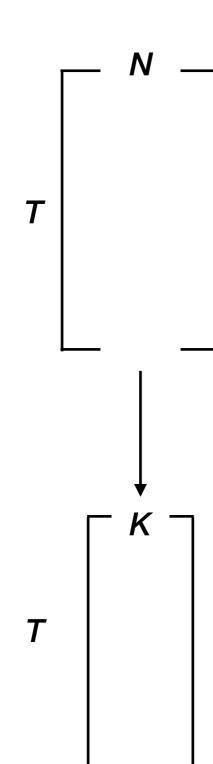
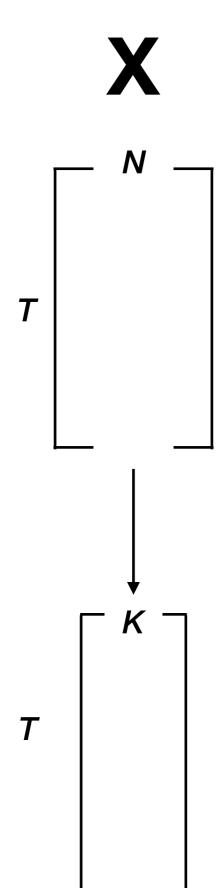
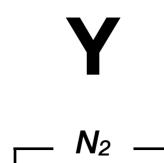
Linear dimensionality reduction across multiple datasets

Josh Glaser Advanced Theory Seminar

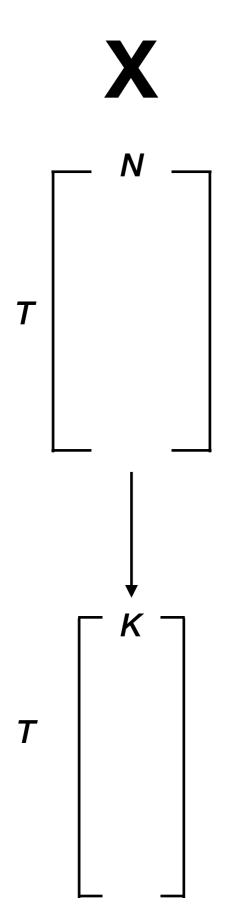




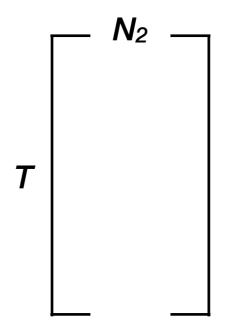


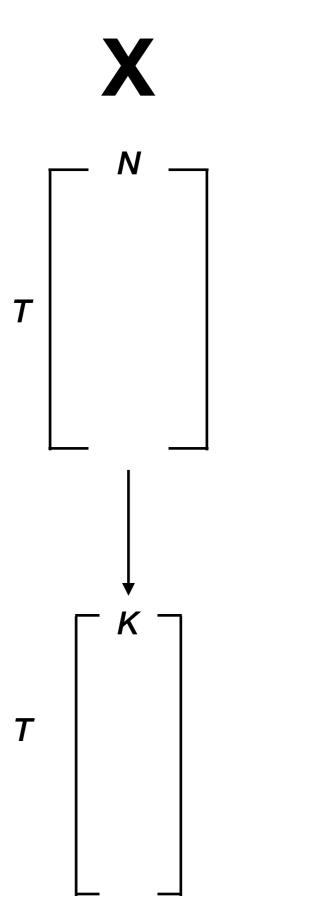


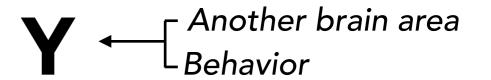
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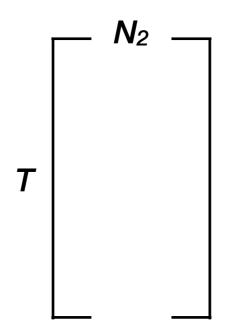












- Reduce noise
- Visualization
- Science!

Overview

- 1. Reducing dimensionality in one space
 - PCA and regression refreshers
 - Principal components regression
 - Reduced rank regression
 - Demixed PCA
- 2. Reducing dimensionality in two spaces
 - Canonical correlation analysis
 - Partial least squares

• Find orthogonal linear low-D transformation that maximizes variance.

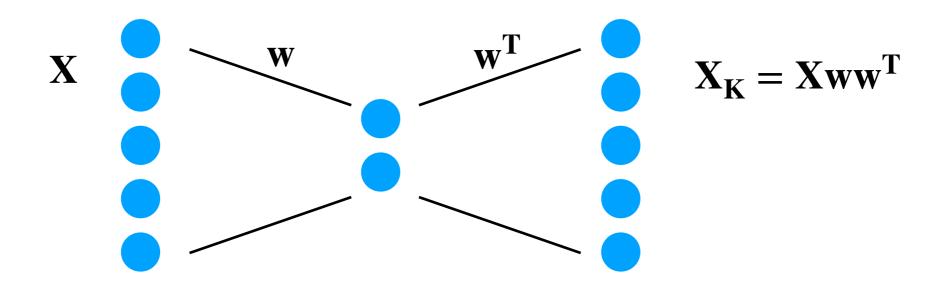
$$\underset{w \in \mathbb{R}^K}{\operatorname{arg\,max}} \left(\| \mathbf{X} \mathbf{w} \|^2 \right) \text{ s.t. } \| \mathbf{w} \| = \mathbf{I}$$

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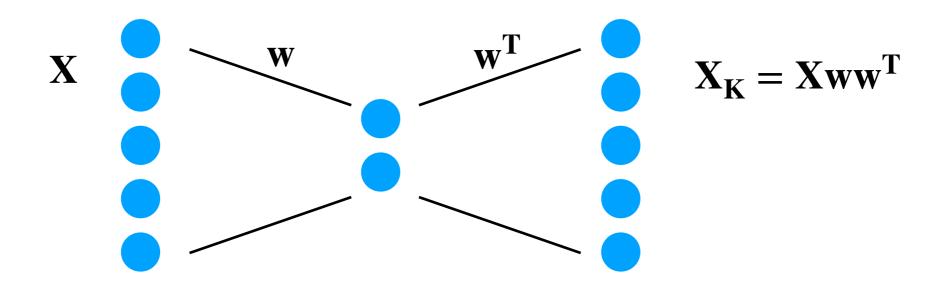
Find transformation that minimizes reconstruction error.

$$\underset{w \in \mathbb{R}^{K}}{\operatorname{arg\,min}} \left(\left\| \mathbf{X} - \mathbf{X} \mathbf{w} \mathbf{w}^{\mathbf{T}} \right\|^{2} \right) \text{ s.t. } \left\| \mathbf{w} \right\| = \mathbf{I}$$



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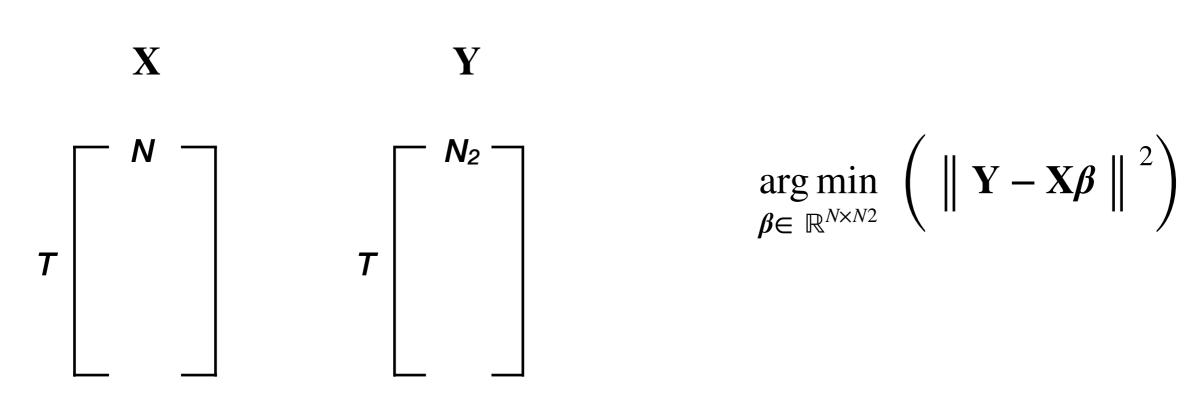
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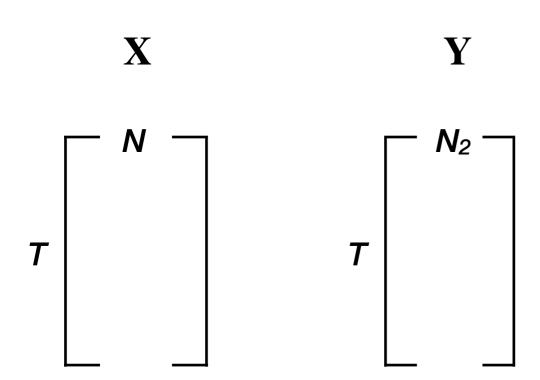


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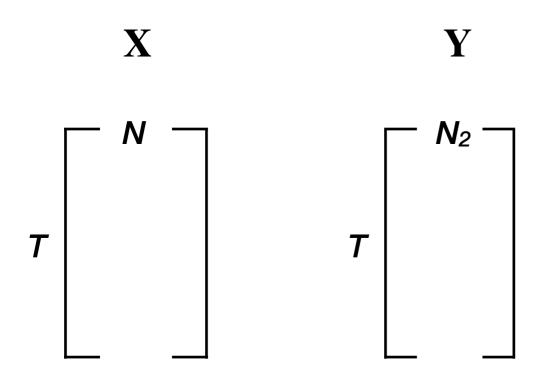
• X_K is the best rank K approximation (in terms of minimizing norm of reconstruction error) when solving with singular value decomposition (Eckart-Young theorem, 1936).

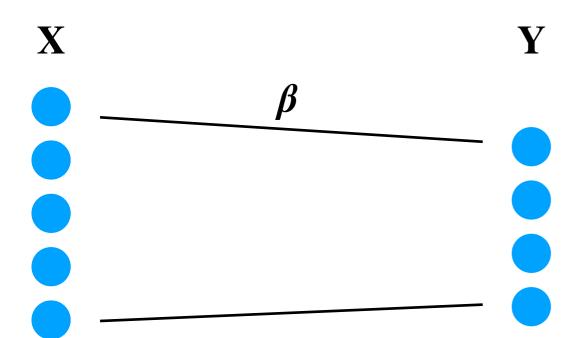




$$\underset{\beta \in \mathbb{R}^{N \times N2}}{\operatorname{arg \, min}} \left(\left\| \mathbf{Y} - \mathbf{X} \boldsymbol{\beta} \right\|^{2} \right)$$
$$\boldsymbol{\beta} = \left(\mathbf{X}^{T} \mathbf{X} \right)^{-1} \mathbf{X}^{T} \mathbf{Y}$$

• This is equivalent to N_2 separate regressions (each for a separate column of **Y** to get a separate column of β).

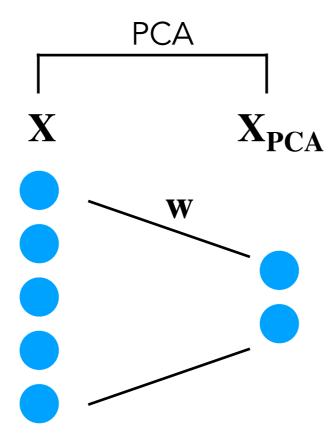




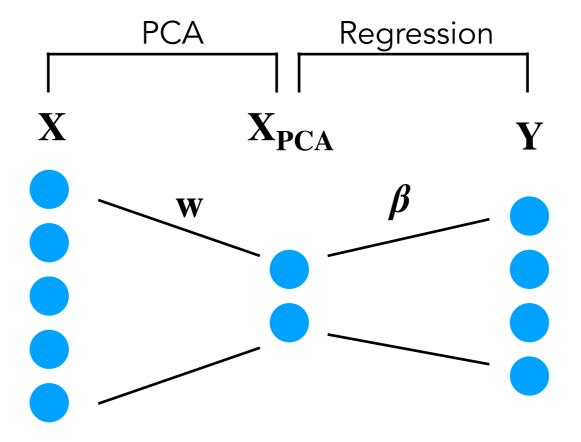
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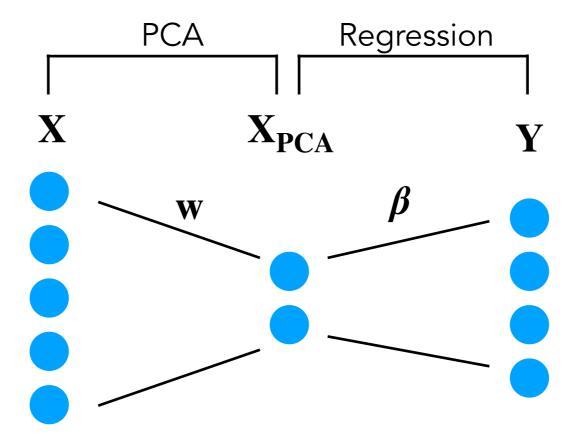
PCA + Regression



PCA + Regression

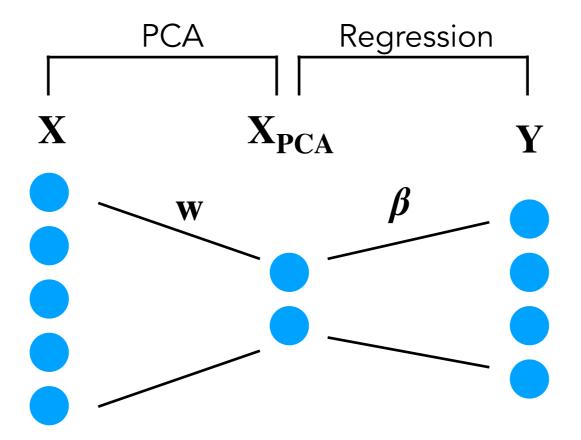


PCA + Regression



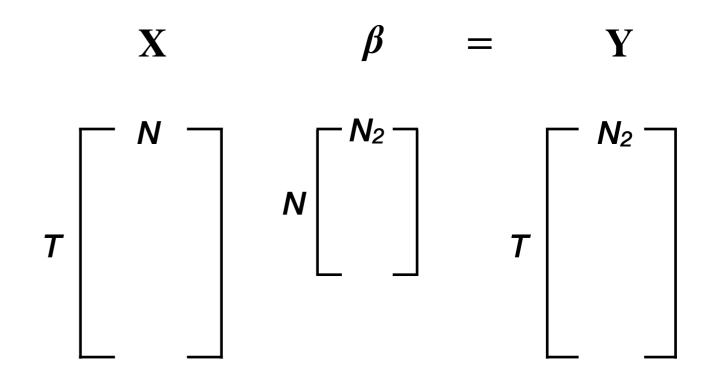
Dimensionality reduction does not take Y into account.

PCA + Regression



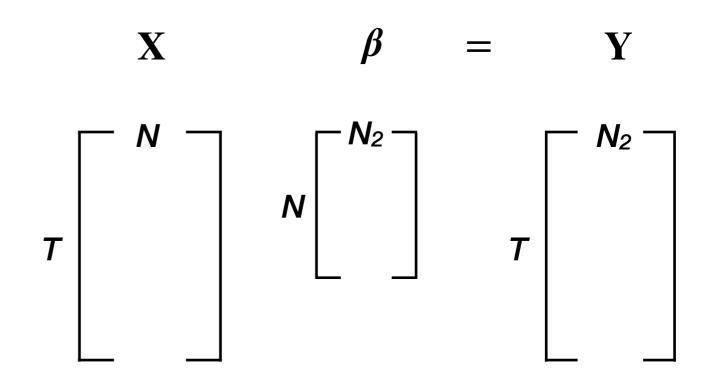
- Dimensionality reduction does not take **Y** into account.
- Dim. reduction acts like denoising / regularization

$$\underset{\beta \in \mathbb{R}^{N \times N2}}{\operatorname{arg\,min}} \left(\left\| \mathbf{Y} - \mathbf{X}\boldsymbol{\beta} \right\|^{2} \right)$$



$$\underset{\beta \in \mathbb{R}^{N \times N2}}{\operatorname{arg \, min}} \left(\| \mathbf{Y} - \mathbf{X} \boldsymbol{\beta} \|^{2} \right)$$

$$\operatorname{rank} (\boldsymbol{\beta}) \leq K$$

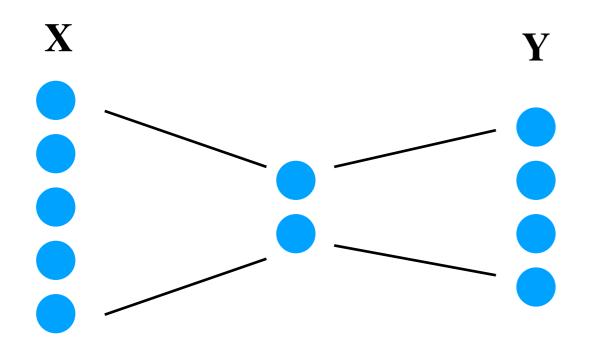


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$$\operatorname{rank} \left(\boldsymbol{\beta} \right) \leq K$$

$$X \qquad \beta \qquad = \qquad Y$$

$$T \qquad N \qquad N \qquad N \qquad T \qquad T \qquad D$$

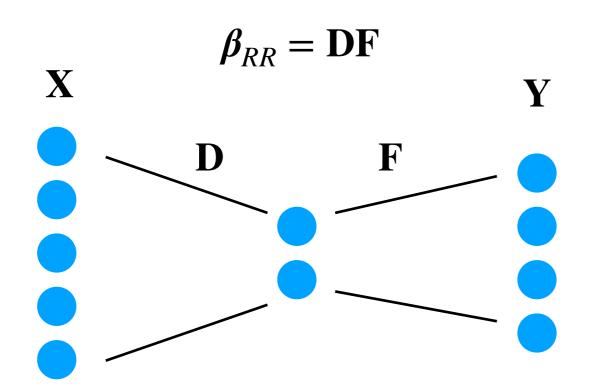


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$$X \qquad \beta \qquad = \qquad Y$$

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$$\underset{\boldsymbol{\beta}_{RR} \in \mathbb{R}^{N \times N2}}{\operatorname{arg \, min}} \left(\left\| \mathbf{Y} - \mathbf{X} \boldsymbol{\beta}_{\mathbf{RR}} \right\|^{2} \right) \qquad \operatorname{rank} \left(\boldsymbol{\beta}_{RR} \right) \leq K$$

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$$\|\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{R}\mathbf{R}}\|^{2} = \|(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{OLS}}) + (\mathbf{X}\boldsymbol{\beta}_{\mathbf{OLS}} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{R}\mathbf{R}})\|^{2} = \|(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{OLS}}) + (\mathbf{X}\boldsymbol{\beta}_{\mathbf{OLS}} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{R}\mathbf{R}})\|^{2} = \|(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{OLS}}) + (\mathbf{X}\boldsymbol{\beta}_{\mathbf{OLS}} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{R}\mathbf{R}})\|^{2} = \|(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{C}\mathbf{L}\mathbf{S}}) + (\mathbf{X}\boldsymbol{\beta}_{\mathbf{C}\mathbf{L}\mathbf{S}} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{C}\mathbf{R}\mathbf{R}})\|^{2} = \|(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{C}\mathbf{L}\mathbf{S}}) + (\mathbf{X}\boldsymbol{\beta}_{\mathbf{C}\mathbf{L}\mathbf{S}} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{C}\mathbf{R}})\|^{2} = \|(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{C}\mathbf{L}\mathbf{S}}) + (\mathbf{X}\boldsymbol{\beta}_{\mathbf{C}\mathbf{L}\mathbf{S}} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{C}\mathbf{R}})\|^{2} = \|(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{C}\mathbf{L}\mathbf{S}}) + (\mathbf{X}\boldsymbol{\beta}_{\mathbf{C}\mathbf{L}\mathbf{S}} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{C}\mathbf{R}})\|^{2} = \|(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{C}\mathbf{L}\mathbf{S}}) + (\mathbf{Y}\boldsymbol{\beta}_{\mathbf{C}\mathbf{L}\mathbf{S}} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{C}\mathbf{R}})\|^{2} = \|(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{C}\mathbf{L}\mathbf{S}}) + (\mathbf{Y}\boldsymbol{\beta}_{\mathbf{C}\mathbf{L}\mathbf{S}} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{C}\mathbf{R}})\|^{2} = \|(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{C}\mathbf{L}\mathbf{S}}) + (\mathbf{Y}\boldsymbol{\beta}_{\mathbf{C}\mathbf{C}\mathbf{S}} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{C}\mathbf{C}\mathbf{S}})\|^{2} + (\mathbf{Y}\boldsymbol{\beta}_{\mathbf{C}\mathbf{C}\mathbf{S}} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{C}\mathbf{C}\mathbf{S}})\|^{2} + (\mathbf{Y}\boldsymbol{\beta}_{\mathbf{C}\mathbf{C}\mathbf{S}} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{C}\mathbf{C}\mathbf{S}})\|^{2} + (\mathbf{Y}\boldsymbol{\beta}_{\mathbf{C}\mathbf{C}\mathbf{S})\|^{2} + (\mathbf{Y}\boldsymbol{\beta}_{\mathbf{C}\mathbf{C}\mathbf{S}} - \mathbf{Y}\boldsymbol{\beta}_{\mathbf{C}\mathbf{C}\mathbf{S}})\|^{2} + (\mathbf{Y}\boldsymbol{\beta}_{\mathbf{C}\mathbf{C}\mathbf{S})\|^{2} + (\mathbf{Y}\boldsymbol{\beta}_{\mathbf{C}\mathbf{C}\mathbf{S}} - \mathbf{Y}\boldsymbol{\beta}_{\mathbf{C}\mathbf{C}\mathbf{S})\|^{2} + (\mathbf{Y}\boldsymbol{\beta}_{\mathbf{C}\mathbf{C}\mathbf{S}} - \mathbf{Y}\boldsymbol{\beta}_{\mathbf{C}\mathbf{C}\mathbf{S})\|^{2} + (\mathbf{Y}\boldsymbol{\beta}_{\mathbf{C}\mathbf{C}\mathbf{S})\|^{2} + (\mathbf{Y}\boldsymbol{\beta}_{\mathbf{C}\mathbf{C}\mathbf{S}} - \mathbf{Y}\boldsymbol{\beta}_{\mathbf{C}\mathbf{C}\mathbf{S})\|^{2} + (\mathbf{Y}\boldsymbol{\beta}_{\mathbf{C}\mathbf{C}\mathbf{S})\|^{2} + (\mathbf{Y}\boldsymbol{\beta}_{$$

$$\underset{\boldsymbol{\beta}_{RR} \in \mathbb{R}^{N \times N2}}{\operatorname{arg \, min}} \left(\left\| \mathbf{Y} - \mathbf{X} \boldsymbol{\beta}_{\mathbf{RR}} \right\|^{2} \right) \qquad \operatorname{rank} \left(\boldsymbol{\beta}_{RR} \right) \leq K$$

$$\| \mathbf{Y} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{R}\mathbf{R}} \|^{2} =$$

$$\| (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{OLS}}) + (\mathbf{X}\boldsymbol{\beta}_{\mathbf{OLS}} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{R}\mathbf{R}}) \|^{2} =$$

$$\| \mathbf{Y} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{OLS}} \|^{2} + \| \mathbf{X}\boldsymbol{\beta}_{\mathbf{OLS}} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{R}\mathbf{R}} \|^{2} + \mathbf{crossterms}$$

$$\underset{\boldsymbol{\beta}_{RR} \in \mathbb{R}^{N \times N2}}{\operatorname{arg \, min}} \left(\left\| \mathbf{Y} - \mathbf{X} \boldsymbol{\beta}_{\mathbf{RR}} \right\|^{2} \right) \qquad \operatorname{rank} \left(\boldsymbol{\beta}_{RR} \right) \leq K$$

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$$\| \mathbf{Y} - \mathbf{X} \boldsymbol{\beta}_{\mathbf{OLS}} \|^{2} + \| \mathbf{X} \boldsymbol{\beta}_{\mathbf{OLS}} - \mathbf{X} \boldsymbol{\beta}_{\mathbf{RR}} \|^{2} + \mathbf{crossterms}$$

Because residuals $(Y - X\beta_{OLS})$ are orthogonal to X

$$\underset{\boldsymbol{\beta}_{RR} \in \mathbb{R}^{N \times N2}}{\operatorname{arg \, min}} \left(\left\| \mathbf{Y} - \mathbf{X} \boldsymbol{\beta}_{\mathbf{RR}} \right\|^{2} \right) \qquad \operatorname{rank} \left(\boldsymbol{\beta}_{RR} \right) \leq K$$

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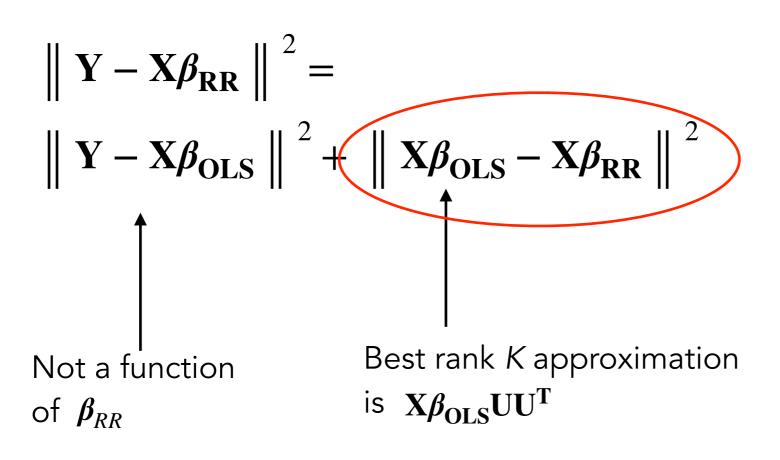
$$\|\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{R}\mathbf{R}}\|^2 = \|\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{OLS}}\|^2 + \|\mathbf{X}\boldsymbol{\beta}_{\mathbf{OLS}} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{R}\mathbf{R}}\|^2$$
Least squares loss

Loss from low-rank approximation

$$\underset{\boldsymbol{\beta}_{RR} \in \mathbb{R}^{N \times N2}}{\operatorname{arg \, min}} \left(\left\| \mathbf{Y} - \mathbf{X} \boldsymbol{\beta}_{\mathbf{RR}} \right\|^{2} \right) \qquad \operatorname{rank} \left(\boldsymbol{\beta}_{RR} \right) \leq K$$

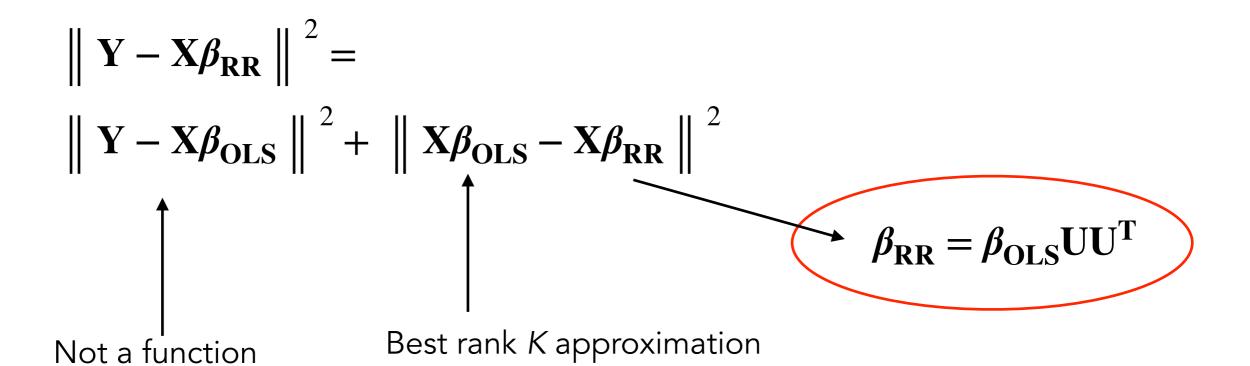
$$\|\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{RR}}\|^2 = \|\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{OLS}}\|^2 + \|\mathbf{X}\boldsymbol{\beta}_{\mathbf{OLS}} - \mathbf{X}\boldsymbol{\beta}_{\mathbf{RR}}\|^2$$
Not a function of $\boldsymbol{\beta}_{RR}$

$$\underset{\boldsymbol{\beta}_{RR} \in \mathbb{R}^{N \times N2}}{\operatorname{arg \, min}} \left(\left\| \mathbf{Y} - \mathbf{X} \boldsymbol{\beta}_{\mathbf{RR}} \right\|^{2} \right) \qquad \operatorname{rank} \left(\boldsymbol{\beta}_{RR} \right) \leq K$$



where **U** are the first K singular vectors of $\mathbf{X}\boldsymbol{\beta}_{\mathbf{OLS}}$ (Eckart-Young theorem)

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where \mathbf{U} are the first K singular vectors of $\mathbf{X}\boldsymbol{\beta}_{\mathbf{OLS}}$ (Eckart-Young theorem)

is $\mathbf{X}oldsymbol{eta}_{\mathrm{OLS}}\mathbf{U}\mathbf{U}^{\mathrm{T}}$

of β_{RR}

Reduced Rank Regression Additional Notes

$$\underset{\boldsymbol{\beta}_{RR} \in \mathbb{R}^{N \times N2}}{\operatorname{arg \, min}} \left(\left\| \mathbf{Y} - \mathbf{X} \boldsymbol{\beta}_{\mathbf{RR}} \right\|^{2} \right) \qquad \operatorname{rank} \left(\boldsymbol{\beta}_{RR} \right) \leq K$$

$$m{eta_{RR}} = m{eta_{OLS}} \mathbf{U} \mathbf{U}^{T}$$
 where \mathbf{U} are the first K singular vectors of $\mathbf{X} m{eta_{OLS}}$

$$= \mathbf{X} \left(\mathbf{X}^T \mathbf{X} \right)^{-1} \mathbf{X}^T \mathbf{Y}$$

 Dimensionality reduction depends on Y, unlike principal components regression

Reduced Rank Regression Additional Notes

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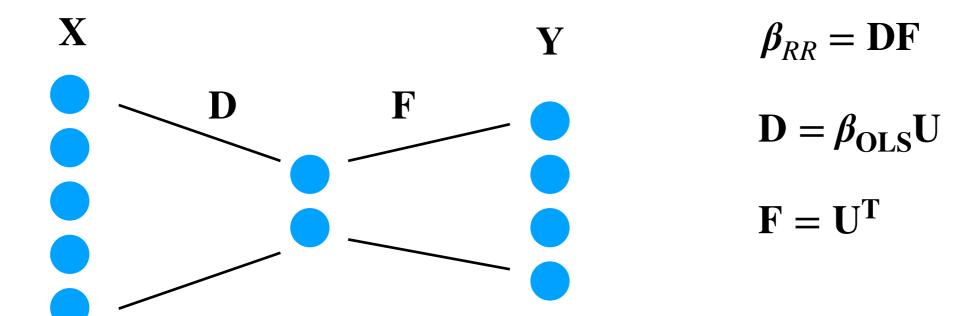
- Dimensionality reduction depends on Y, unlike principal components regression
- Reduced Rank Regression turns into PCA when Y = X.

Reduced Rank Regression Fun-facts

$$\underset{\boldsymbol{\beta}_{RR} \in \mathbb{R}^{N \times N2}}{\operatorname{arg \, min}} \left(\left\| \mathbf{Y} - \mathbf{X} \boldsymbol{\beta}_{\mathbf{RR}} \right\|^{2} \right) \qquad \operatorname{rank} \left(\boldsymbol{\beta}_{RR} \right) \leq K$$

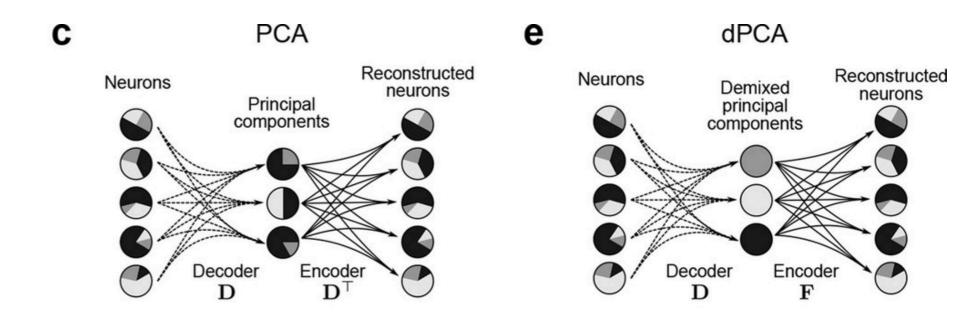
$$m{eta_{RR}} = m{eta_{OLS}} \mathbf{U} \mathbf{U}^{\mathbf{T}}$$
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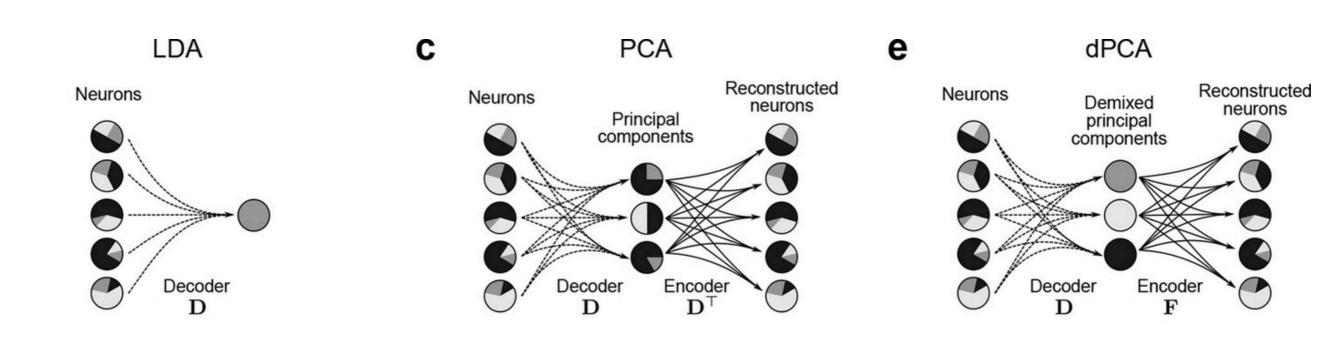
Demixed PCA

- Aims to find a latent representation that both reconstructs neural data (as in PCA) and maps the latents onto task parameters.
- Kobak,..., Machens. eLife (2016).

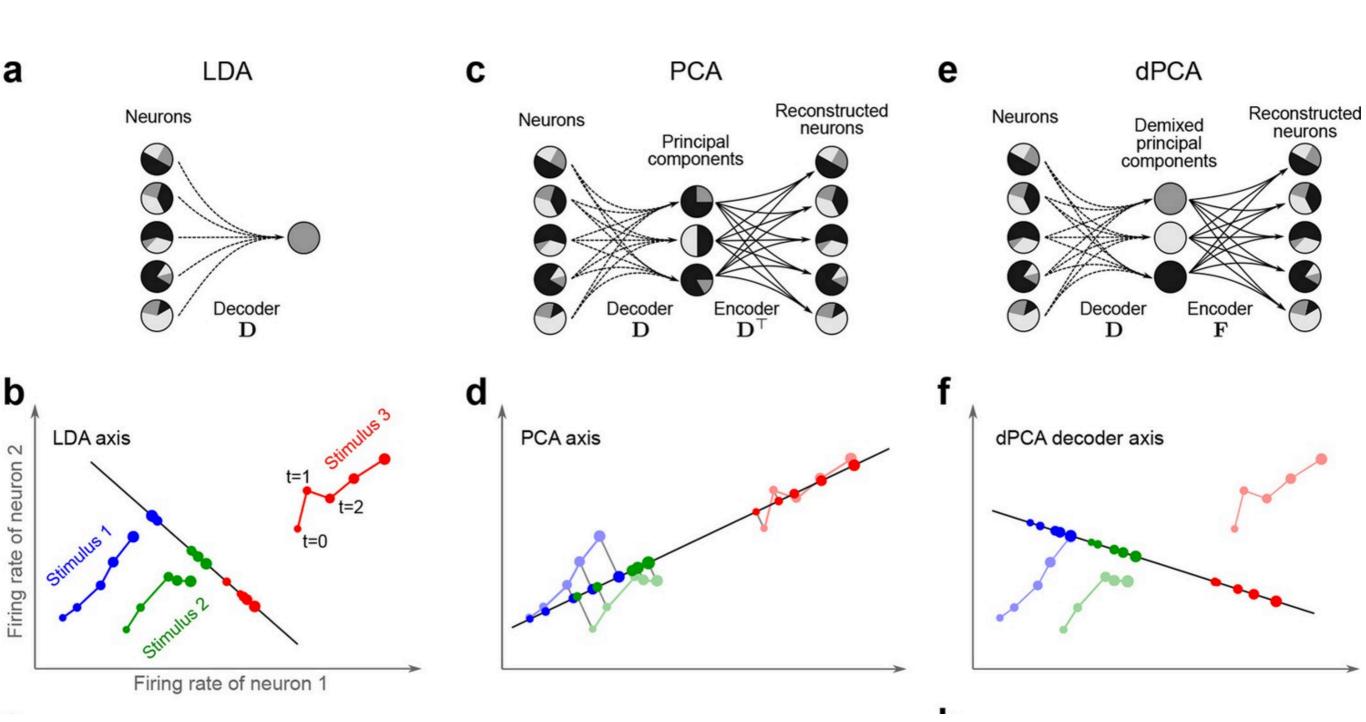


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Demixed PCA

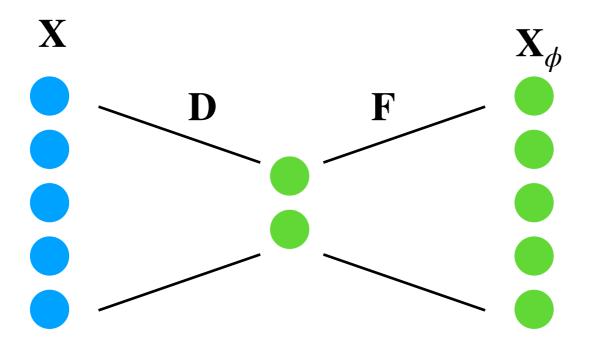


Demixed PCA

$$\mathbf{X} = \mathbf{X}_t + \mathbf{X}_{st} + \mathbf{X}_{dt} + \mathbf{X}_{sdt} + \mathbf{X}_{noise} = \sum_{\phi} \mathbf{X}_{\phi} + \mathbf{X}_{noise}.$$

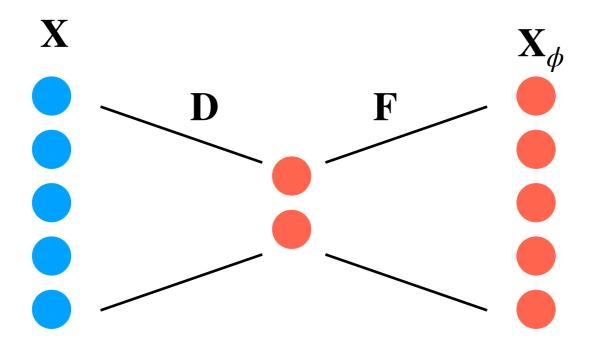
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$$L_{\text{dPCA}} = \sum_{\phi} \|\mathbf{X}_{\phi} - \mathbf{F}_{\phi} \mathbf{D}_{\phi} \mathbf{X}\|^{2}.$$



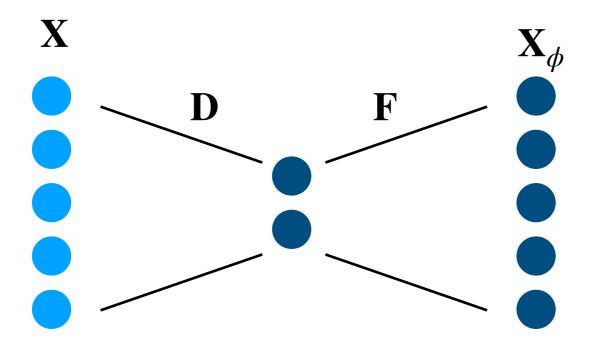
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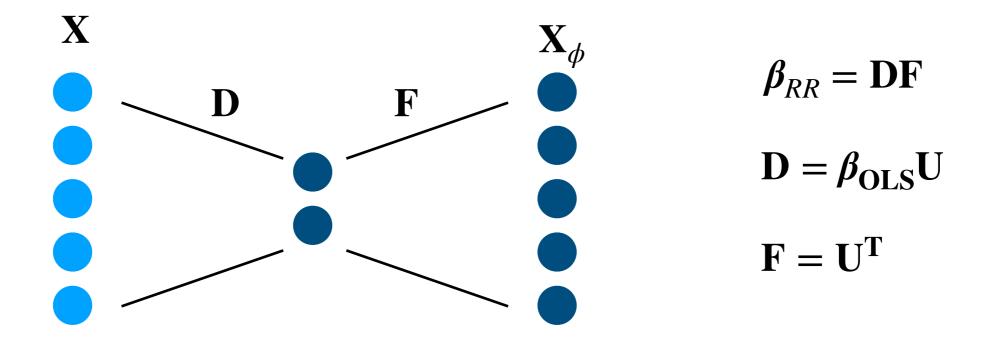
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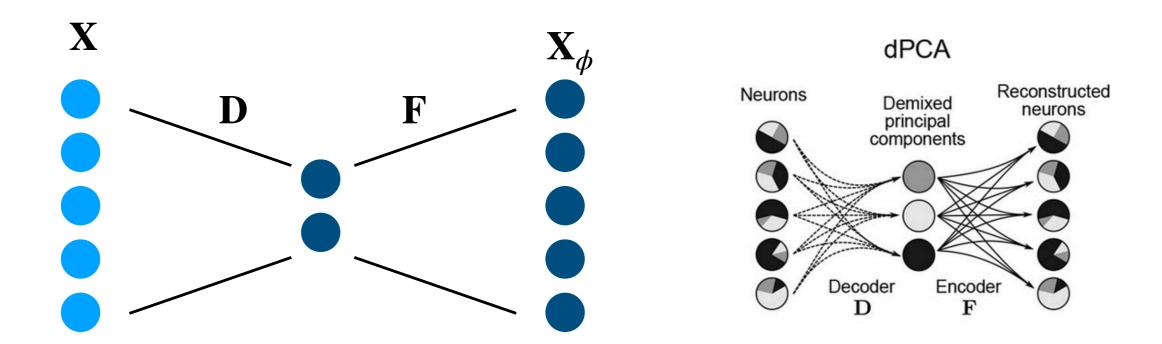
$$L_{\text{dPCA}} = \sum_{\phi} \|\mathbf{X}_{\phi} - \mathbf{F}_{\phi} \mathbf{D}_{\phi} \mathbf{X}\|^{2}.$$



Just do Reduced Rank Regression for each condition!

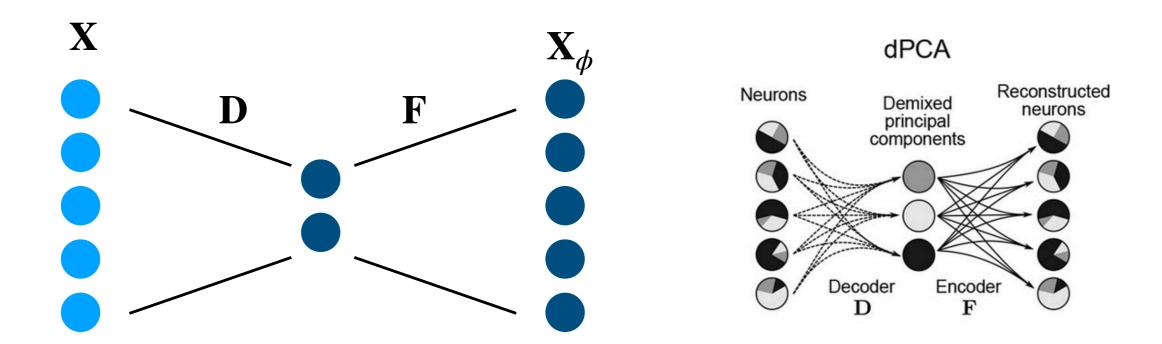
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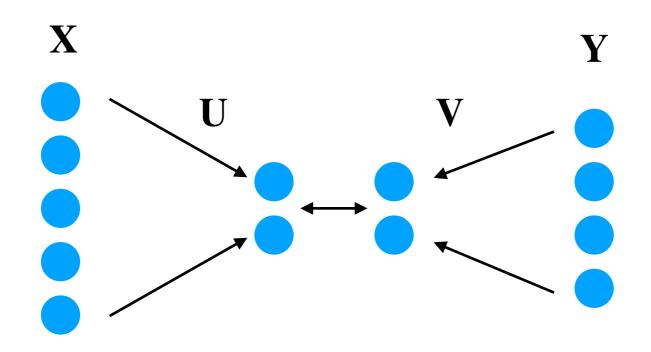


- Related methods include:
 - Targeted dimensionality reduction (Mante,...,Newsome, 2013)
 - Model-based targeted dimensionality reduction (Aoi,...,Pillow, 2019)

Overview

- 1. Reducing dimensionality in one space
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 - Partial least squares

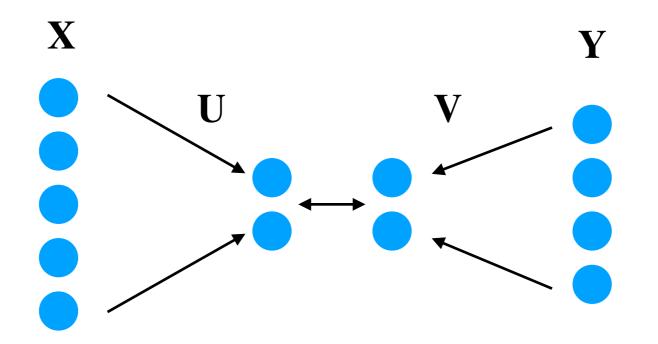
Reducing dimensionality in two spaces



Partial Least Squares

Maximize covariance between XU and YV

$$\underset{\mathbf{U},\mathbf{V}}{\text{arg max}} \left(\ \left\| \ (\mathbf{X}\mathbf{U})^{\mathbf{T}}\mathbf{Y}\mathbf{V} \ \right\|^{2} \right) \text{ s.t. } \left\| \ \mathbf{U} \ \right\| \ = \mathbf{I}, \ \left\| \ \mathbf{V} \ \right\| \ = \mathbf{I}$$

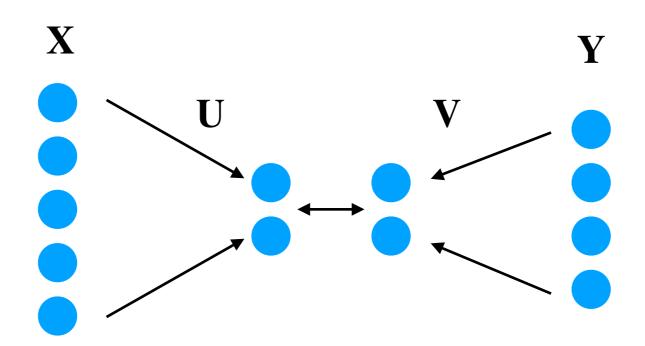


Partial Least Squares

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- Solution is to take first K singular vectors of $\mathbf{X}^{\mathbf{T}}\mathbf{Y}$
 - \mathbf{U} = left singular vectors, \mathbf{V} = right singular vectors



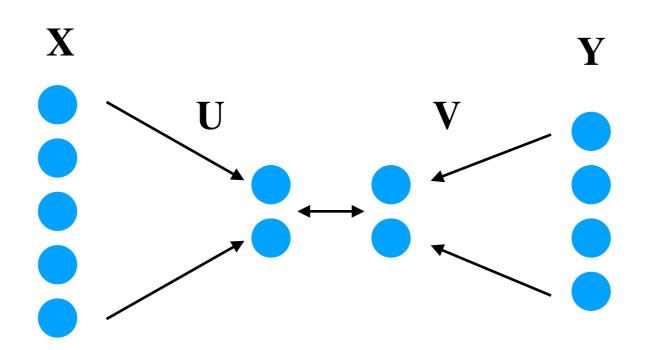
Partial Least Squares

Maximize covariance between XU and YV

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Minimize error between XU and YV

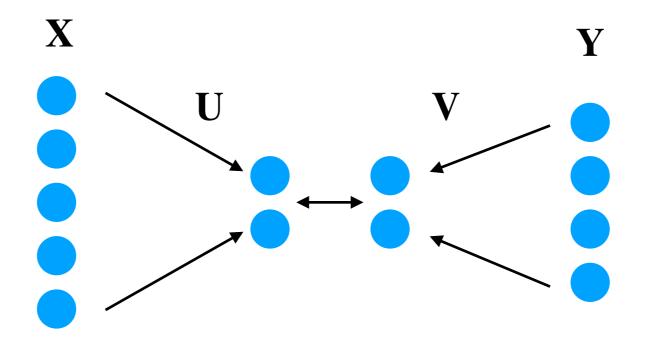
$$\underset{\mathbf{U},\mathbf{V}}{\text{arg min}} \ \left(\ \left\| \ \mathbf{X}\mathbf{U} - \mathbf{Y}\mathbf{V} \ \right\|^{2} \right) \ \text{s.t.} \quad \left\| \ \mathbf{U} \ \right\| \ = \mathbf{I}, \ \left\| \ \mathbf{V} \ \right\| \ = \mathbf{I}$$



Canonical Correlation Analysis

Maximize correlation between XU and YV

$$\underset{\mathbf{U},\mathbf{V}}{\operatorname{arg\,max}} \left(\frac{ \left\| (\mathbf{X}\mathbf{U})^{\mathbf{T}}\mathbf{Y}\mathbf{V} \right\|^{2}}{ \left\| \mathbf{X}\mathbf{U} \right\| \| \mathbf{Y}\mathbf{V} \|} \right) \text{ s.t. } \| \mathbf{U} \| = \mathbf{I}, \| \mathbf{V} \| = \mathbf{I}$$

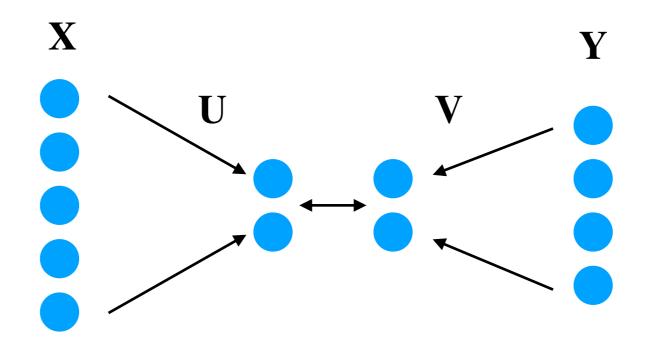


Canonical Correlation Analysis

Maximize correlation between XU and YV

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- Solution is to take first K singular vectors of $(\mathbf{X}^T\mathbf{X})^{-1/2}\mathbf{X}^T\mathbf{Y}(\mathbf{Y}^T\mathbf{Y})^{-1/2}$
 - U = left singular vectors, V = right singular vectors



PLS:
$$\underset{\mathbf{U},\mathbf{V}}{\operatorname{arg\,max}} \left(\| (\mathbf{X}\mathbf{U})^{\mathsf{T}}\mathbf{Y}\mathbf{V} \|^{2} \right) \text{ s.t. } \| \mathbf{U} \| = \mathbf{I}, \| \mathbf{V} \| = \mathbf{I}$$

CCA:
$$\underset{\mathbf{U},\mathbf{V}}{\operatorname{arg\,max}} \left(\frac{ \left\| (\mathbf{X}\mathbf{U})^{\mathbf{T}}\mathbf{Y}\mathbf{V} \right\|^{2}}{ \left\| \mathbf{X}\mathbf{U} \right\| \| \mathbf{Y}\mathbf{V} \|} \right)$$
 s.t. $\| \mathbf{U} \| = \mathbf{I}, \| \mathbf{V} \| = \mathbf{I}$

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PLS:
$$\underset{\mathbf{U},\mathbf{V}}{\operatorname{arg\,min}} \left(\| \mathbf{X}\mathbf{U} - \mathbf{Y}\mathbf{V} \|^2 \right) \text{ s.t. } \| \mathbf{U} \| = \mathbf{I}, \| \mathbf{V} \| = \mathbf{I}$$

CCA:

PLS:
$$\underset{\mathbf{U},\mathbf{V}}{\operatorname{arg\,min}} \left(\| \mathbf{X}\mathbf{U} - \mathbf{Y}\mathbf{V} \|^2 \right) \text{ s.t. } \| \mathbf{U} \| = \mathbf{I}, \| \mathbf{V} \| = \mathbf{I}$$

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 s.t. $\| \mathbf{U} \| = \mathbf{I}, \| \mathbf{V} \| = \mathbf{I}$

PLS: Solution is to take first K singular vectors of $\mathbf{X}^{T}\mathbf{Y}$

CCA: Solution is to take first K singular vectors of $(\mathbf{X}^T\mathbf{X})^{-1/2}\mathbf{X}^T\mathbf{Y}(\mathbf{Y}^T\mathbf{Y})^{-1/2}$

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CCA solution "whitens" X and Y

CCA vs PLS vs RRR

PLS:
$$\underset{\mathbf{U},\mathbf{V}}{\operatorname{arg\,max}} \left(\| (\mathbf{X}\mathbf{U})^{\mathsf{T}}\mathbf{Y}\mathbf{V} \|^{2} \right) \text{ s.t. } \| \mathbf{U} \| = \mathbf{I}, \| \mathbf{V} \| = \mathbf{I}$$

CCA:
$$\underset{\mathbf{U},\mathbf{V}}{\operatorname{arg\,max}} \left(\frac{\left\| (\mathbf{X}\mathbf{U})^{\mathbf{T}}\mathbf{Y}\mathbf{V} \right\|^{2}}{\left\| \mathbf{X}\mathbf{U} \right\| \|\mathbf{Y}\mathbf{V} \|} \right) \text{ s.t. } \|\mathbf{U}\| = \mathbf{I}, \|\mathbf{V}\| = \mathbf{I}$$

RRR:
$$\underset{\mathbf{U},\mathbf{V}}{\operatorname{arg\,max}} \left(\frac{ \left\| (\mathbf{X}\mathbf{U})^{\mathbf{T}}\mathbf{Y}\mathbf{V} \right\|^{2}}{ \left\| \mathbf{X}\mathbf{U} \right\|} \right) \text{ s.t. } \left\| \mathbf{V} \right\| = \mathbf{I}$$

- CCA solution "whitens" X and Y
- RRR solution "whitens" X, but not Y

$$\beta = \left(\mathbf{X}^{\mathrm{T}}\mathbf{X}\right)^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{Y}$$

Many extensions

- Adding regularization
- Reduced Rank GLMs
- Kernel CCA
- Neural networks with bottlenecks
- Multiple factor analysis (for >2 populations)
- Probabilistic versions (pCCA)