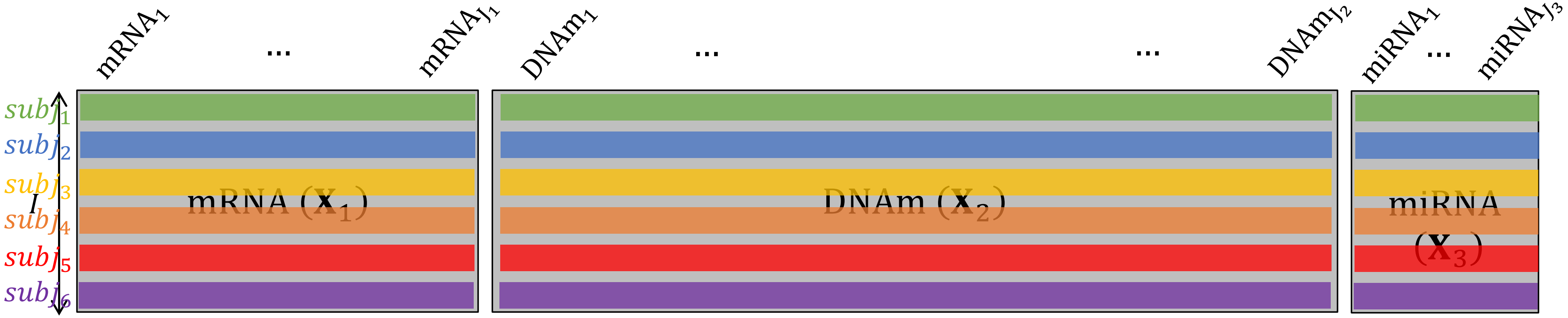

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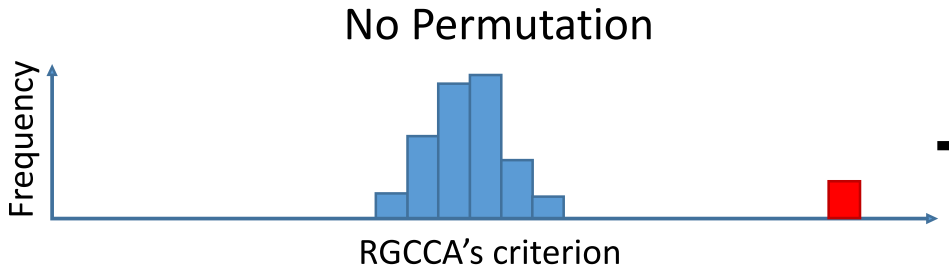

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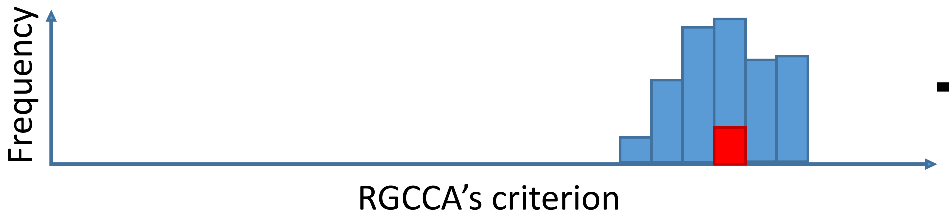
⋮

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



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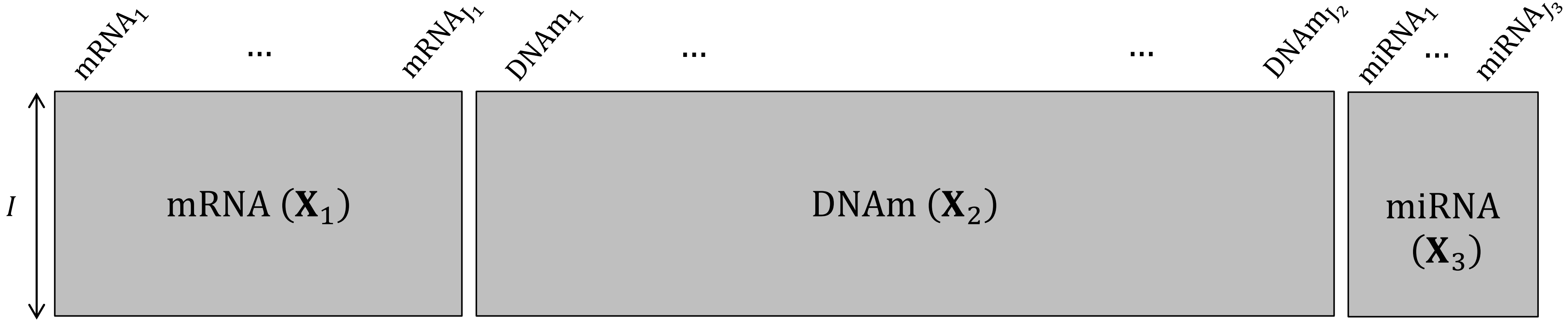
Evaluate the robustness of the model by bootstrapping.



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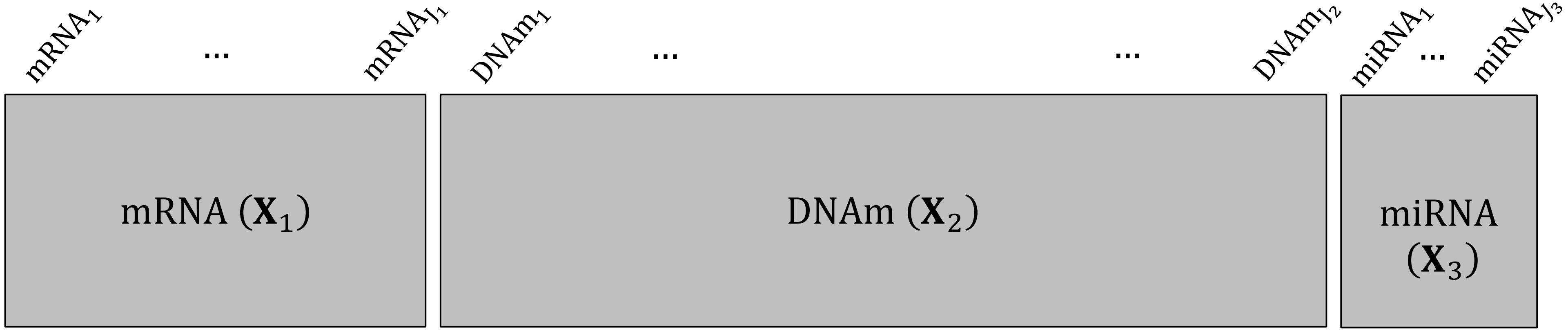

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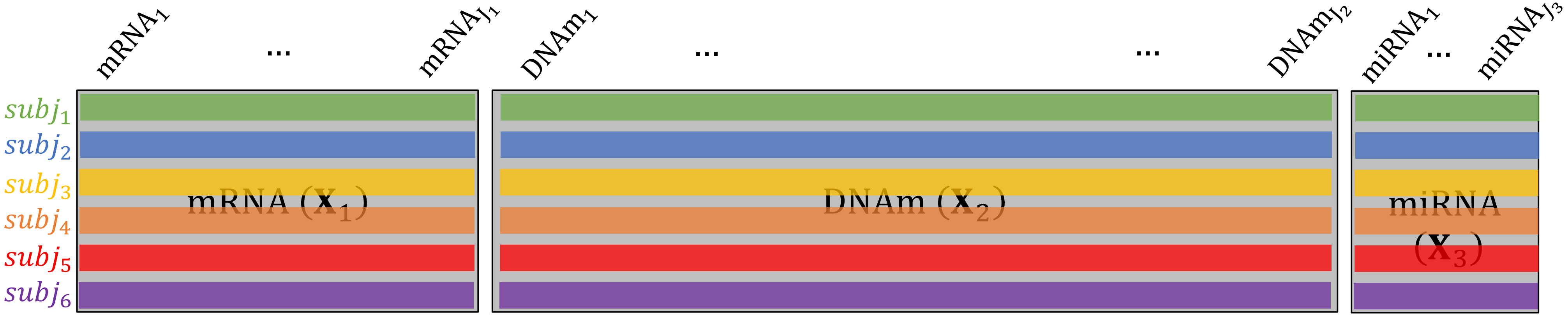

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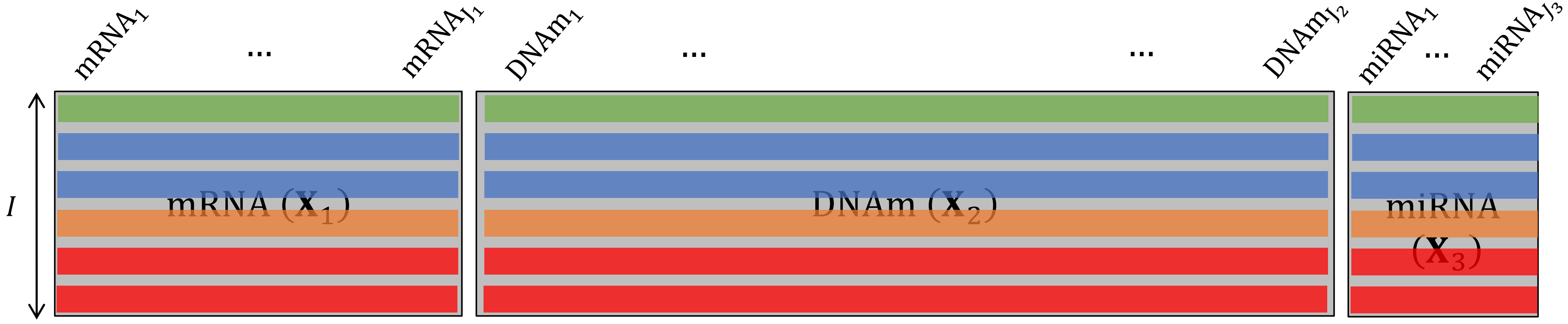

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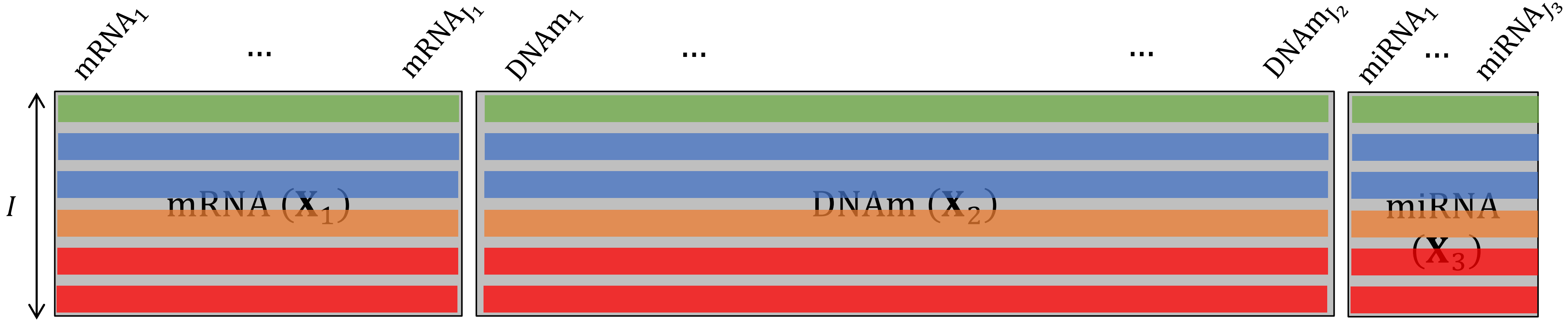

Bootstrap sample n°1

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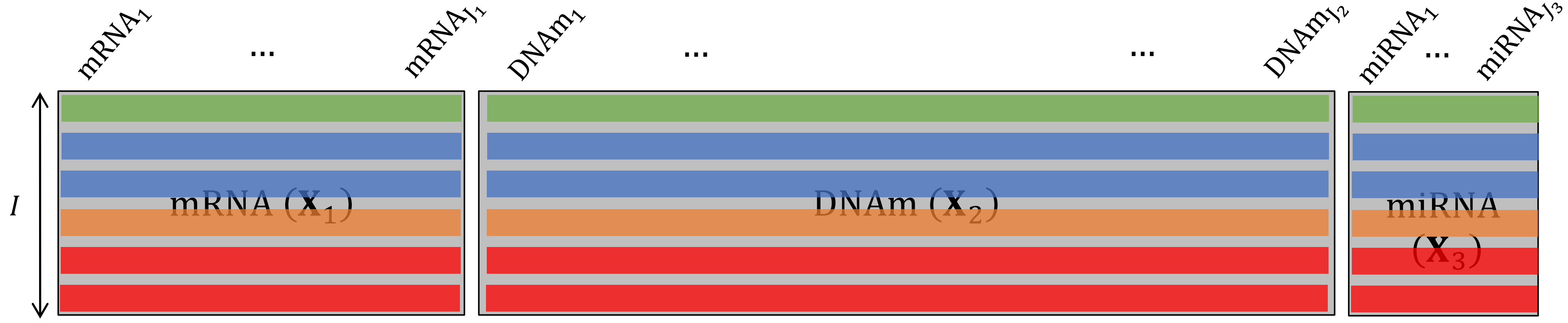

Bootstrap sample n°1

Weight for mRNA$_1$

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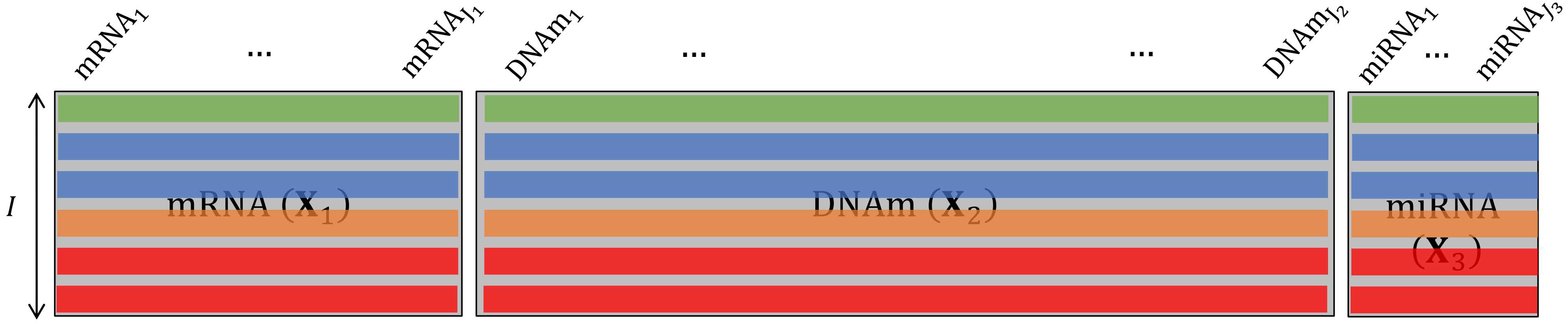
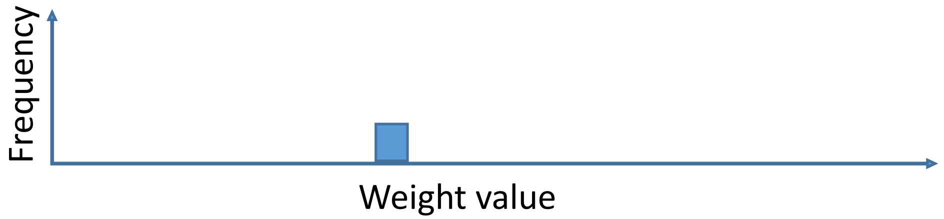
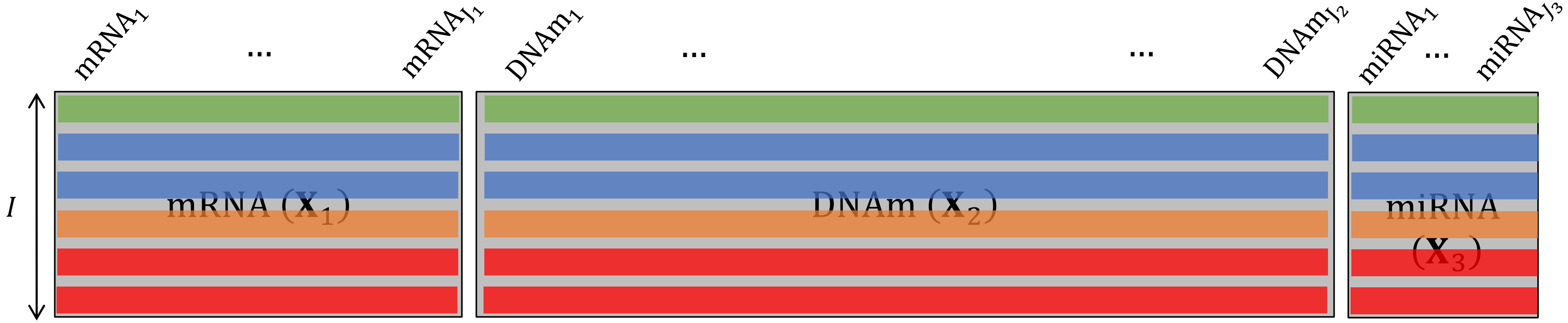


Bootstrap sample n°1

Weight for mRNA_1

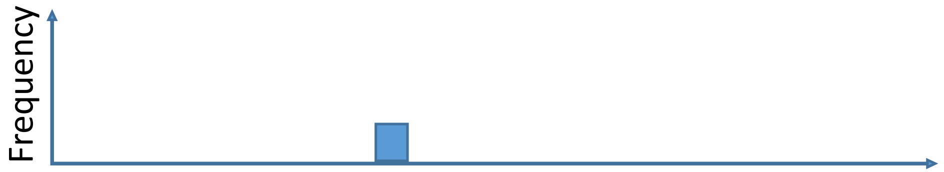


Evaluate the robustness of the model by bootstrapping.



Bootstrap sample n°1

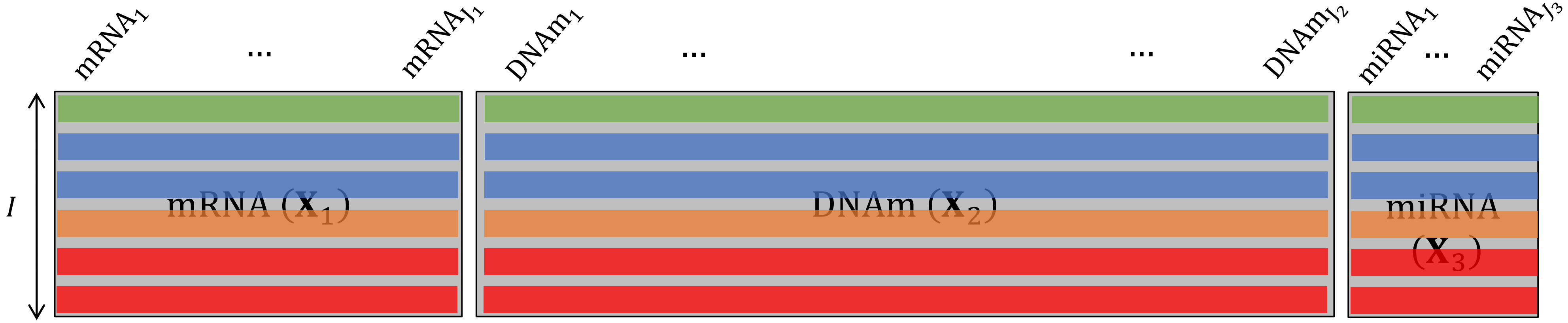
Weight for mRNA$_1$



⋮

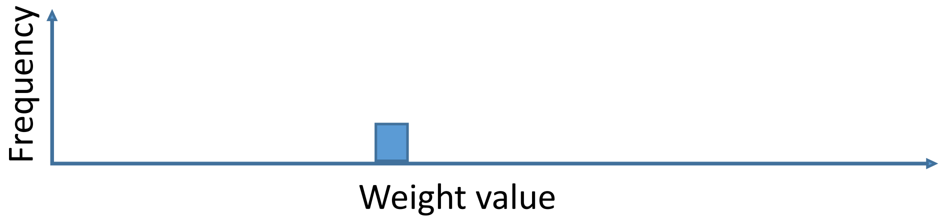
Weight for miRNA$_{J_3}$

Evaluate the robustness of the model by bootstrapping.



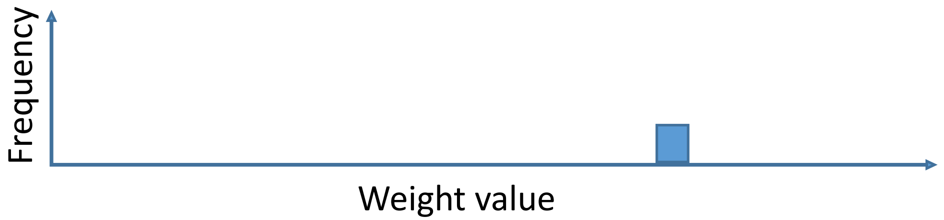
Bootstrap sample n°1

Weight for mRNA_1



⋮ ⋮

Weight for miRNA_{J_3}



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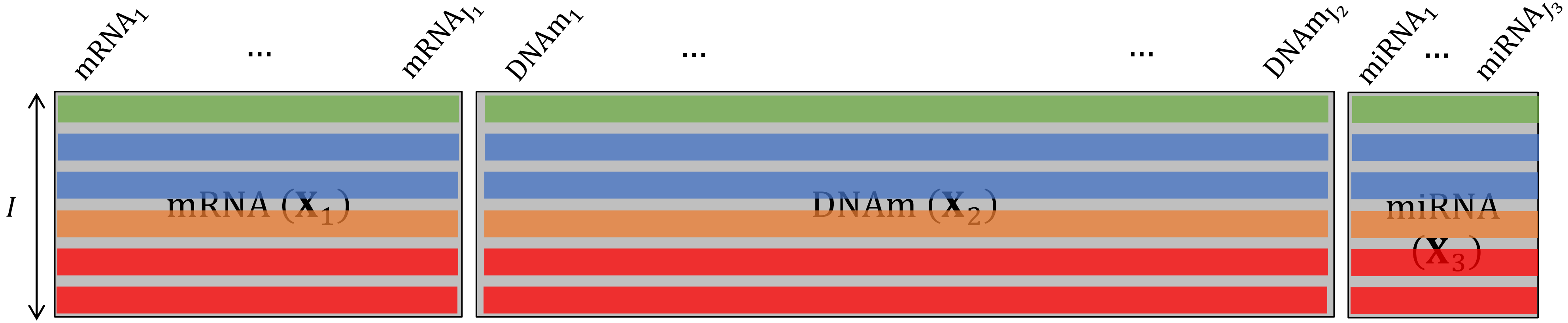
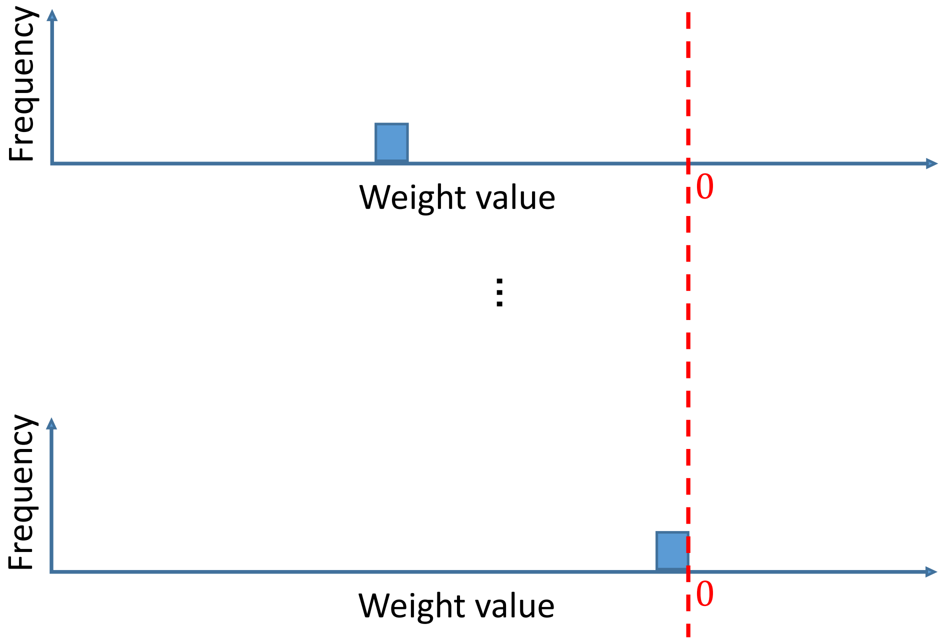


Bootstrap sample n°1

Weight for mRNA$_1$

⋮

Weight for miRNA$_{J_3}$



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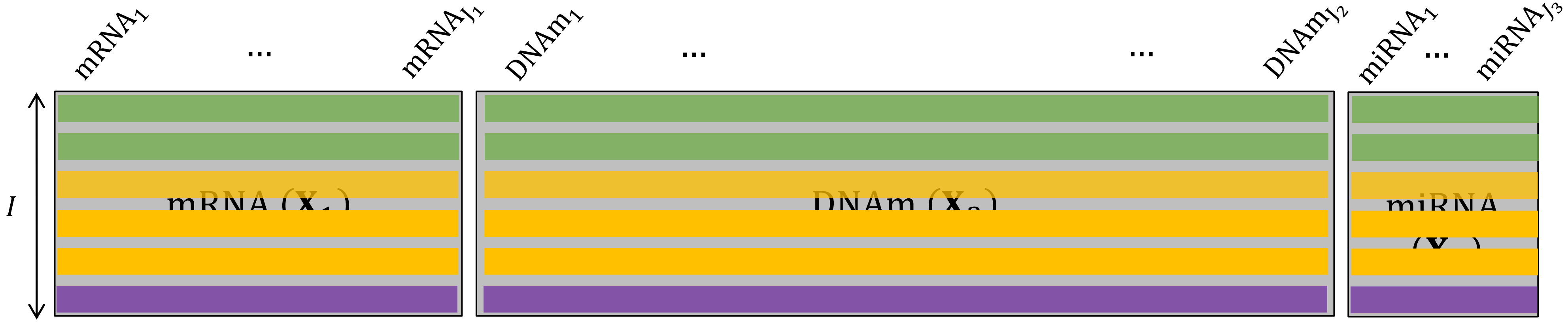
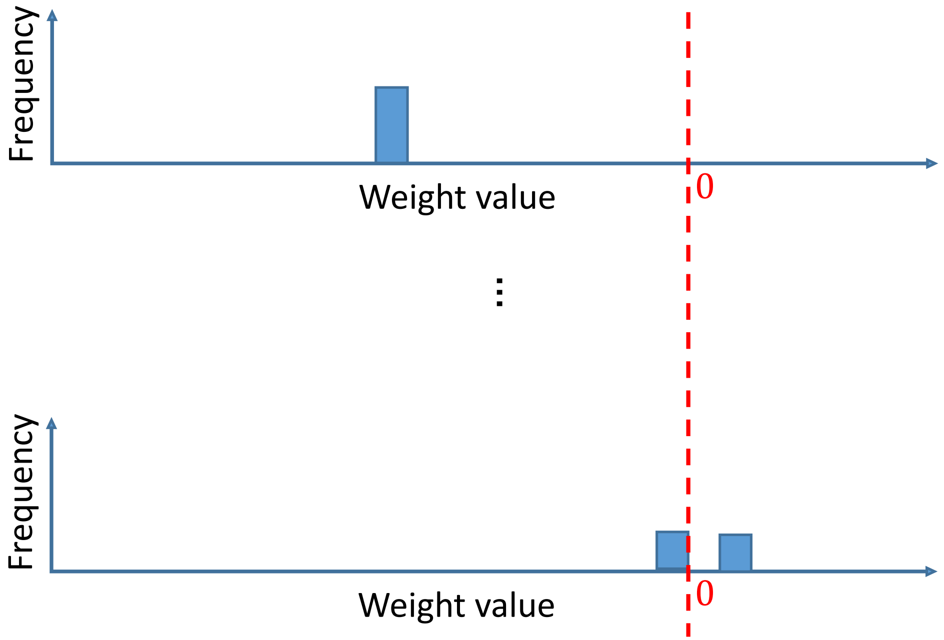


Bootstrap sample n°2

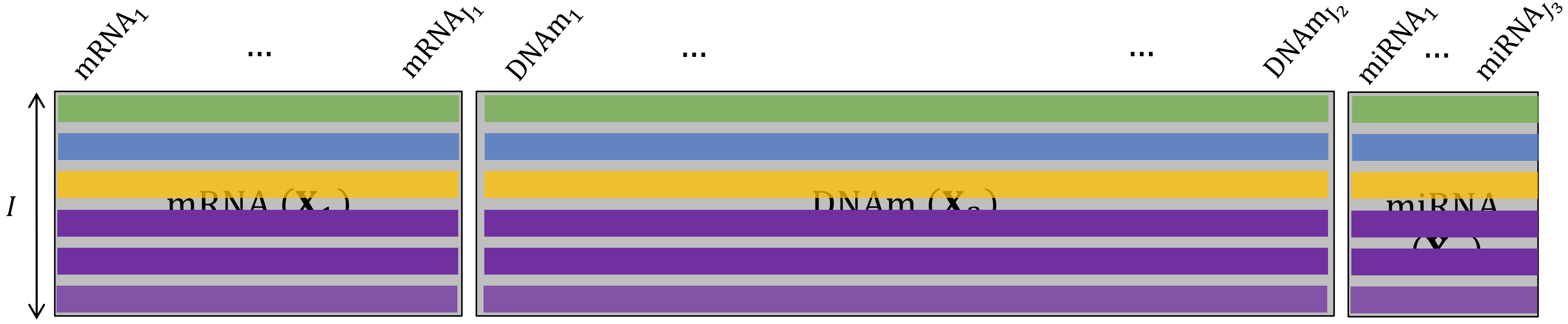
Weight for mRNA_1

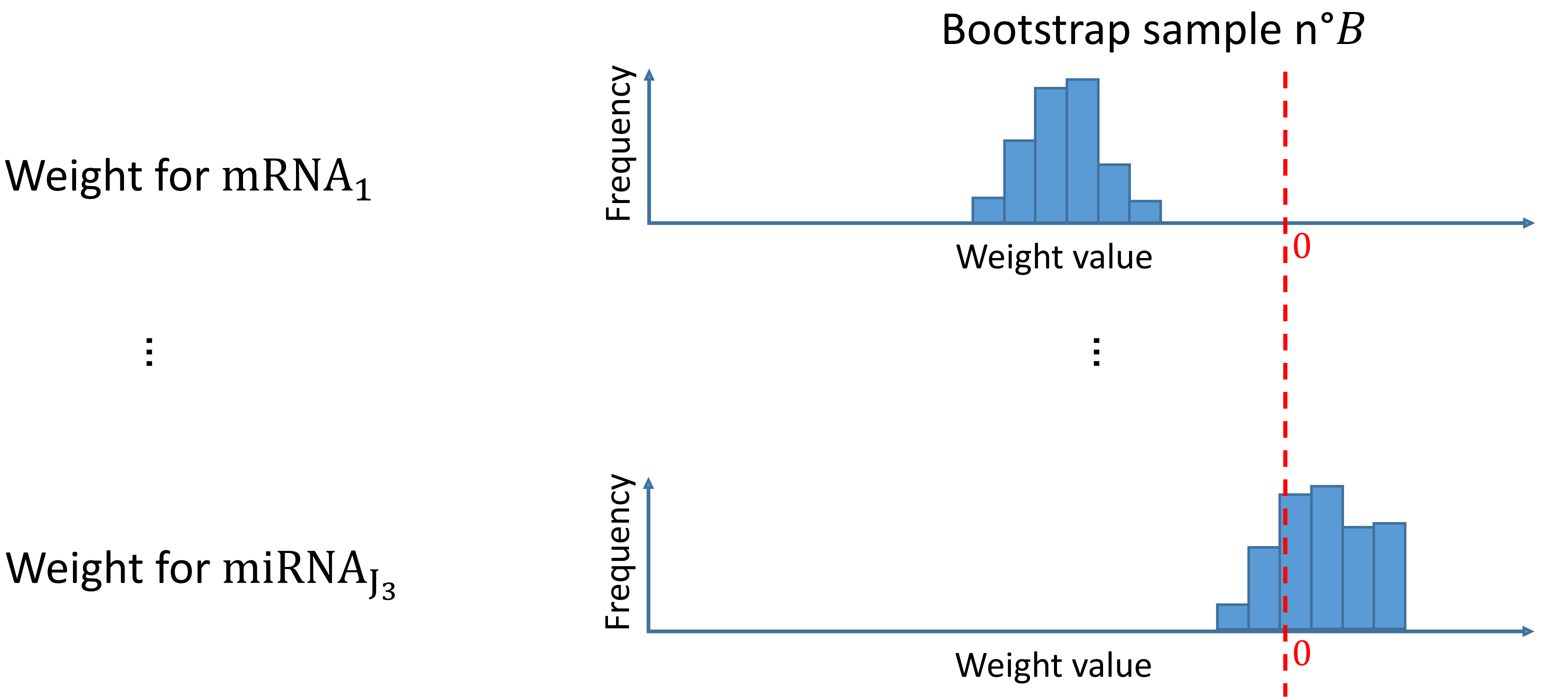
⋮

Weight for miRNA_{J_3}

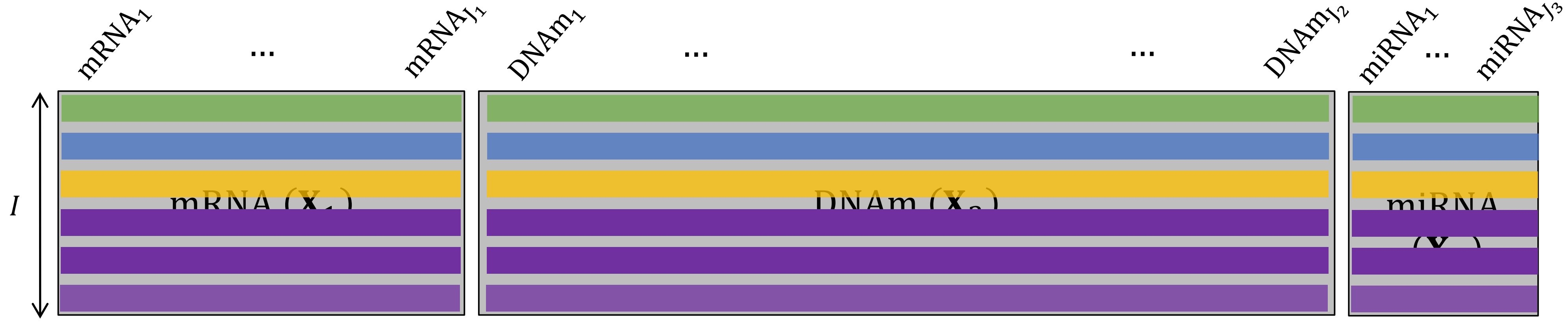


Evaluate the robustness of the model by bootstrapping.



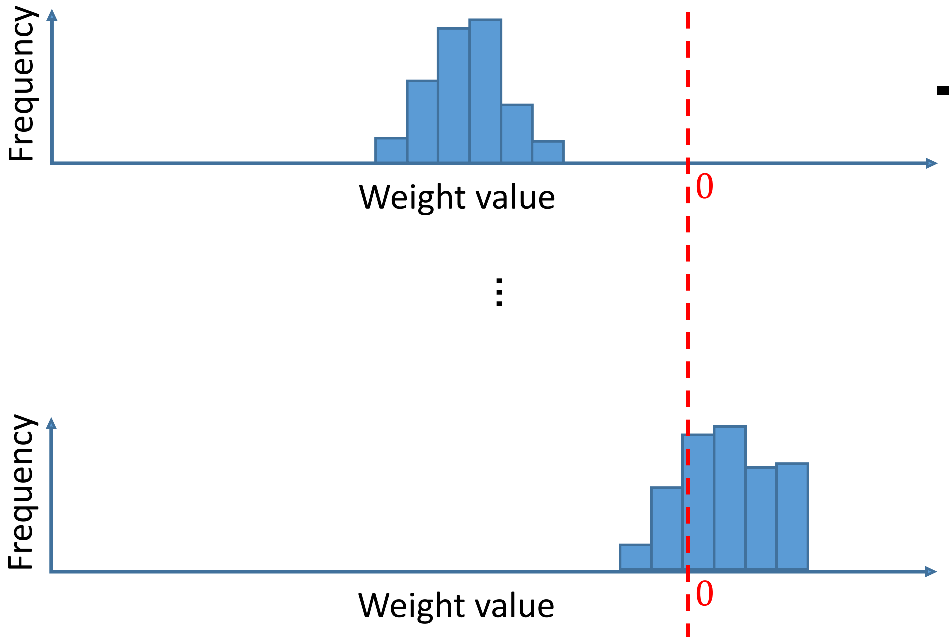


Evaluate the robustness of the model by bootstrapping.



Bootstrap sample n°B

Weight for mRNA_1

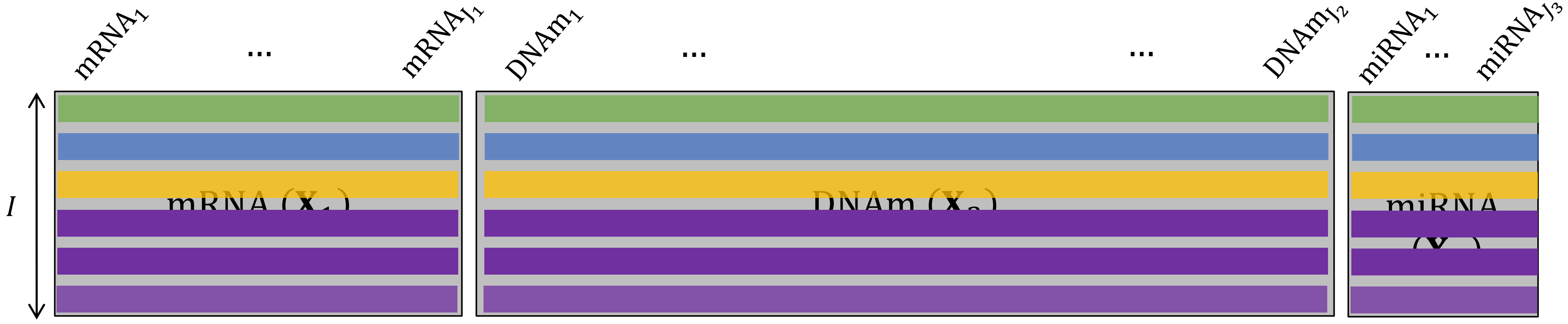


⋮

Weight for miRNA_{J_3}

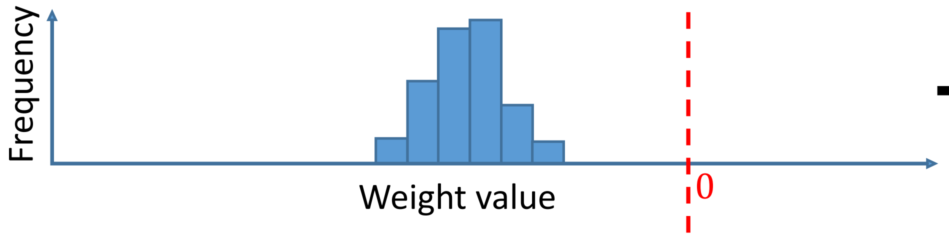
➔ The weight is likely to be considered as significantly different from 0.

Evaluate the robustness of the model by bootstrapping.



Bootstrap sample n°B

Weight for mRNA$_1$



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⋮

Weight for miRNA$_{J_3}$

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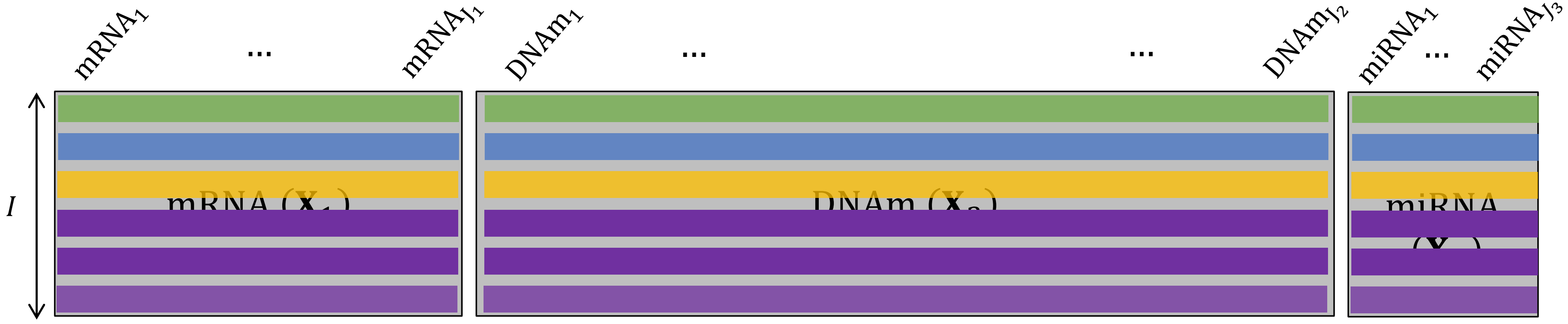

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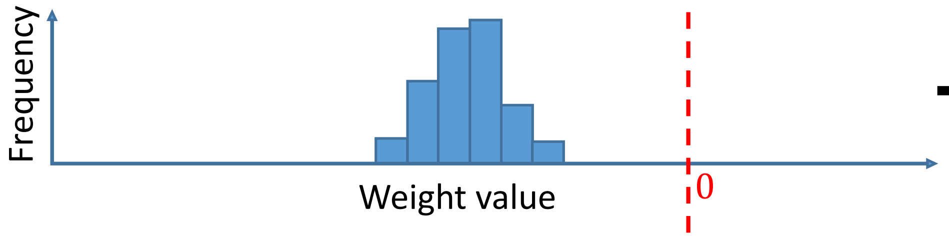
Weight for mRNA$_1$



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

⋮

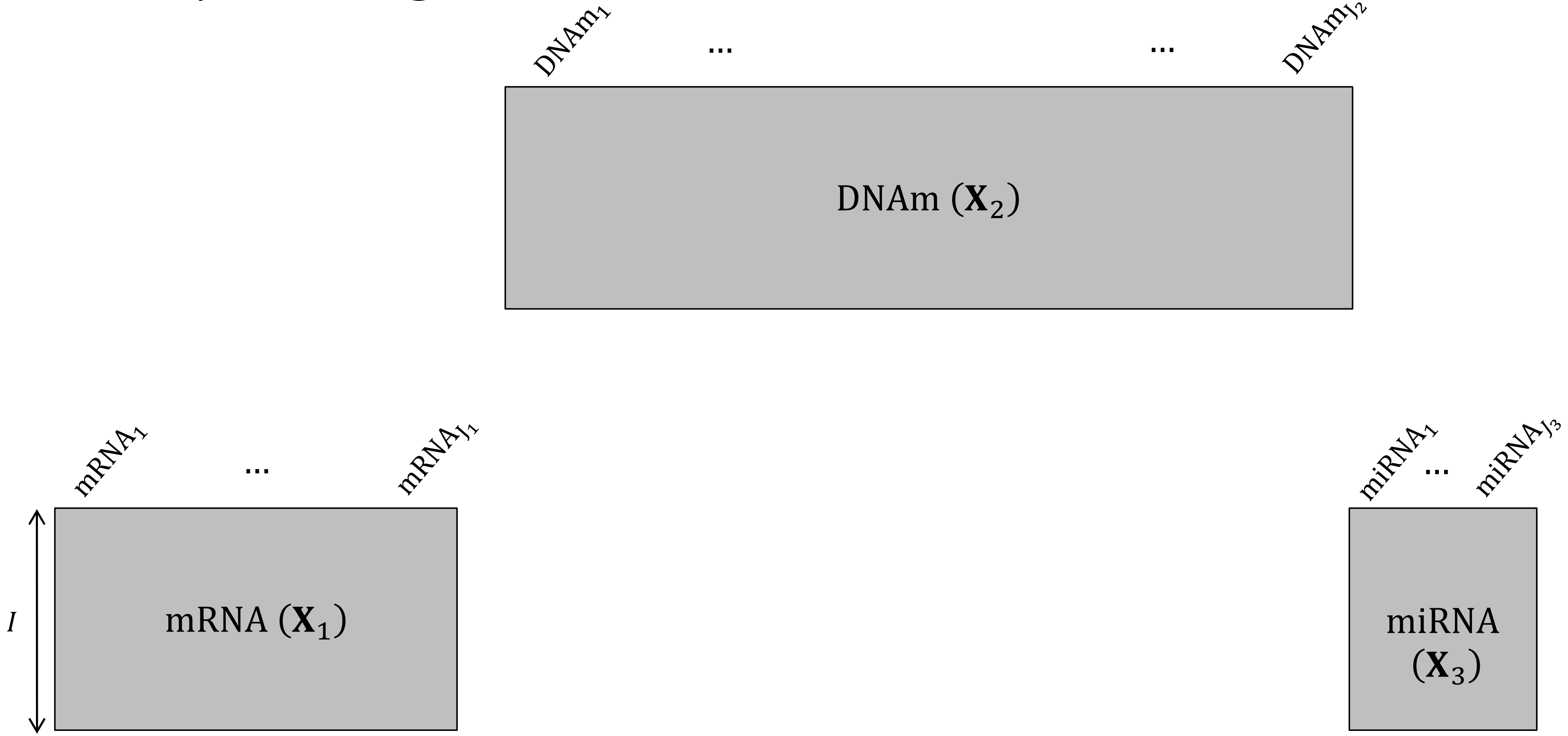
Out of these distributions, RGCCA non-parametrically estimates confidence intervals $([q_{0.025}, q_{0.975}])$ and p-values $\left(min(Nb_{\geq 0}, Nb_{\leq 0})/max(Nb_{\geq 0}, Nb_{\leq 0})\right)$.

Weight for miRNA$_{J_3}$

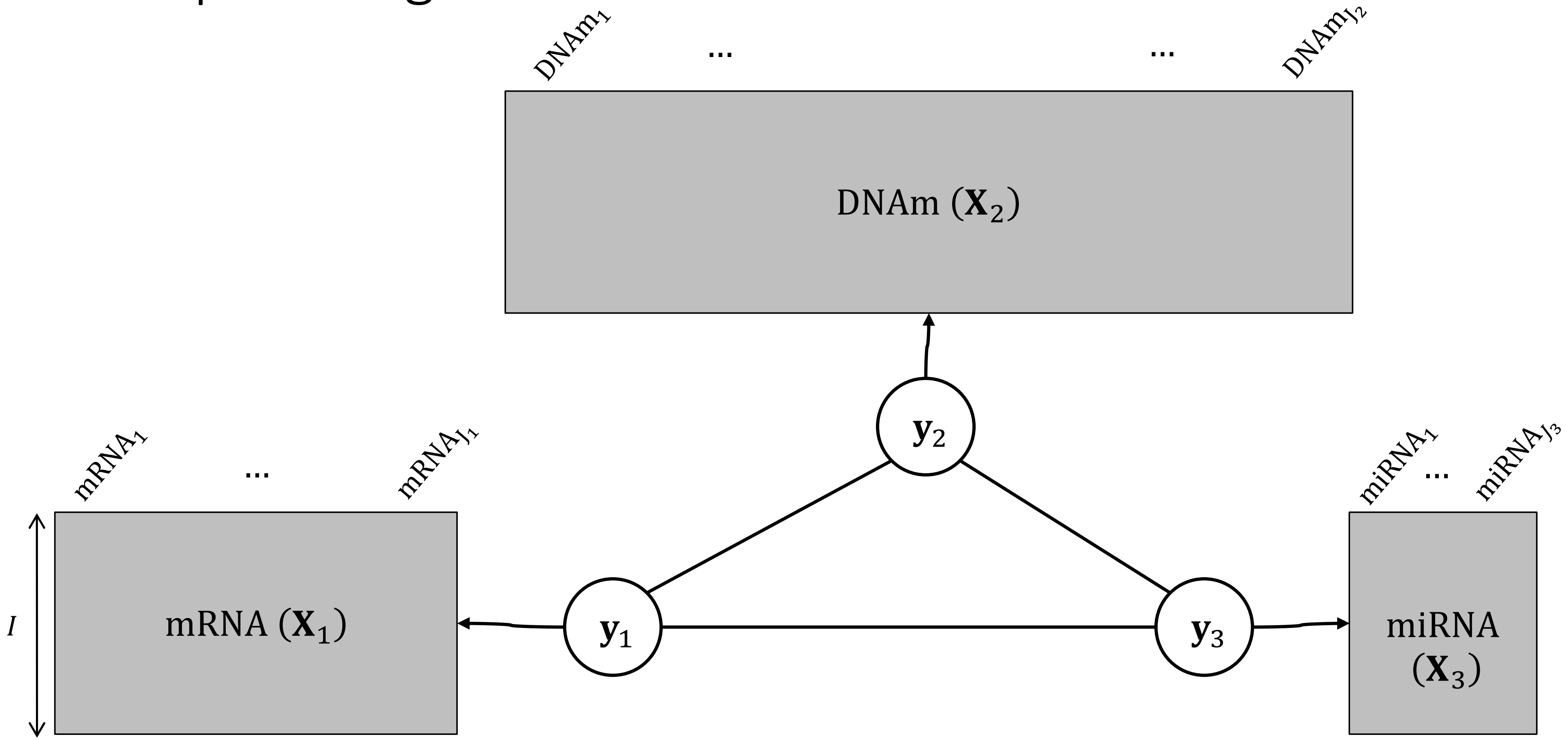
➔ The weight is unlikely to be considered as significantly different from 0.

5. Supervised analysis with L-blocks

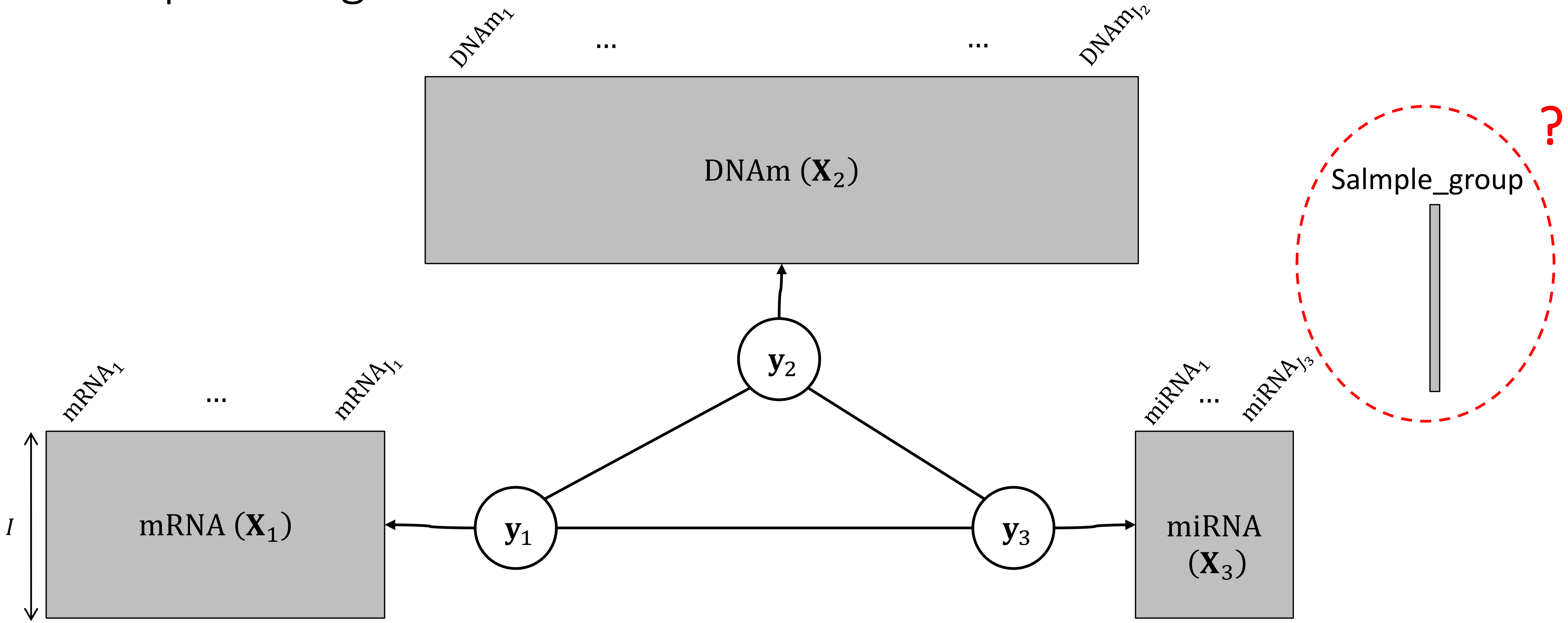
Supervising with RGCCA



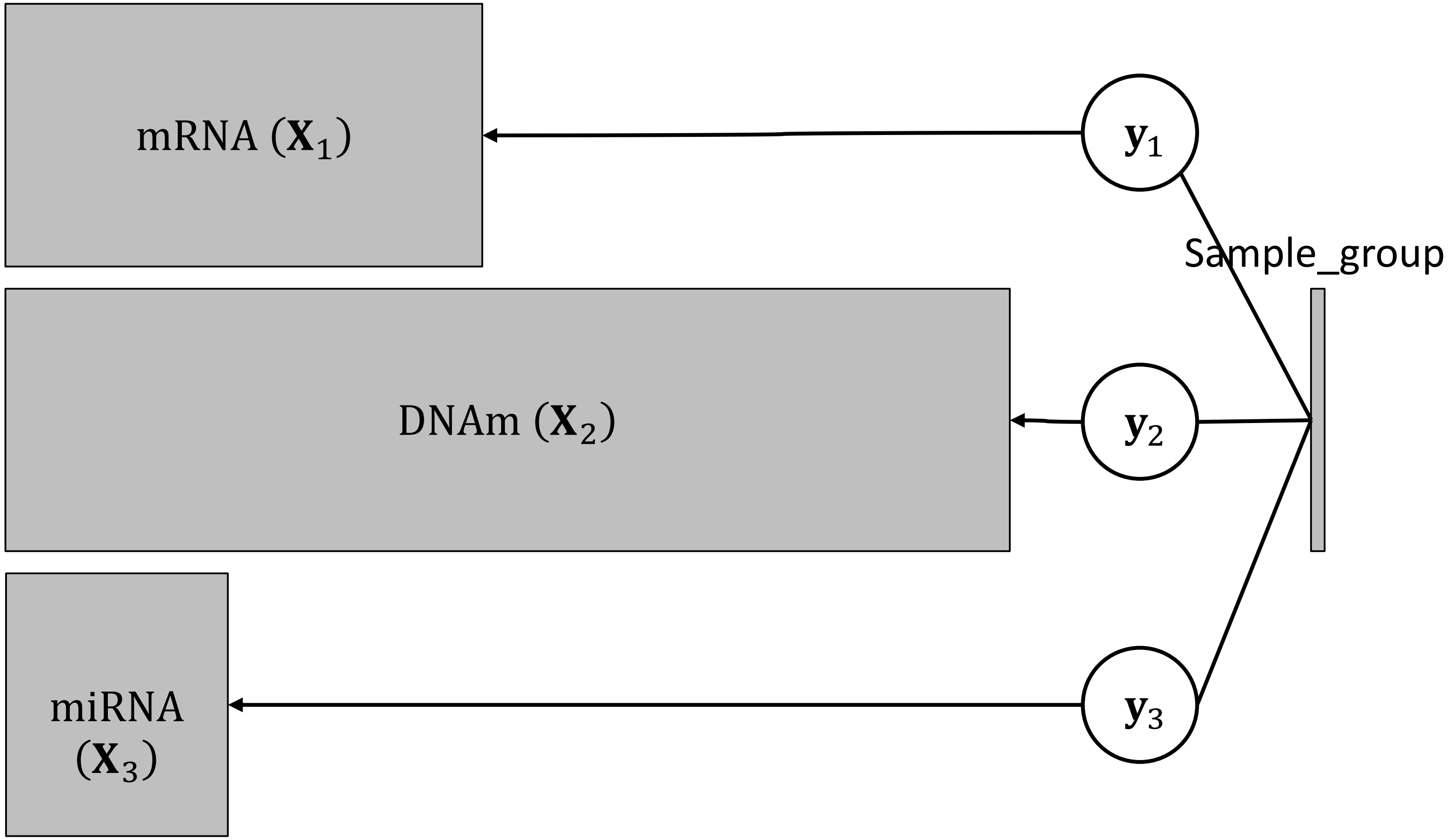
Supervising with RGCCA



Supervising with RGCCA



Supervising with RGCCA



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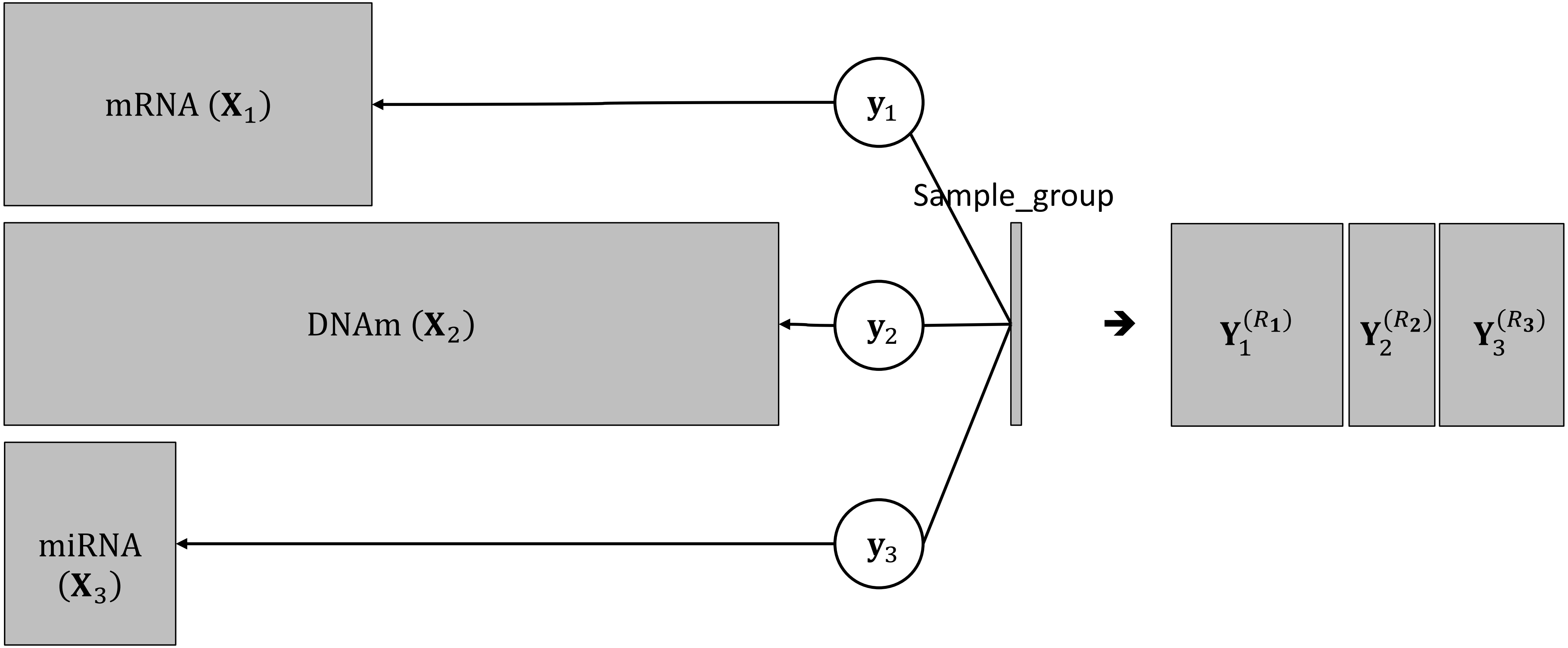

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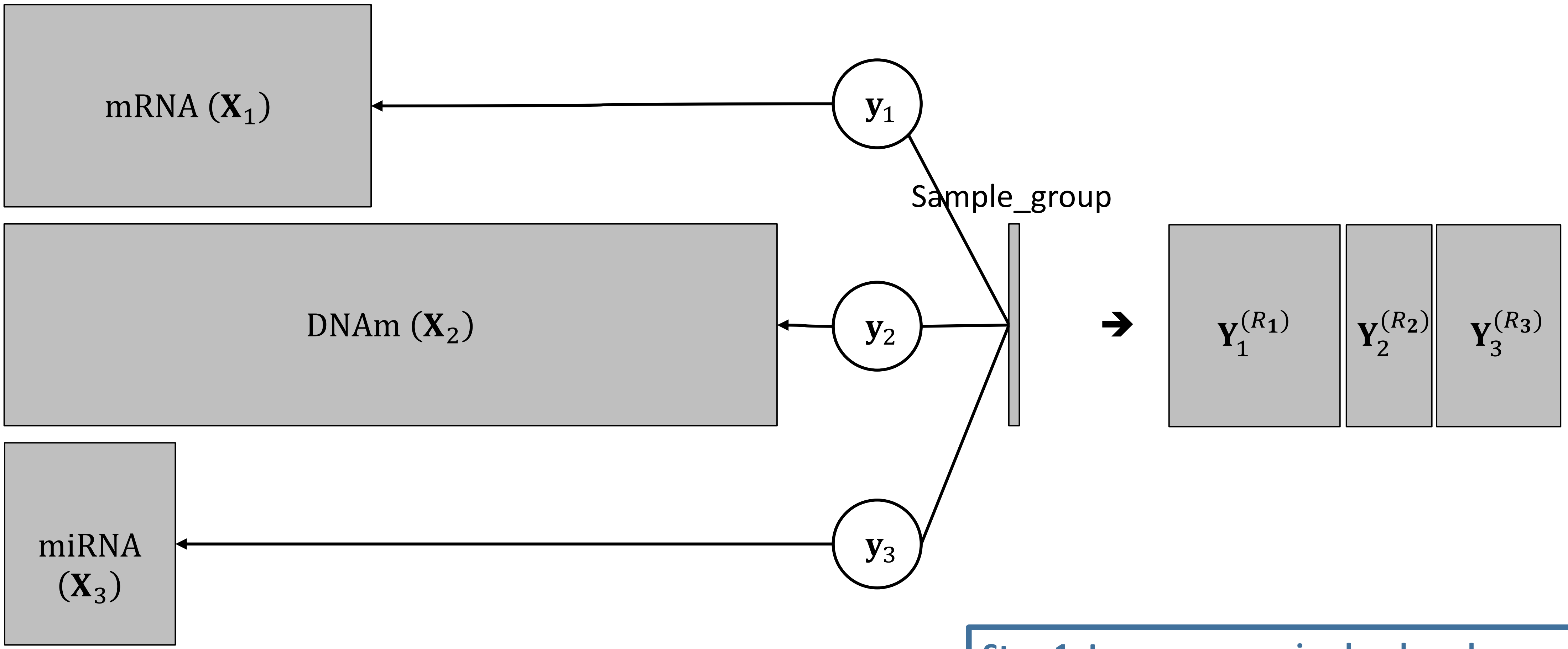
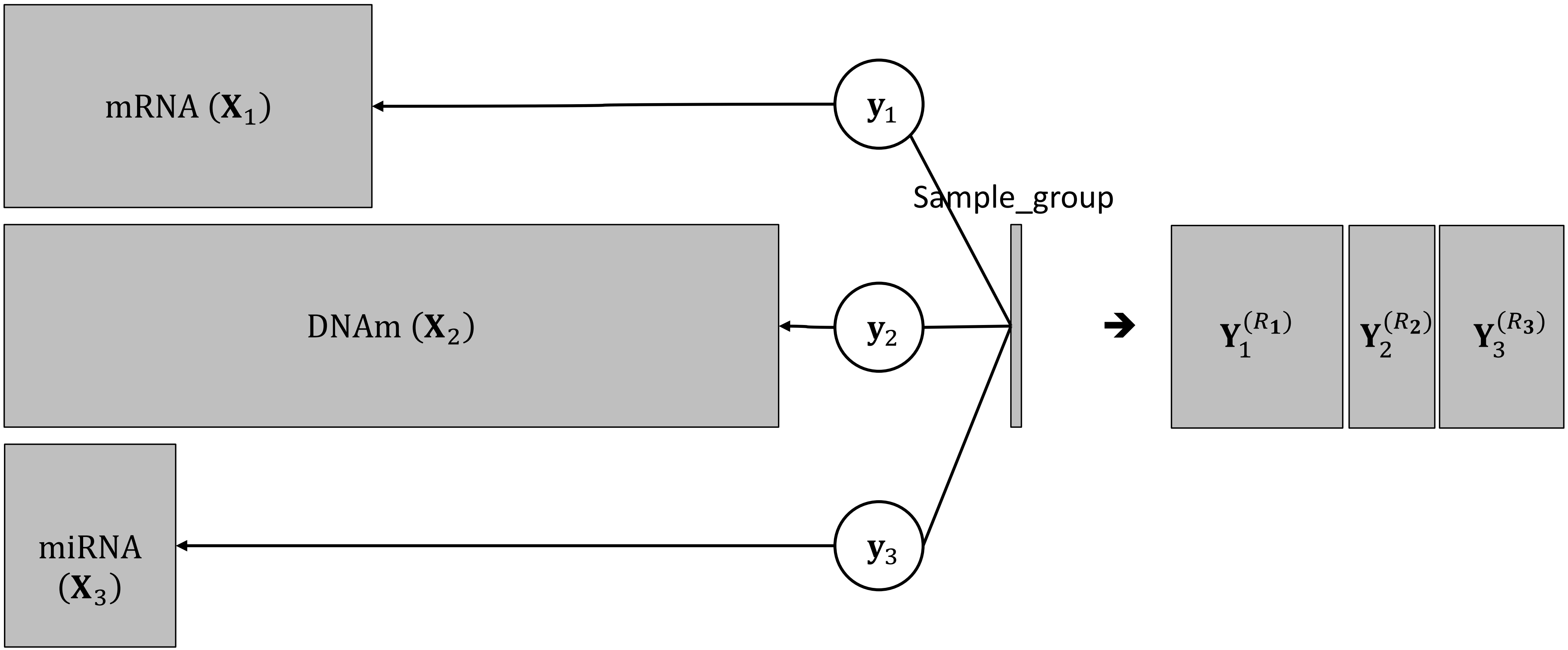
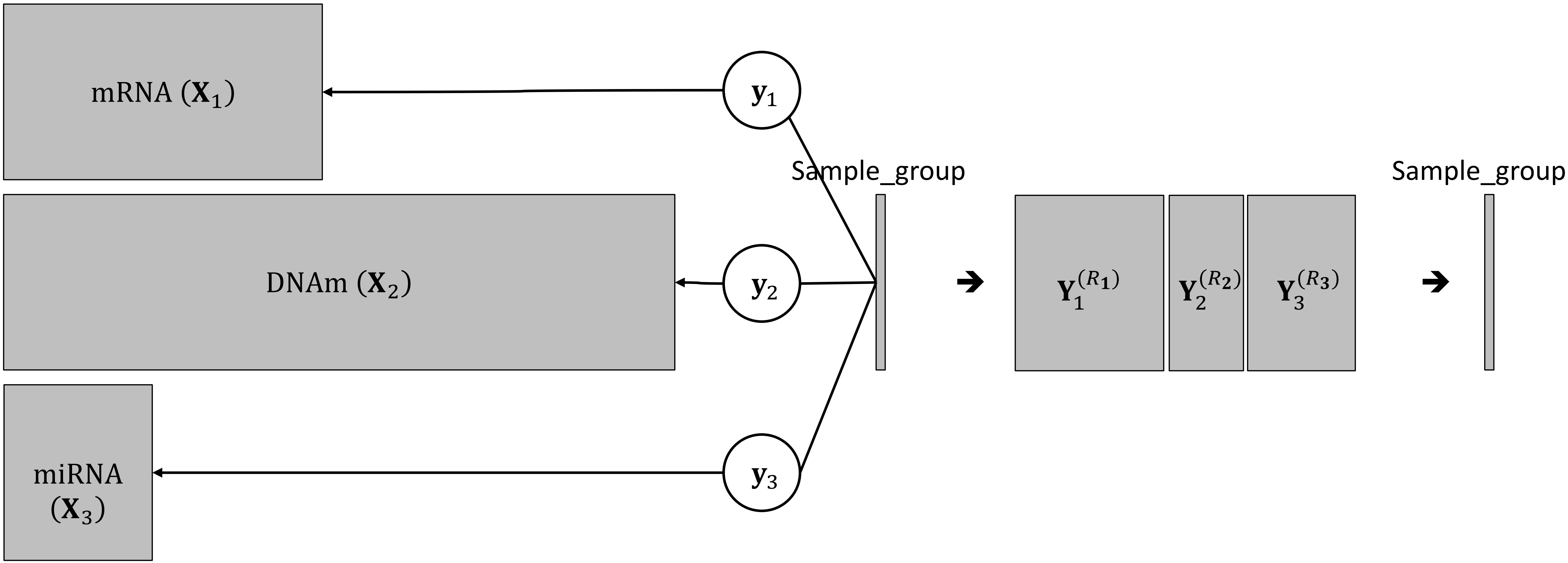


Step 1: Learn a supervised reduced space

Supervising with RGCCA



Supervising with RGCCA



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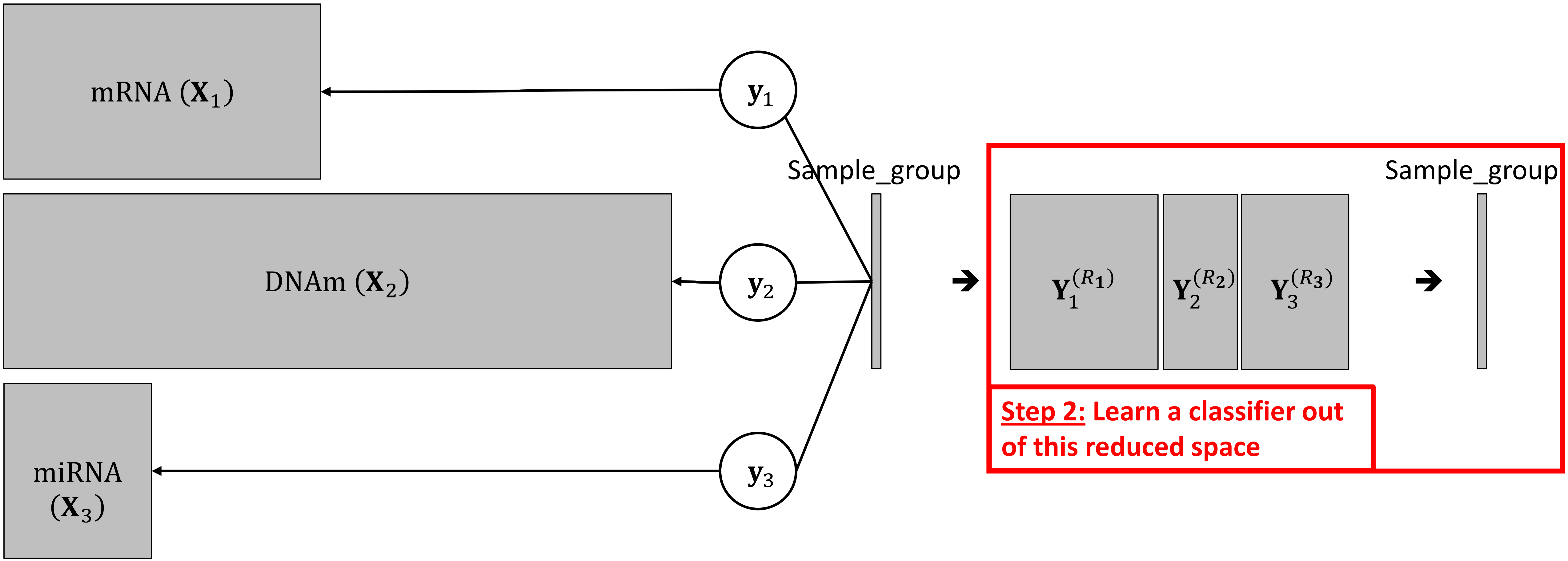

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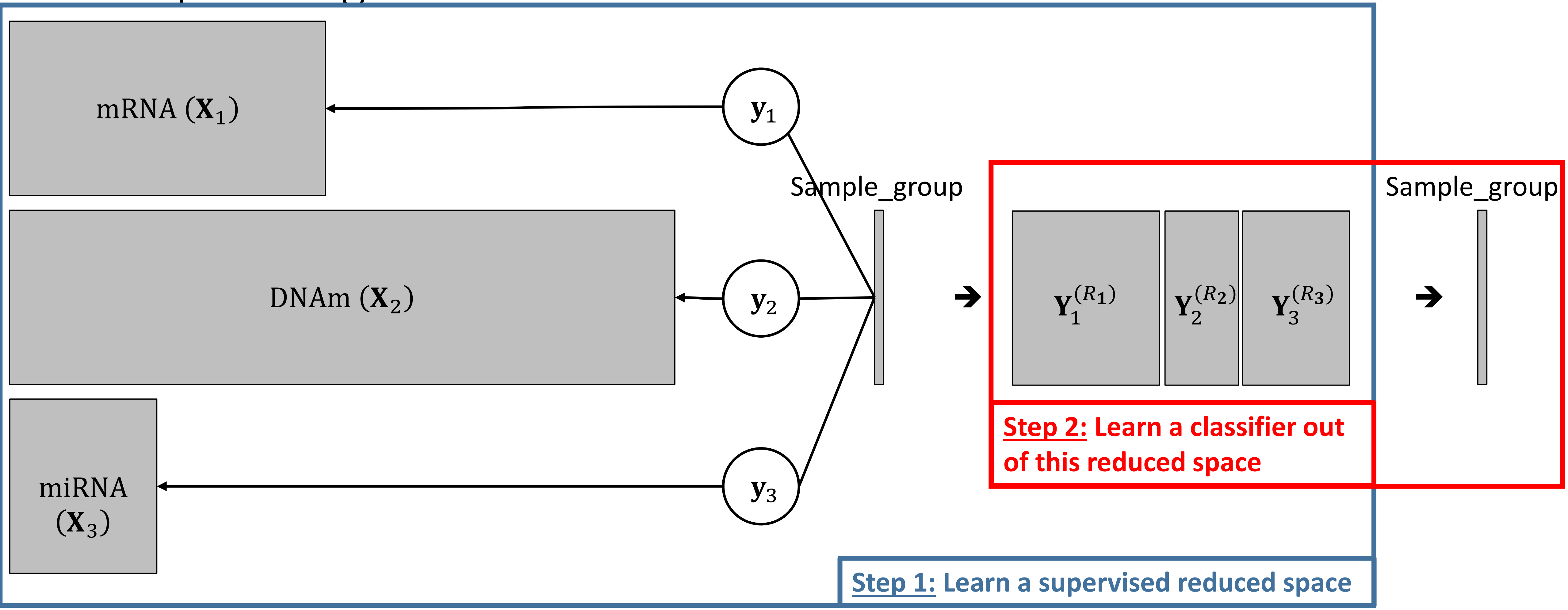
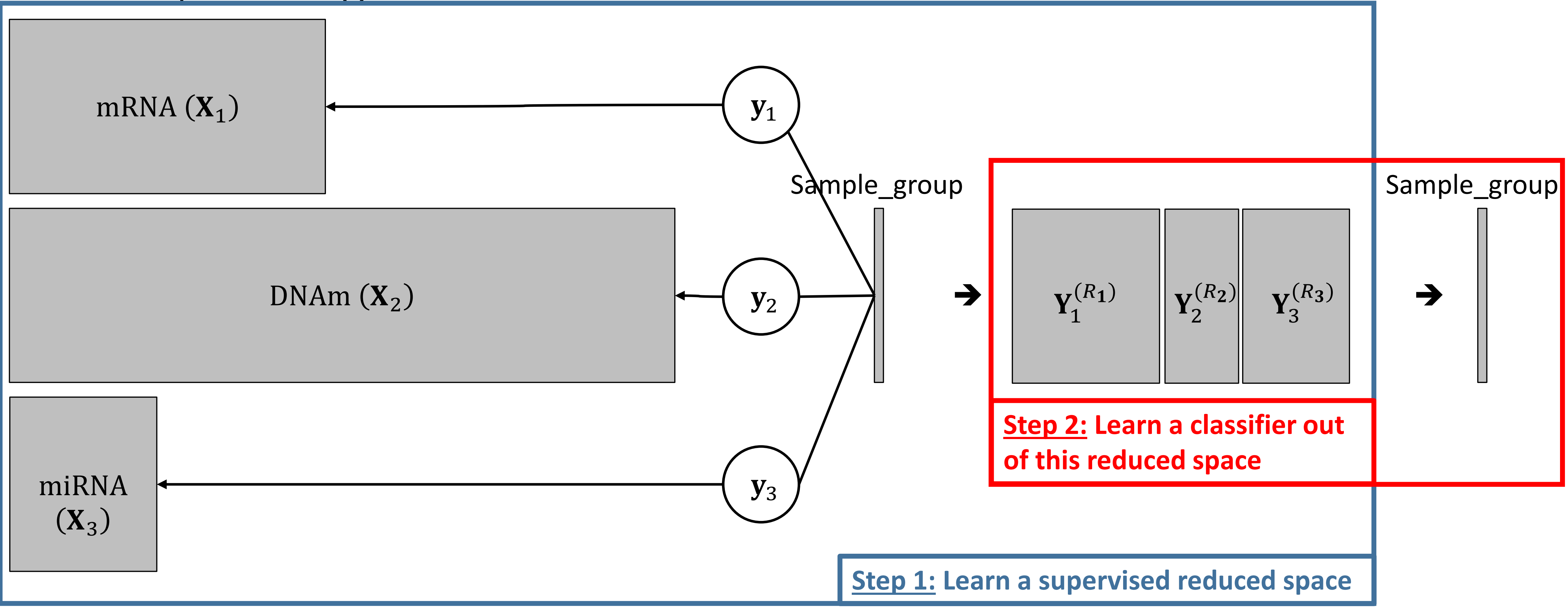
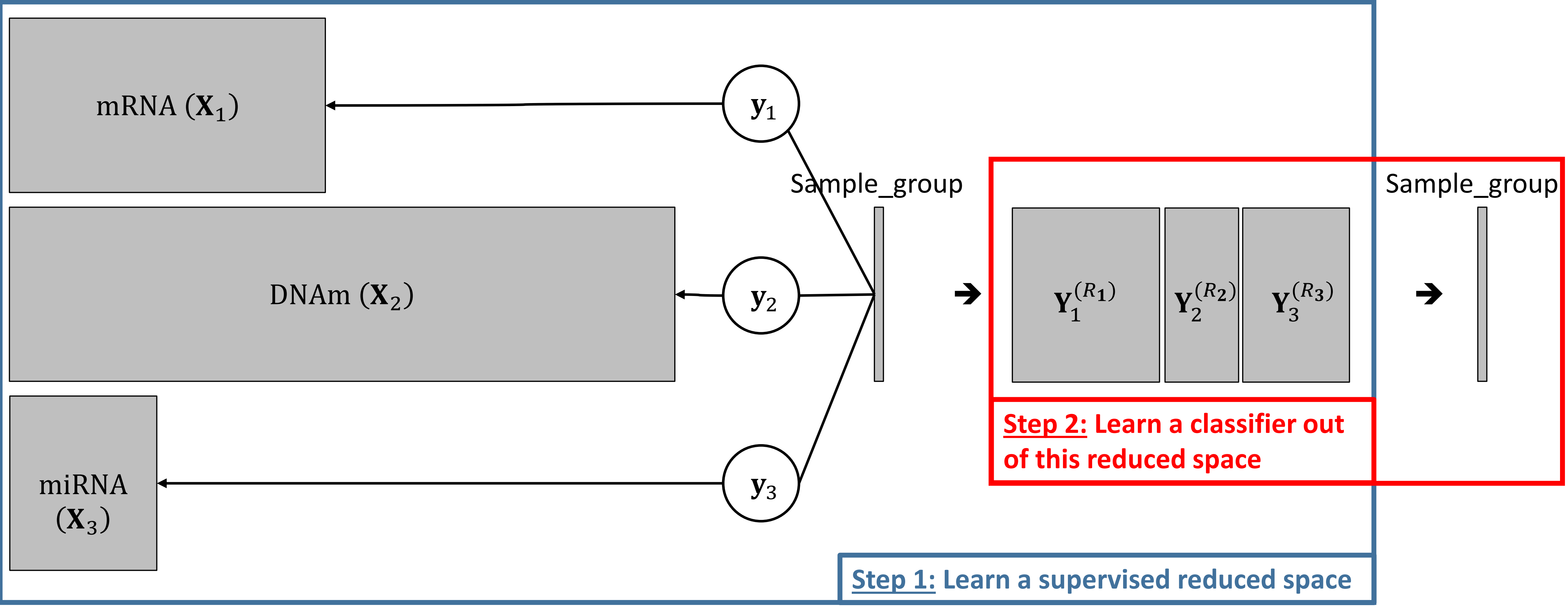


Supervising with RGCCA



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

F1-score

Confusion Matrix:

		True labels	
		Positive	Negative
Predicted labels	Positive	True Positive (TP)	False Positive (FP)
	Negative	False Negative (FN)	True Negative (TN)

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$$precision = \frac{TP}{TP + FP}$$

➔ How many positive predicted labels are true ?

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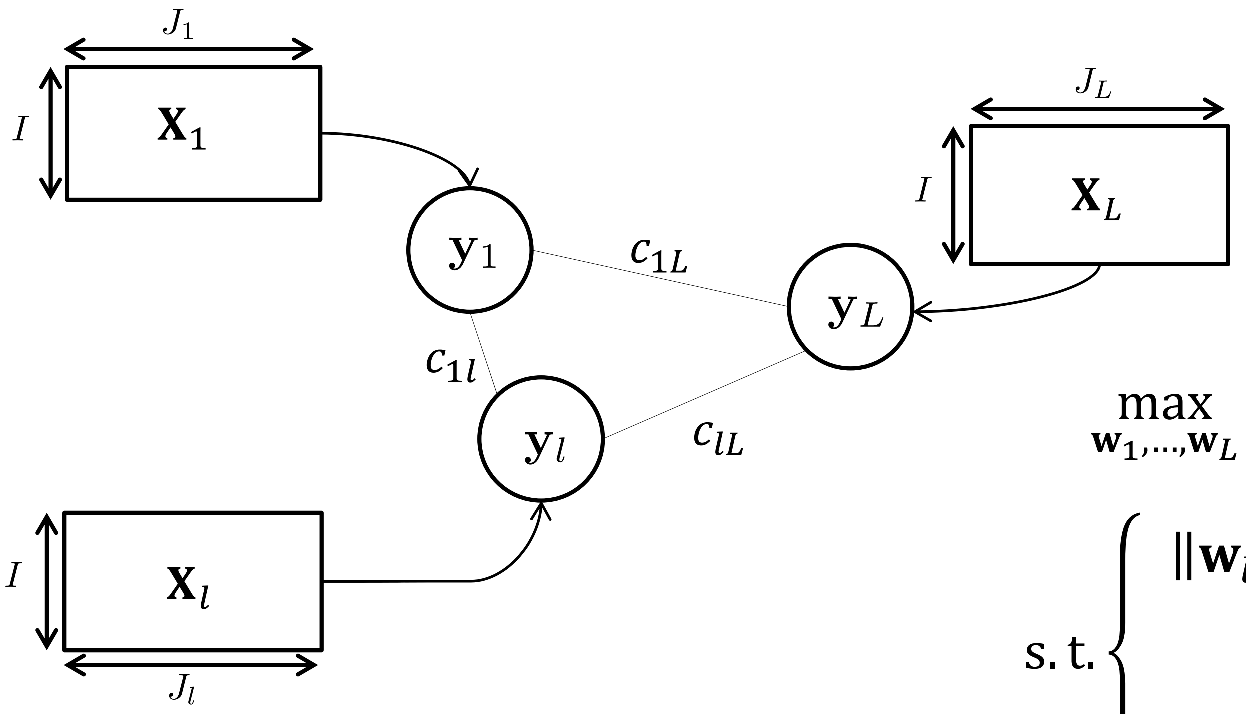
➔ How many true positive labels are retrieved ?

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

6. Going further with RGCCA

Sparse Generalized Canonical Correlation Analysis (SGCCA)



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

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

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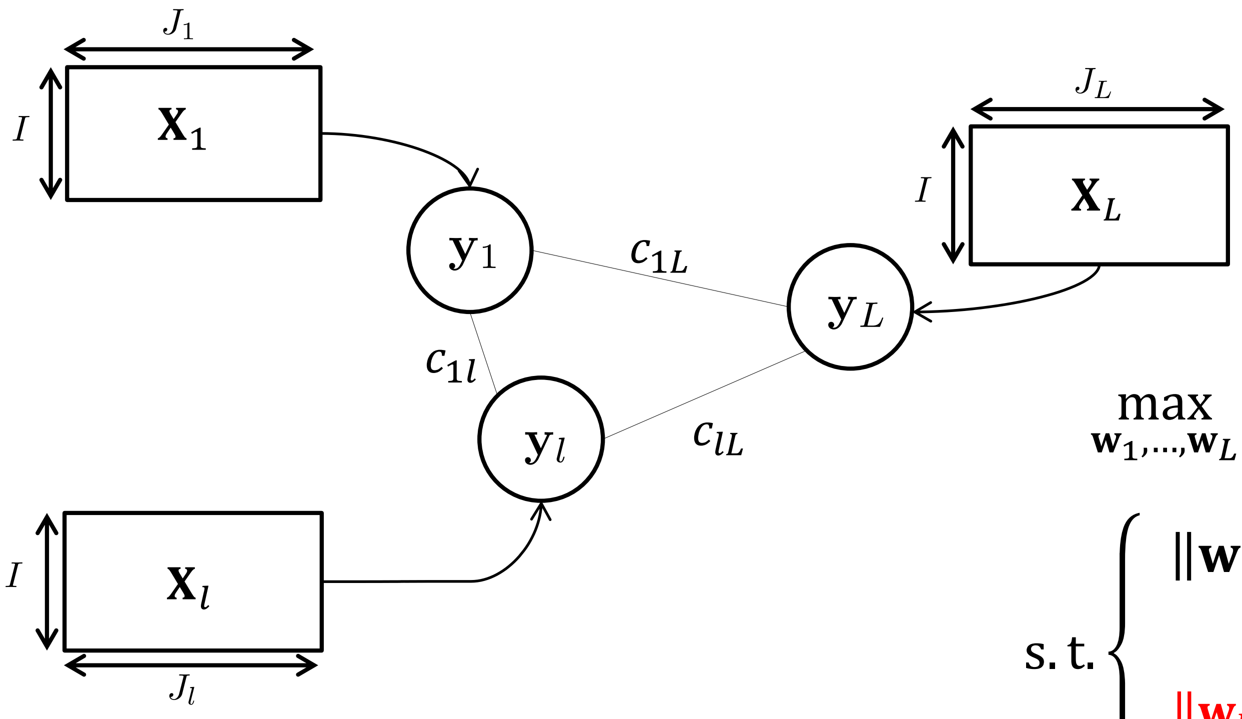

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$$\text{s.t.} \begin{cases} \|\mathbf{w}_l\|_2^2 = 1 \\ \|\mathbf{w}_l\|_1 = \sum_{j=1}^{J_l} |w_{lj}| \leq s_l \end{cases}, l = 1, \ldots, L.$$

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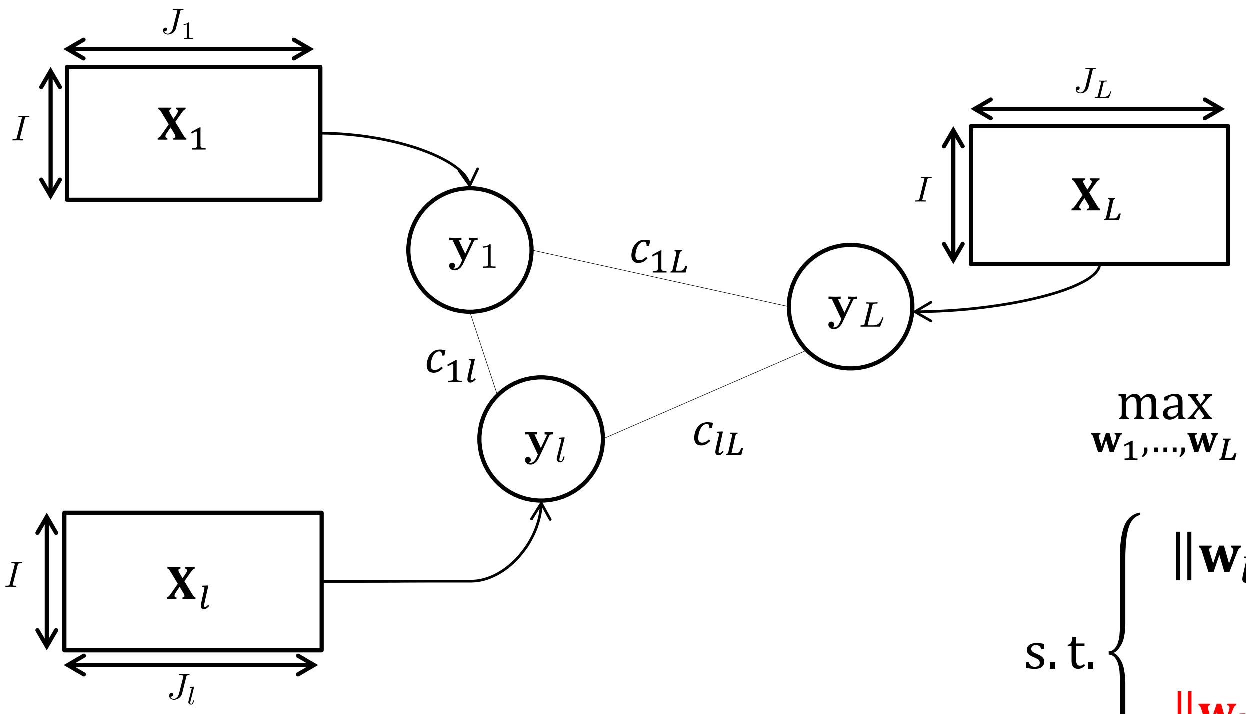

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The LASSO regularization allows to perform variable selection.

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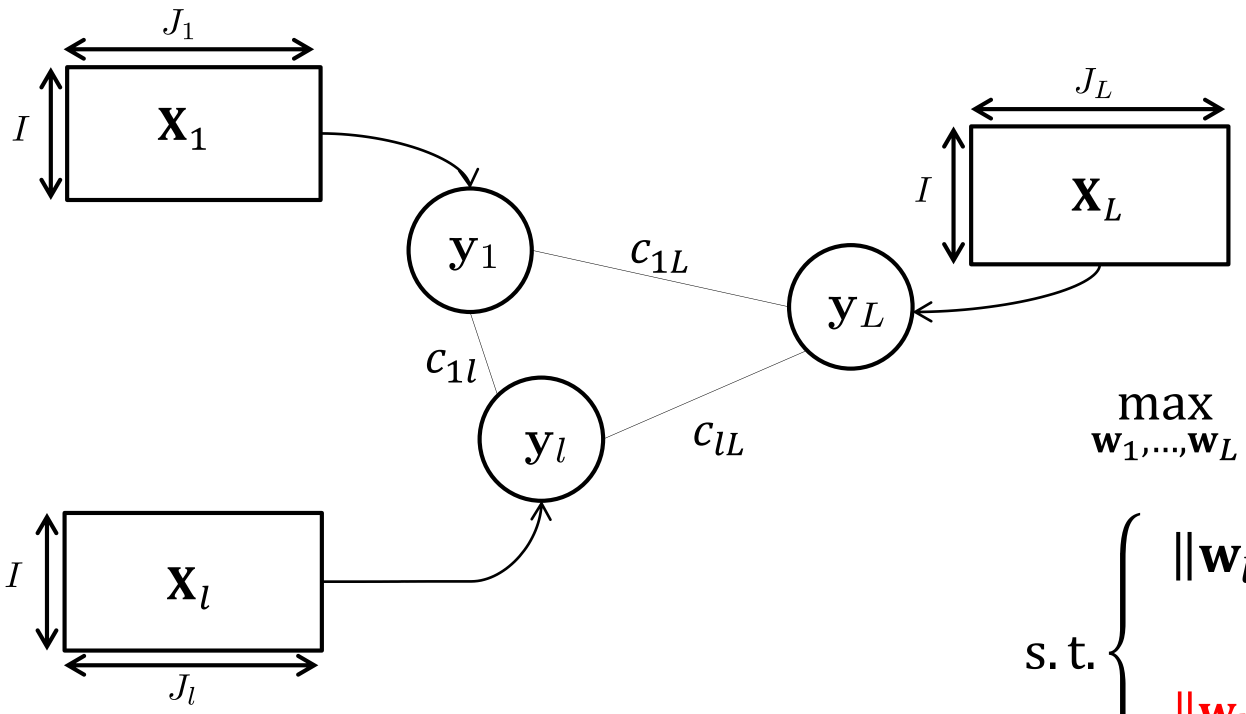

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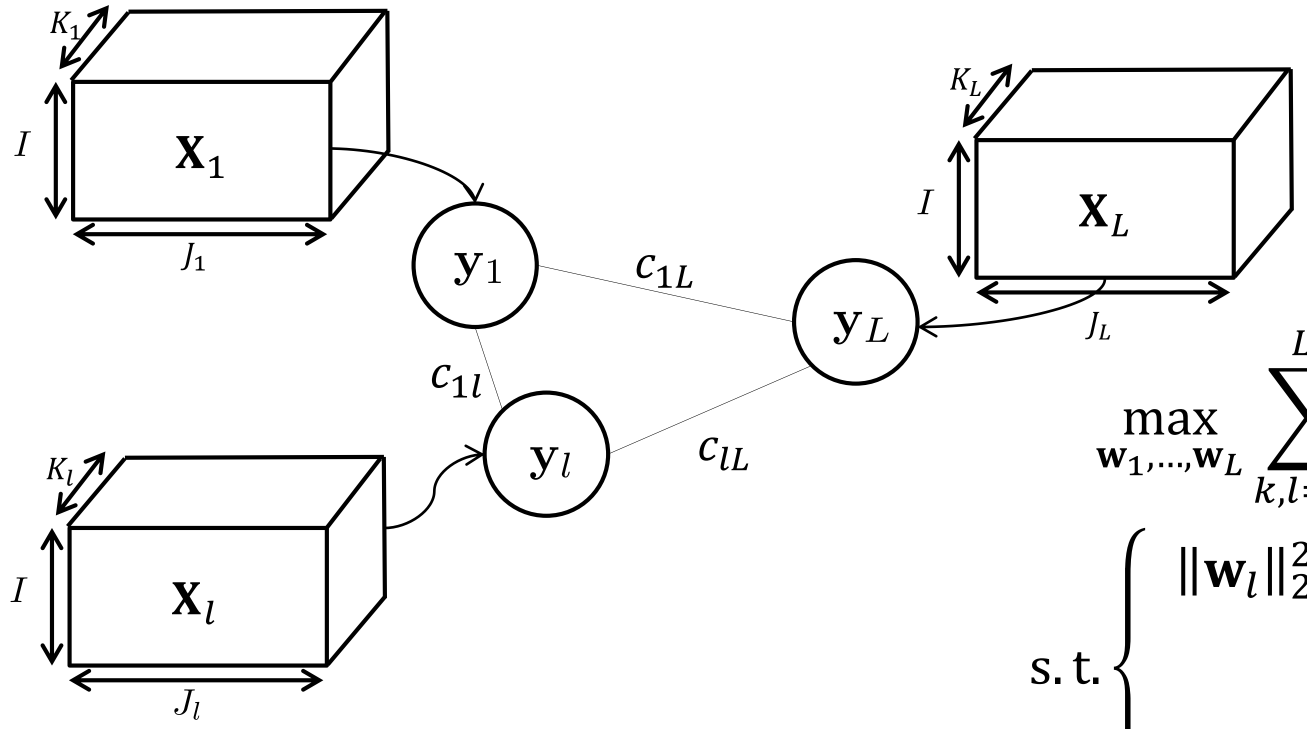
Controls the level of sparsity (has to be tuned).

The LASSO regularization allows to perform variable selection.

Multiway Generalized Canonical Correlation Analysis (MGCCA)



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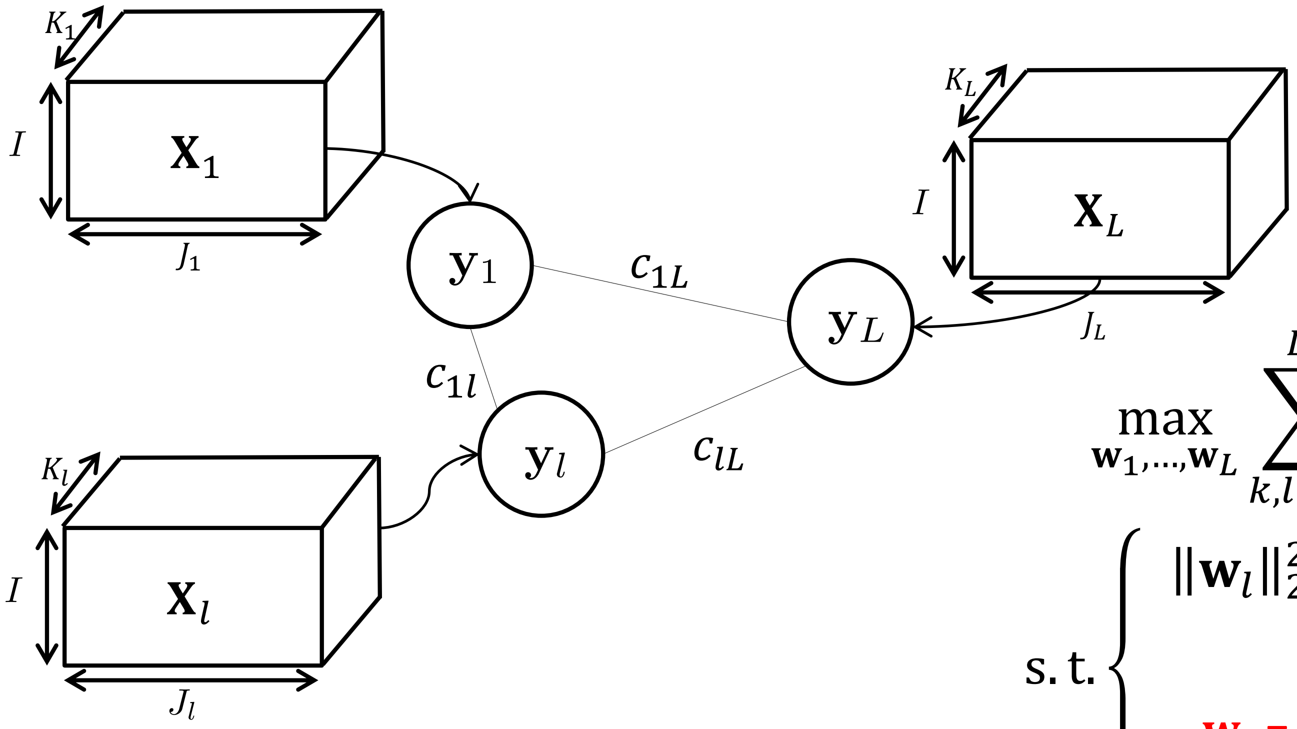

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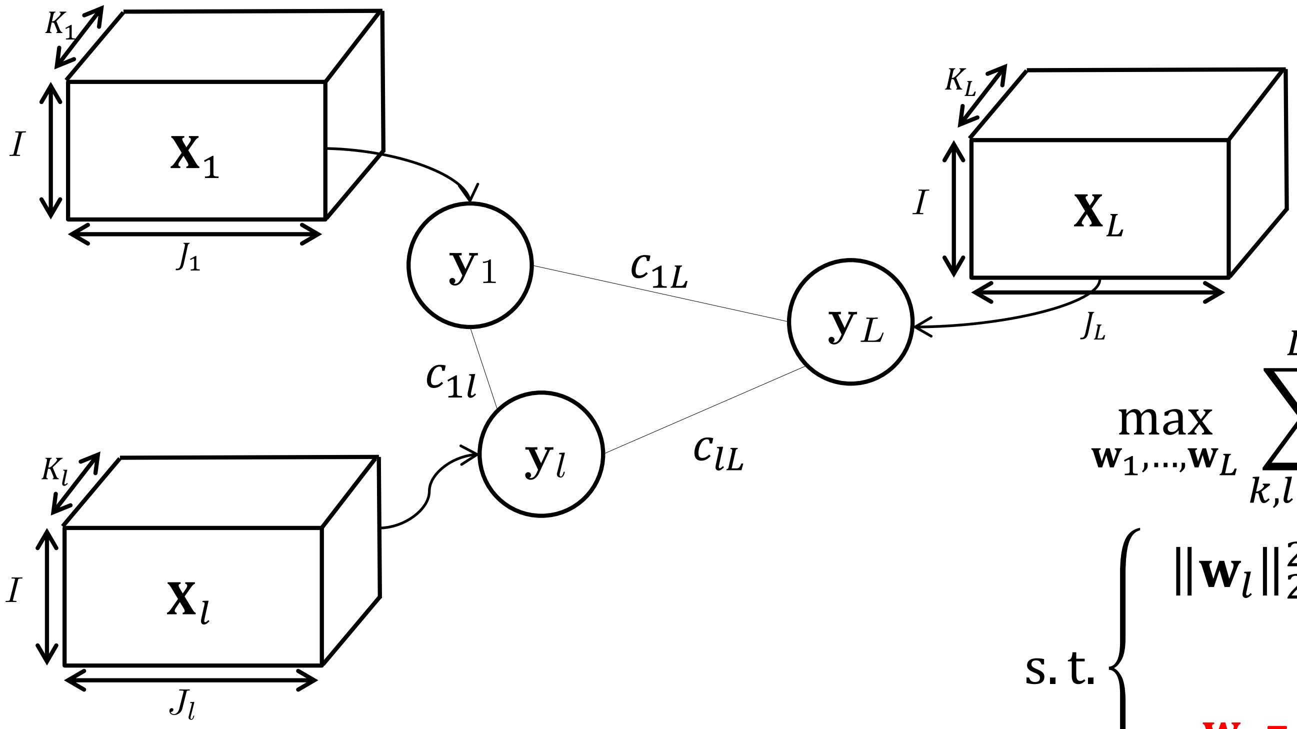

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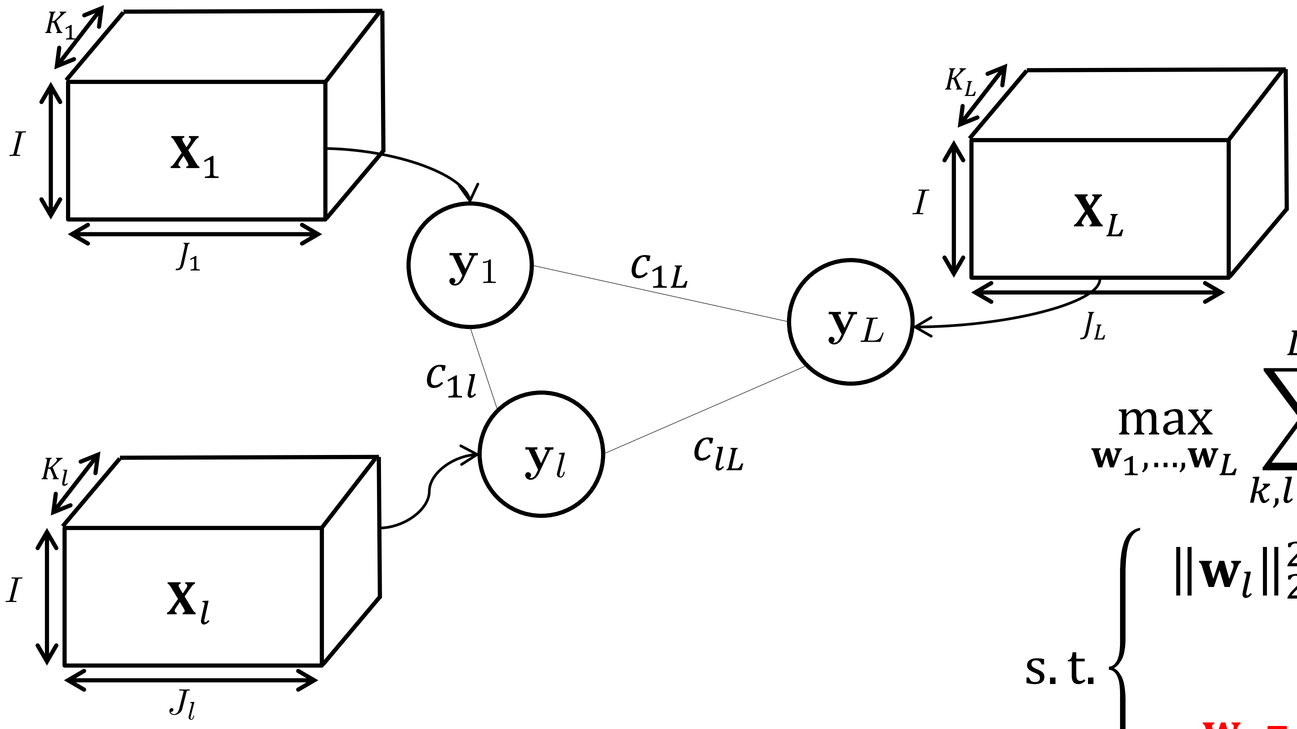

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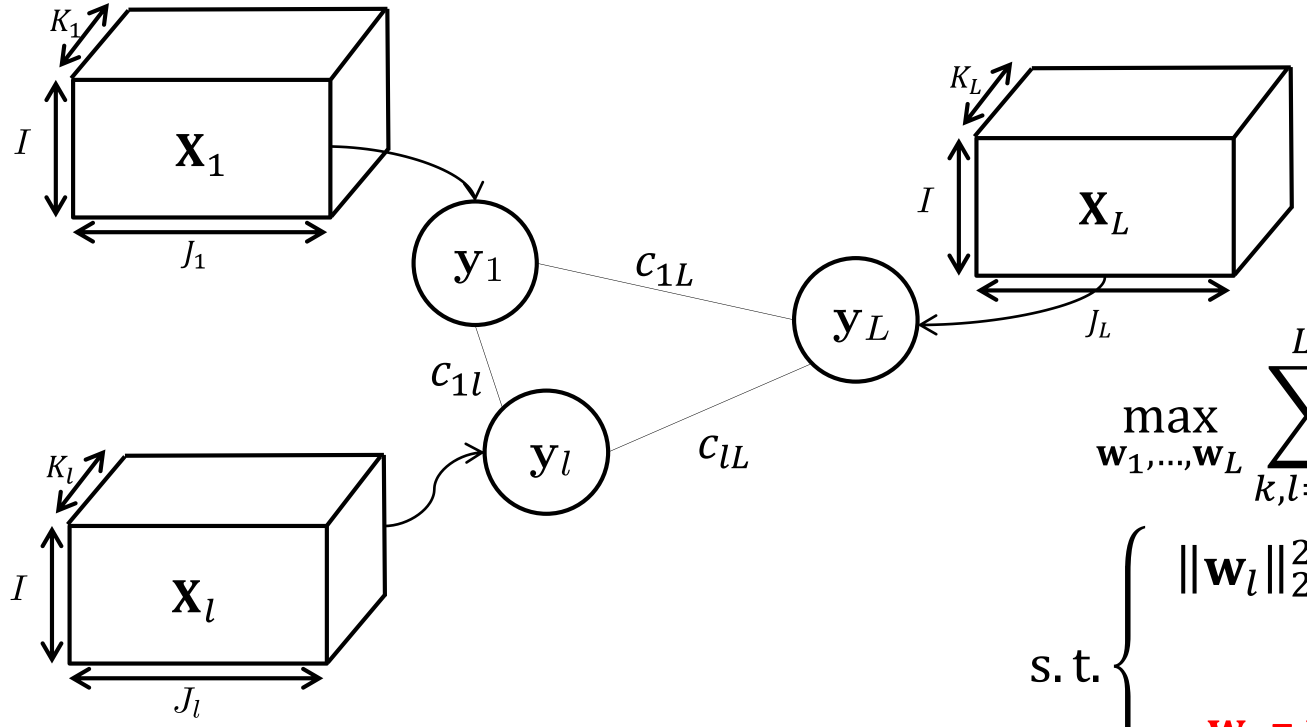

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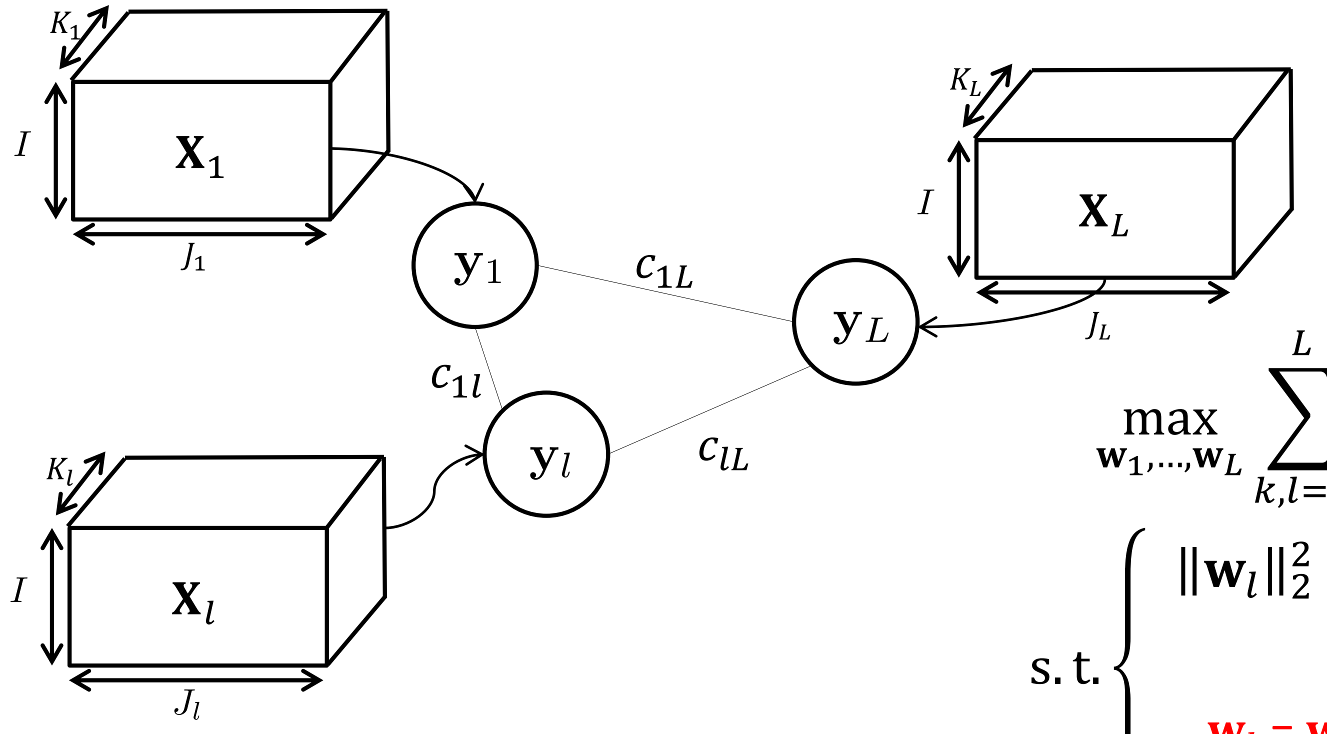

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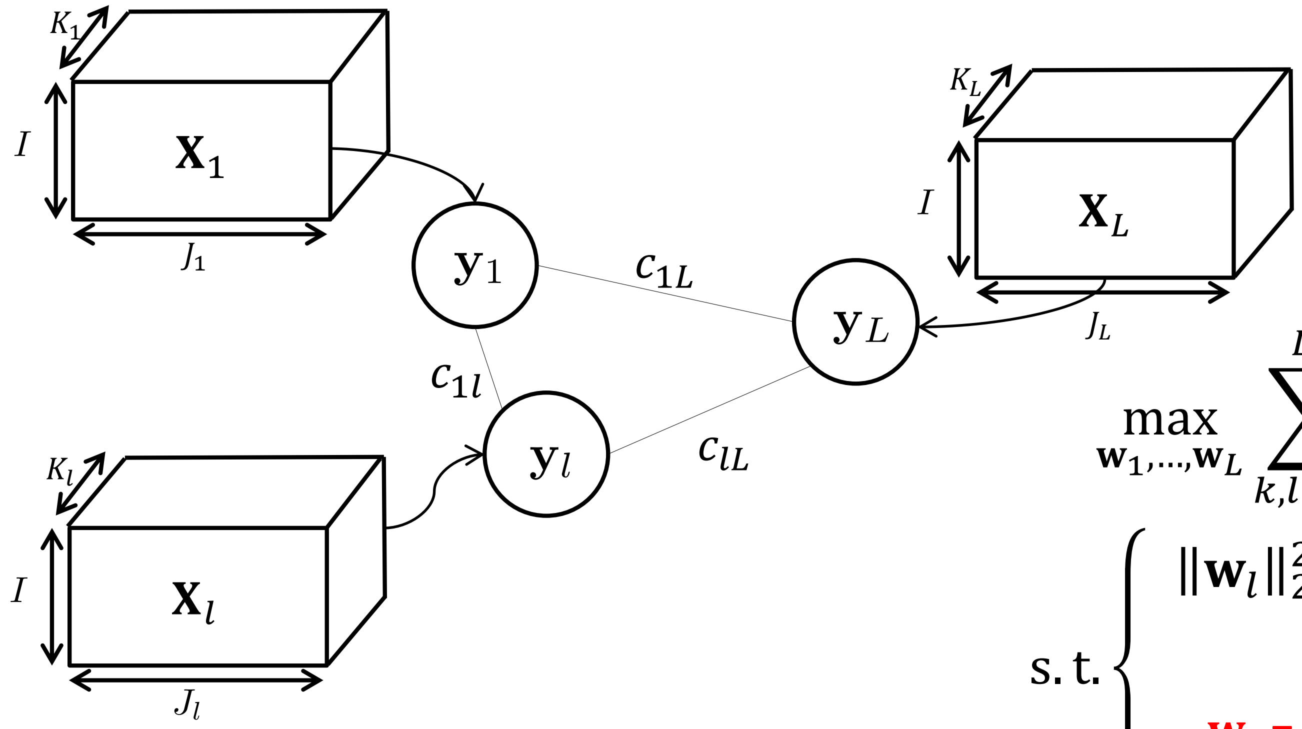

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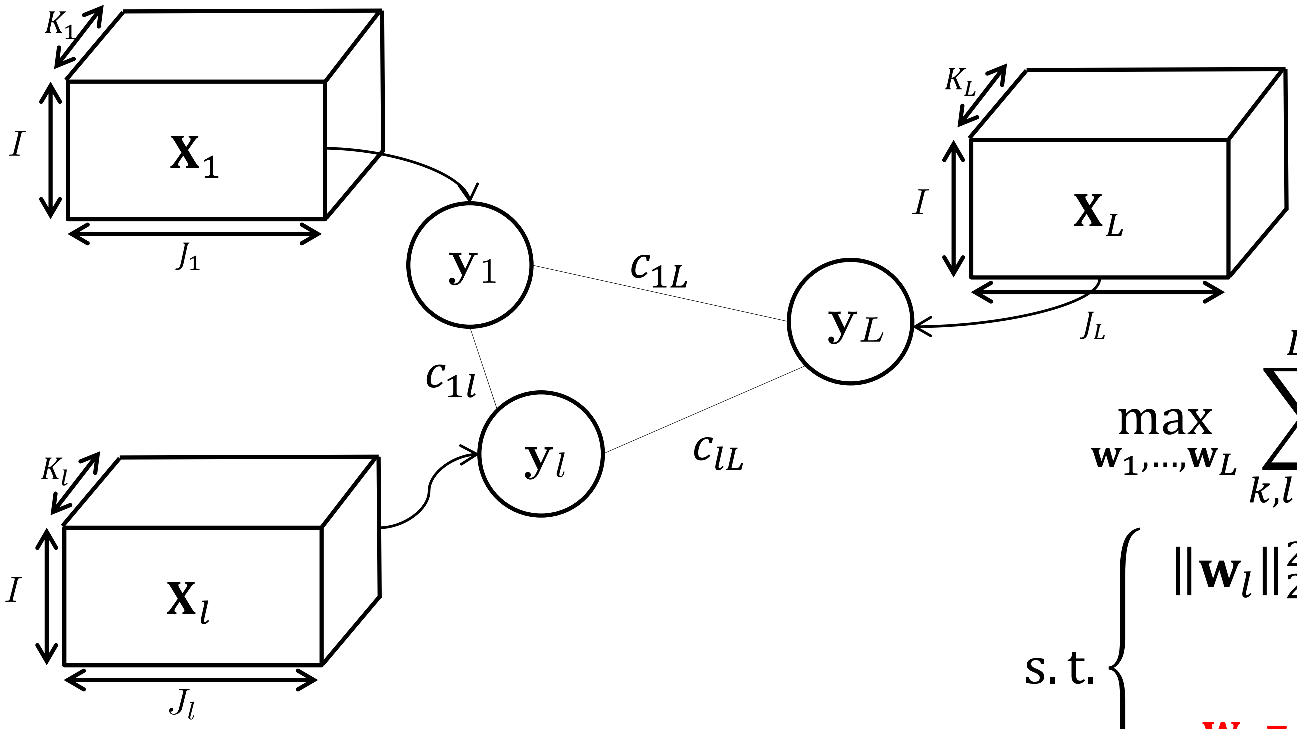

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New extension with Tensor GCCA

Other extensions of RGCCA

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Kernel GCCA: in order to take estimate non-linear links between blocks.

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Group SGCCA: perform group selection.

Acknowledgment

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Dr El Chérif Ibrahim

Dr Belzeaux Raoul

Dr Gascon Gonzalo

Pr Isabelle Mansuy

Summer School:

Dr Florence Mehl

Dr Olivier Sand

Dr Grégoire Rossier

Dr Jimmy Vandel

Dr Guillemette Marot

Dr Marie-Galadriel Briere

Dr Morgane Tereeol

Dr Anaïs Baudot

Dr Maxime Delmas

Dr Jean-Clément Gallardo

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Edith Le Floch

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Dr Belzeaux Raoul

Dr Gascon Gonzalo

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Dr Anaïs Baudot

Dr Maxime Delmas

Dr Jean-Clément Gallardo

Dr Marco Pagni

Slides:

Dr Arthur Tenenhaus

Dr Laurent Le Brusquet

Dr Julien Bect

Vincent Le Goff

CNRGH – Math-Stat Team:

Edith Le Floch

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QUESTIONS ?