Canonical Correlation Analysis (CCA)

Lecture #13

BIOE 597, Spring 2017,

Penn State University

By Xiao Liu

Agenda

- Review
- CCA Basics
- CCA Solution
- Hypothesis Testing
- Examples
- Final Project
- Midterm Review

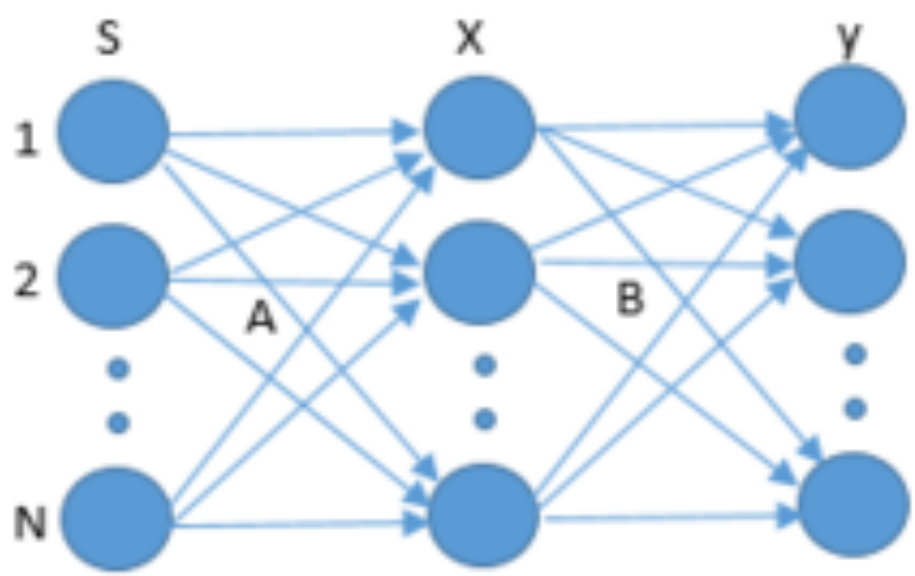
Independent Component Analysis (Review)

- **What is ICA**

"Independent component analysis (ICA) is a method for finding underlying factors or components from multivariate (multi-dimensional) statistical data. What distinguishes ICA from other methods is that it looks for components that are both *statistically independent*, and *nonGaussian*."

Independent Component Analysis (Review)

- **Blind Signal Separation**
  - Blind signal separation (BSS), also known as blind source separation, is the separation of a set of source signals from a set of mixed signals, without the aid of information (or with very little information) about the source signals or the mixing process.



Independent Component Analysis (Review)

- **Mathematical Description**

$$x_i = a_{i1}s_1 + ai_2s_2 + \ldots + a_{im}s_m, \text{ for all } i = 1, \ldots, m$$

$$\boldsymbol{X}_{n\times r} = \boldsymbol{S}_{n\times m}\boldsymbol{A}_{m\times r}$$

- Giving:
  observation "$\boldsymbol{X}$"
- Find:
  Original independent components "$\boldsymbol{S}$"

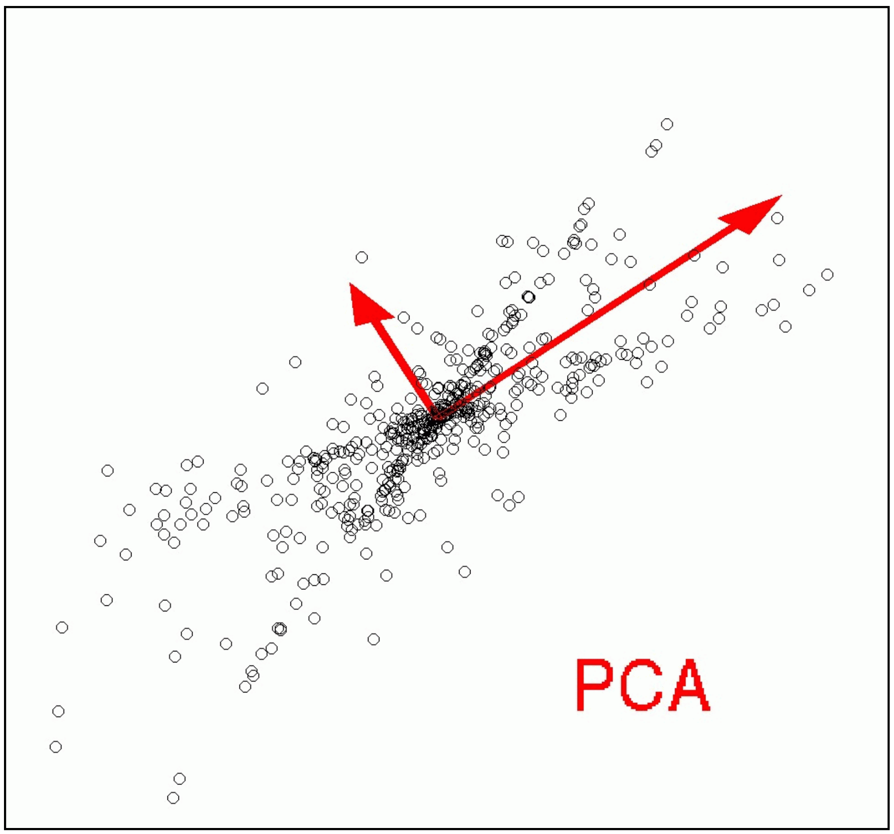
$$\boldsymbol{S}_{n\times m} = \boldsymbol{X}_{n\times r}\boldsymbol{W}_{r\times m}$$

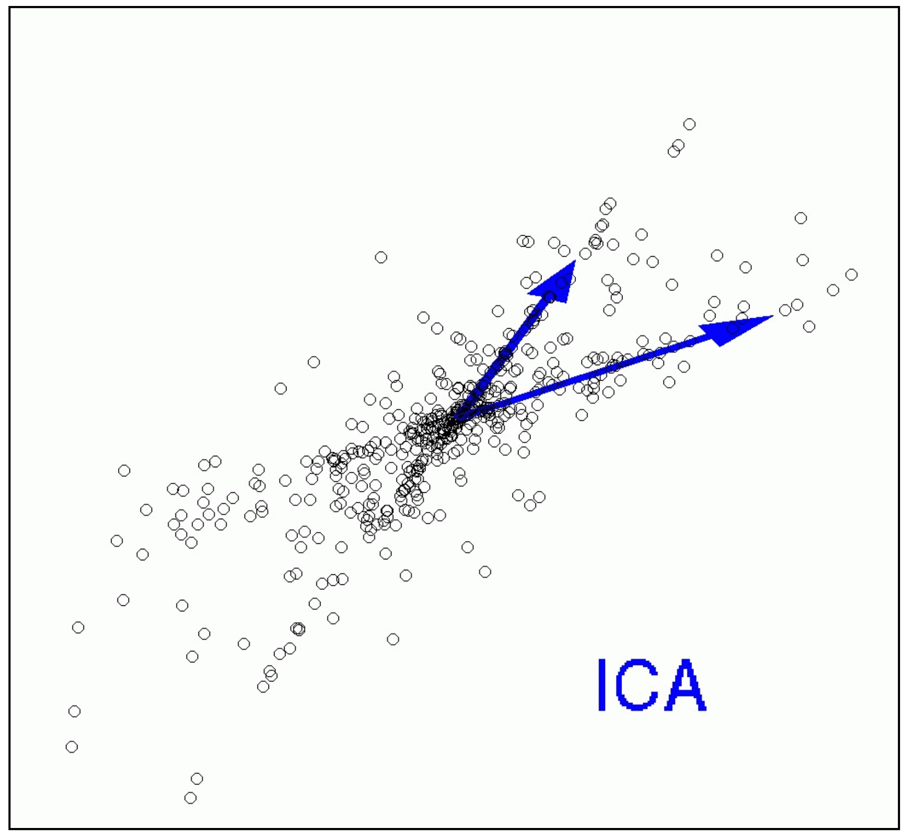
Independent Component Analysis (Review)

- **Identifiability**
  - s_i are statistically independent
  - At most one of the sources s_i is Gaussian
  - The number of observed mixtures, r, must be at least as large as the number of estimated components m: $r \geq m$

Independent Component Analysis (Review)

- **PCA versus ICA**
  - PCA: Finds directions of maximal variance in gaussian data
  - ICA: Finds directions of maximal independence in nongaussian data





Independent Component Analysis (Review)

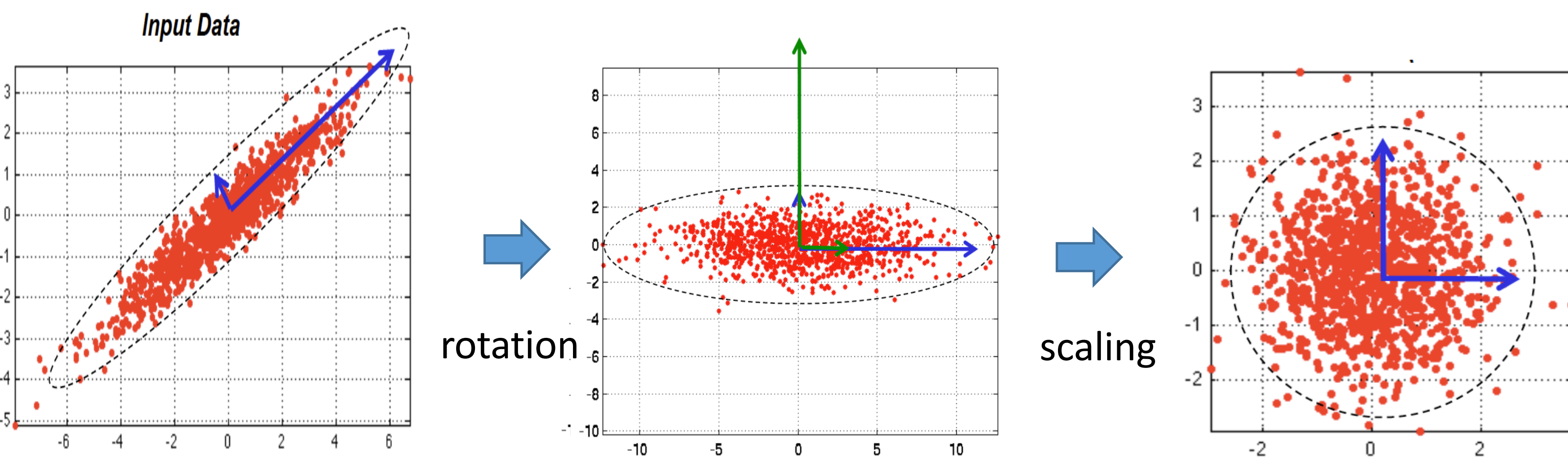
- **ICA Steps: Whitening**
- Whitenning/Sphering, i.e., PCA

$$Z = XW \qquad C_Z = W^T C_X W = \mathrm{diag}(\lambda_i)$$

$$Y = XW_N \qquad C_Y = {W_N}^T C_X W_N = I$$

SVD: $XV = U\Sigma \qquad XV\Sigma^{-1} = U \qquad \Sigma = diag(\sigma_i)$

$$XW = Z \qquad XW_N = Y \qquad \Sigma^{-1} = diag(1/\sigma_i)$$



Independent Component Analysis (Review)

- **ICA Steps: Whitening**
  - Why do we do ”whitening/sphering”?

$$Y = XW_N \qquad\qquad C_Y = I$$

for any orthogonal rotation R

$$S = YR$$

$$C_S = R^T C_Y R = R^T C_Y R = I$$

- No matter how we rotate the whitened data, the resulting columns will be ”uncorrelated”

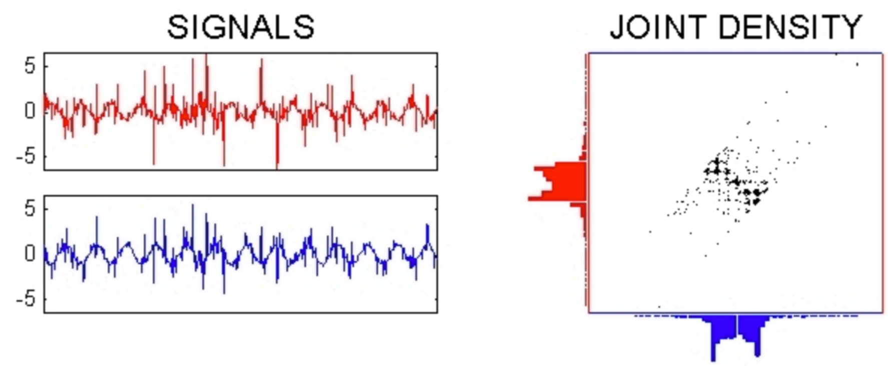
Independent Component Analysis (Review)

- **ICA Steps: Rotation**

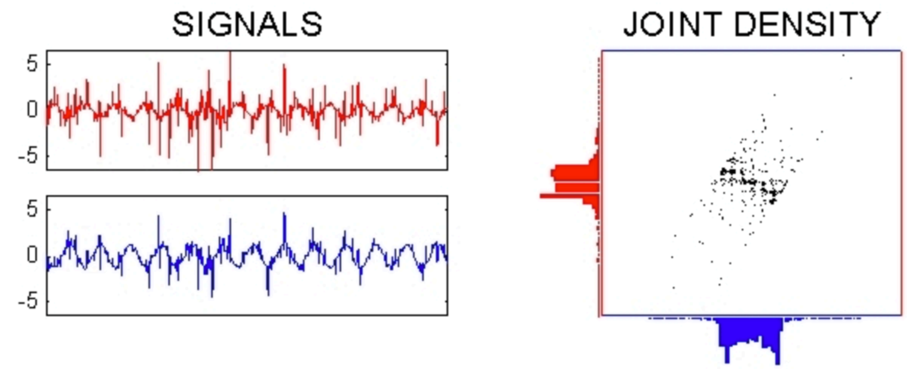
- Maximize the statistical independence of the estimated components
  - Maximize non-Gaussianity
  - Minimize mutual information
- Measures of non-Gaussianity and independence
  - Kurtosis: $kurt(y) = E\{y^4\} - 3(E\{y^2\})^2$
  - Entropy: $H(y) = -\int f(y) \log f(y) dy$
  - Negentropy: $J(y) = H(y_{gauss}) - H(y)$
  - Kullback–Leibler divergence (relative entropy)
  - …

Independent Component Analysis (Review)

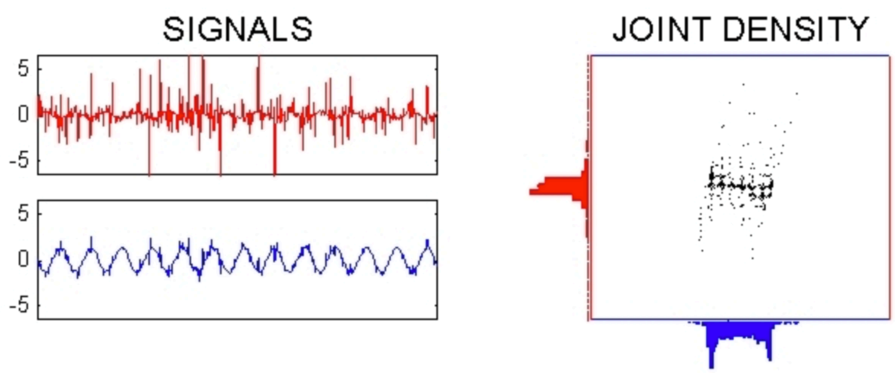
- **ICA Steps: Rotation**



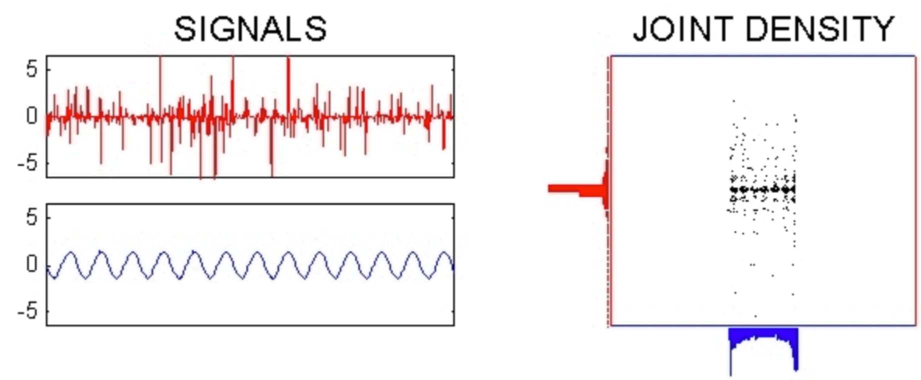
Separated signals after 1 step of FastICA



Separated signals after 2 steps of FastICA



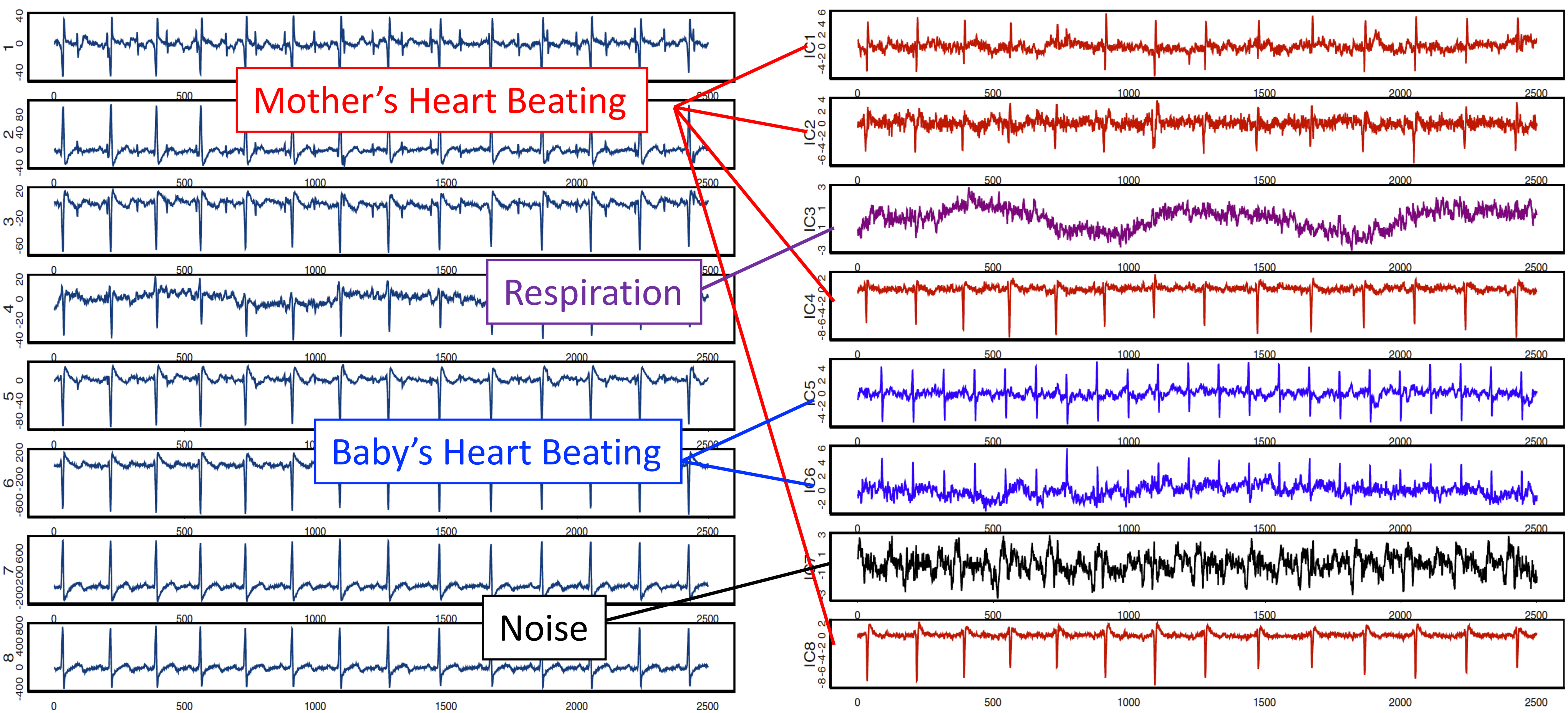
Separated signals after 3 steps of FastICA



Separated signals after 4 steps of FastICA

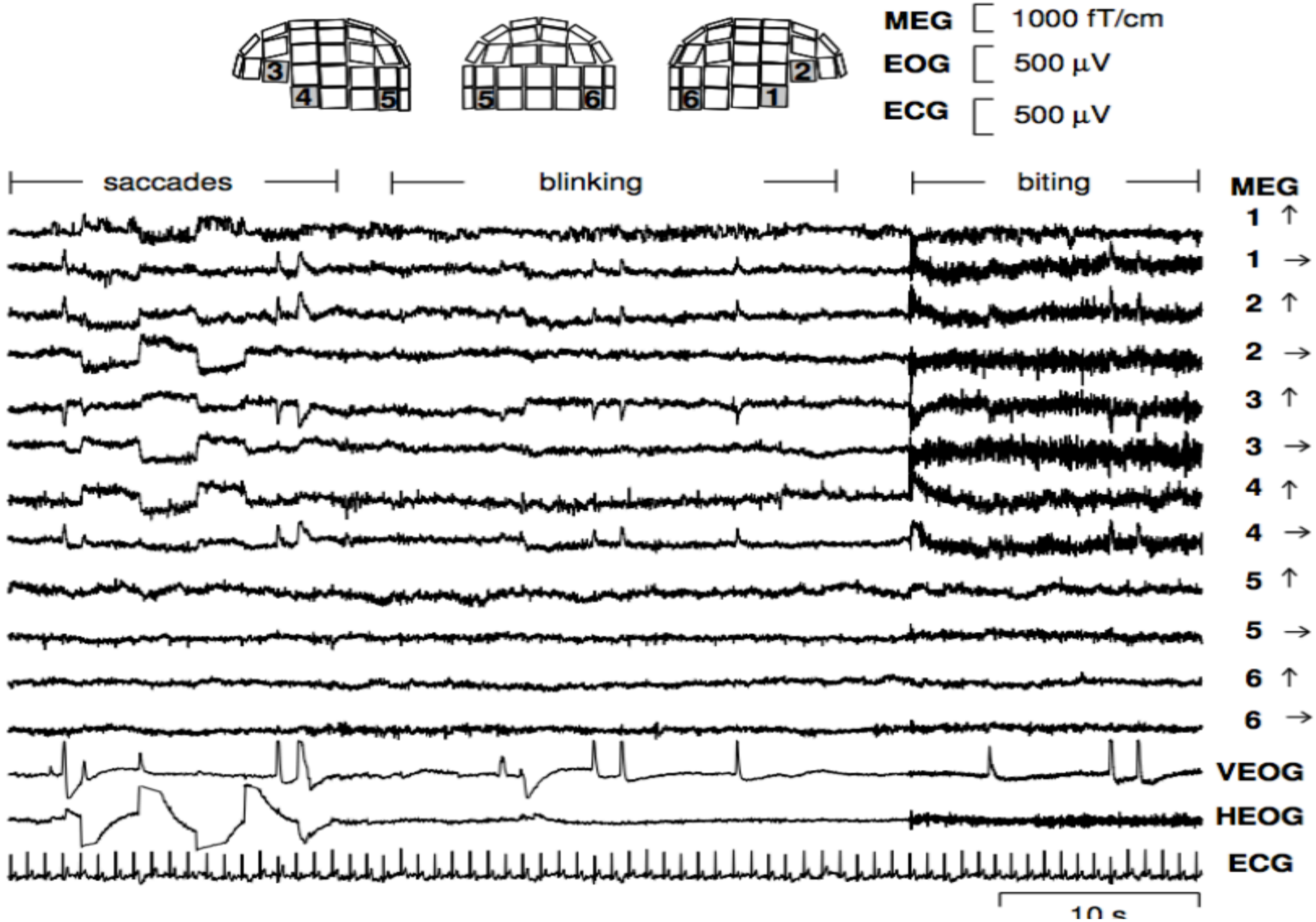
Independent Component Analysis (Review)

- **Examples**
  - Original Signals
  - Independent Components



Independent Component Analysis (Review)

- **Examples**
- Clearing up MEG (Magnetoencephalography) data



Introduction

- When we have univariate data there are times when we would like to measure the linear relationship between things
    - Simple Linear Regression: we have 2 variables and all we are interested in is measuring their linear relationship.
    - Multiple linear regression: we have several independent variables and one dependent variable.

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_1 x_{i2} + \cdots + \beta_1 x_{ik} + e_i \quad e_i \sim N(0, \sigma^2)$$

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- What if we have several dependent variables and several independent variables?
  - Multivariate Regression
  - Canonical Correlation Analysis

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- Finding two sets of basis vectors such that the correlation between the projections of the variables onto these basis vectors is maximized
- Determine correlation coefficients

Jargon

- Variables: two sets of variables X and Y

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- Canonical Variates --- Linear combinations of variables
- Canonical Variates Pair --- Two Canonical Variates with each from one set showing non-zero correlations
- Canonical Correlations--- Correlation between Canonical Variate Pairs

CCA Definition

- Two groups of multidimensional variables $X = [\boldsymbol{x_1}, \boldsymbol{x_2}, \ldots, \boldsymbol{x_p}]$ and $Y = [\boldsymbol{y_1}, \boldsymbol{y_2}, \ldots, \boldsymbol{y_q}]$

where $$\boldsymbol{x_i} = \begin{bmatrix} x_{i1} \\ x_{i2} \\ x_{i3} \\ \ldots \\ x_{in} \end{bmatrix} \qquad \boldsymbol{y_i} = \begin{bmatrix} y_{j1} \\ y_{j2} \\ y_{j3} \\ \ldots \\ y_{jn} \end{bmatrix}$$

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- Purpose of CCA: find coefficient vectors $\boldsymbol{a_1} = (a_{11}, a_{21}, \dots, ap_1)^T$, and $\boldsymbol{b_1} = (b_{11}, b_{21}, \dots, b_{q1})^T$ to maximize the correlation $\rho = corr(X\boldsymbol{a_1}, Y\boldsymbol{b_1})$

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- $U_1 = X\boldsymbol{a_1}$ and $V_1 = Y\boldsymbol{b_1}$, i.e., linear combinations of X and Y respectively, are the first pair of canonical variates.

CCA Definition

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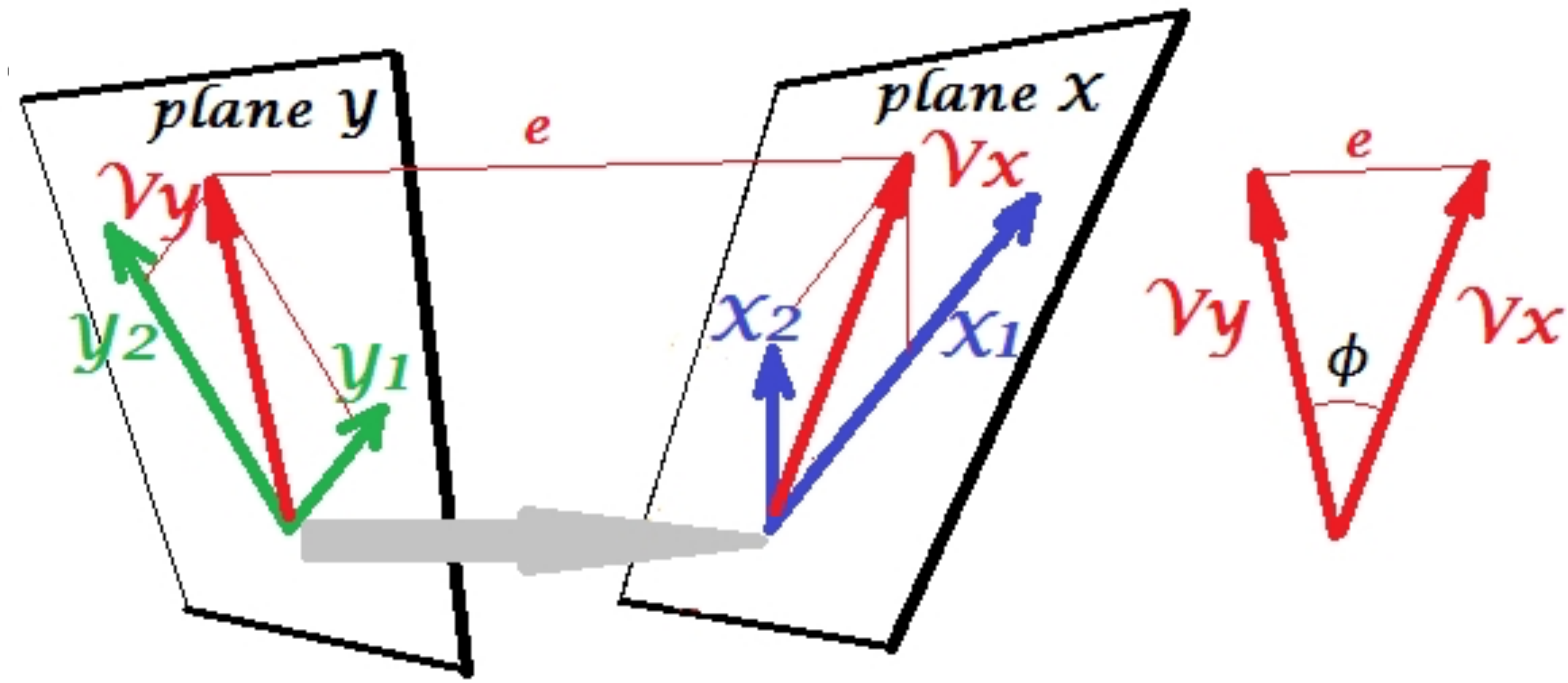
- Then, the second pair of canonical variates can be found in the same way subject to the constraint that they are uncorrelated with the first pair of variables.
- $r = \min\{p, q\}$ pairs of canonical variate pairs can be found by repeating this procedure
- We will finally get two matrices $A = [\boldsymbol{a_1}, \boldsymbol{a_2}, \dots, \boldsymbol{a_r}]$ and $B = [\boldsymbol{b_1}, \boldsymbol{b_2}, \dots, \boldsymbol{b_r}]$ to transfer the X and Y to canonical variates U and V.

$$U_{n\times r} = X_{n\times p}A_{p\times r}$$

$$V_{n\times r} = Y_{n\times q}B_{q\times r}$$

Geometric Interpretation



PCA versus CCA

- PCA looks for patterns with a single multivariate dataset that represent maximum amounts of the variation in the data

- In CCA, the patterns are chosen such that the projected data onto these patterns exhibit maximum correlation – while being uncorrelated with the projections onto any other pattern

- In other words: CCA identifies new variables that maximize the inter-relationships between two data sets, in contrast to the patterns describing the internal variability within a single dataset from PCA.

Mathematical Description

- IF X and Y are both centered, we can concatenate them and calculate the covariance matrix

$$C = Cov([X\ Y]) = \frac{1}{n-1}[X\ Y]^T[X\ Y] = \begin{bmatrix} C_{xx} & C_{xy} \\ C_{yx} & C_{yy} \end{bmatrix}$$

where C_{xx} and C_{xx} are within-set covariance matrices, and $C_{xy} = {C_{yx}}^T$ are between-set covariance matrices

- The first canonical variates $\boldsymbol{a_1}$ and $\boldsymbol{b_1}$ maximizes

$$\rho_1 = \frac{\boldsymbol{a_1}^T C_{xy} \boldsymbol{b_1}}{\sqrt{\boldsymbol{a_1}^T C_{xx} a_{\boldsymbol{1}}}\sqrt{\boldsymbol{b_1}^T C_{yy} b_{\boldsymbol{1}}}}$$

Mathematical Description

- The subsequent pairs of canonical variates $\boldsymbol{a_i}$ and $\boldsymbol{b_i}$ $(i \geq 2)$ maximizes

$$\rho_i = \frac{\boldsymbol{a}_i{}^T C_{xy} \boldsymbol{b_i}}{\sqrt{\boldsymbol{a}_i{}^T C_{xx} \boldsymbol{a_i}} \sqrt{\boldsymbol{b_i}{}^T C_{yy} \boldsymbol{b_i}}}$$

subject to the constraint

$$\boldsymbol{a}_i{}^T C_{xx} \boldsymbol{a_j} = 0 \qquad for\ all\ j < i$$

$$\boldsymbol{b}_i{}^T C_{yy} \boldsymbol{b_j} = 0 \qquad for\ all\ j < i$$

Solution

- The solution for this problem

$$\begin{cases} C_{xx}^{-1} C_{xy} C_{yy}^{-1} C_{yx} \boldsymbol{a_i} = {\rho_i}^2 \boldsymbol{a_i} \\ C_{yy}^{-1} C_{yx} C_{xx}^{-1} C_{xy} \boldsymbol{b_i} = {\rho_i}^2 \boldsymbol{b_i} \end{cases}$$

- So, the $\boldsymbol{a_i}$ are eigenvectors of $C_{xx}^{-1} C_{xy} C_{yy}^{-1} C_{yx}$ corresponding to eigenvalues of ${\rho_i}^2$

- So, the $\boldsymbol{b_i}$ are eigenvectors of $C_{yy}^{-1} C_{yx} C_{xx}^{-1} C_{xy}$ corresponding to eigenvalues of ${\rho_i}^2$

- They are related to each other by

$$\begin{cases} C_{xy} \boldsymbol{b_i} = \rho_i \lambda_x C_{xx} \boldsymbol{a_i} \\ C_{yx} \boldsymbol{a_i} = \rho_i \lambda_y C_{yy} \boldsymbol{b_i} \end{cases} \quad \text{where} \quad \lambda_x = \frac{1}{\lambda_y} = \sqrt{\frac{{\boldsymbol{b_i}}^T C_{yy} \boldsymbol{b_i}}{{\boldsymbol{a_i}}^T C_{xx} \boldsymbol{a_i}}}$$

Steps via Eigendecomposition

- Compute the matrix $C_{xx}^{-1}C_{xy}C_{yy}^{-1}C_{yx}$, and then eigendecompose it to get the square root of its eigenvalues $= [\rho_1, \rho_2, \dots, \rho_r]$ and eigenvectors $A = [\boldsymbol{a_1}, \boldsymbol{a_2}, \dots, \boldsymbol{a_r}]$

- Compute the matrix $C_{yy}^{-1}C_{yx}C_{xx}^{-1}C_{xy}$, and then eigendecompose it to get the square root of its eigenvalues $= [\rho_1, \rho_2, \dots, \rho_r]$ and eigenvectors $B = [\boldsymbol{b_1}, \boldsymbol{b_2}, \dots, \boldsymbol{b_r}]$

- The eigenvalues for both equations are equal and between zero and one. Their square root is the canonical correlation.

- The eigenvectors are weights for constructing the linear combinations of original data, i.e., canonical variates

Hypothesis Testing

- We can also test whether the canonical correlations are significant different from zero

- The test statistic is called Wilks's Lambda

$$\Lambda_k = \prod_{i=k}^{\min(p,q)} (1 - \rho_i{}^2)$$

$-\left(n - 1 - \frac{1}{2}(p + q + 1)\right)\ln(\Lambda_k)$ is asymptotically distribute as a chi-squared with $(p - k + 1)(p - k + 1)$ degree of freedom

CCA Properties

- Canonical correlations are invariant.
  - scale changes (such as standardizing) will not change the correlation
  - Actually, they are invariant after nonsingular linear transformations on X and Y.

- The first canonical correlation is the best we can do with associations.
  - it is larger than any of the simple correlations or any multiple correlation with the variables under study

Matlab Function

- [A, B, r, U, V, stat] = canoncorr(x, y)
  - x, y : set of variables in the form of matrices
    - Each row is an observation
    - Each column is an attribute/feature
  - A, B: Matrices containing the correlation coefficient
  - r : Column matrix containing the canonical correlations (Successively decreasing)
  - U, V: Canonical variates/basis vectors for A,B respectively
  - stat: statistics for hypothesis testing

Example

- Suppose we have two sets of variables X and Y

$$\mathbf{X} = \begin{pmatrix} 1 & 1 & 3 \\ 2 & 3 & 2 \\ 1 & 1 & 1 \\ 1 & 1 & 2 \\ 2 & 2 & 3 \\ 3 & 3 & 2 \\ 1 & 3 & 2 \\ 4 & 3 & 5 \\ 5 & 5 & 5 \end{pmatrix}, \quad \mathbf{Y} = \begin{pmatrix} 4 & 4 & -1.07846 \\ 3 & 3 & 1.214359 \\ 2 & 2 & 0.307180 \\ 2 & 3 & -0.385641 \\ 2 & 1 & -0.078461 \\ 1 & 1 & 1.61436 \\ 1 & 2 & 0.814359 \\ 2 & 1 & -0.0641016 \\ 1 & 2 & 1.535900 \end{pmatrix}$$

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- **Note:** the third column of Y is a linear combination of X:

$$Y(:,3) = 0.4 * X(:,1) + 0.6 * X(:,2) - \sqrt{0.48} * X(:,3)$$

Example

[A, B, r, U, V, stat] = canoncorr(X, Y);

```
A =

  -0.4324   -1.4468   -0.8180
  -0.6485    1.0610    0.6070
   0.7489    0.2902    0.9838

>> B

B =

  -0.0000   -0.8487   -1.5200
   0.0000    1.3346    0.2524
  -1.0809    0.0216   -0.9702
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A1 =

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  -0.6928   -0.1597    0.6947

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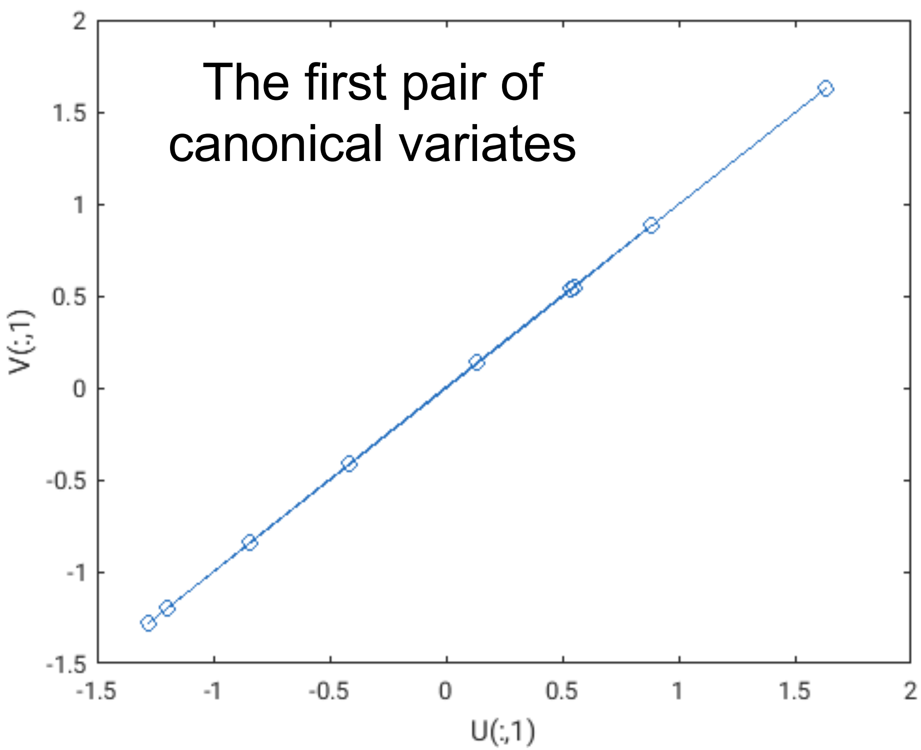
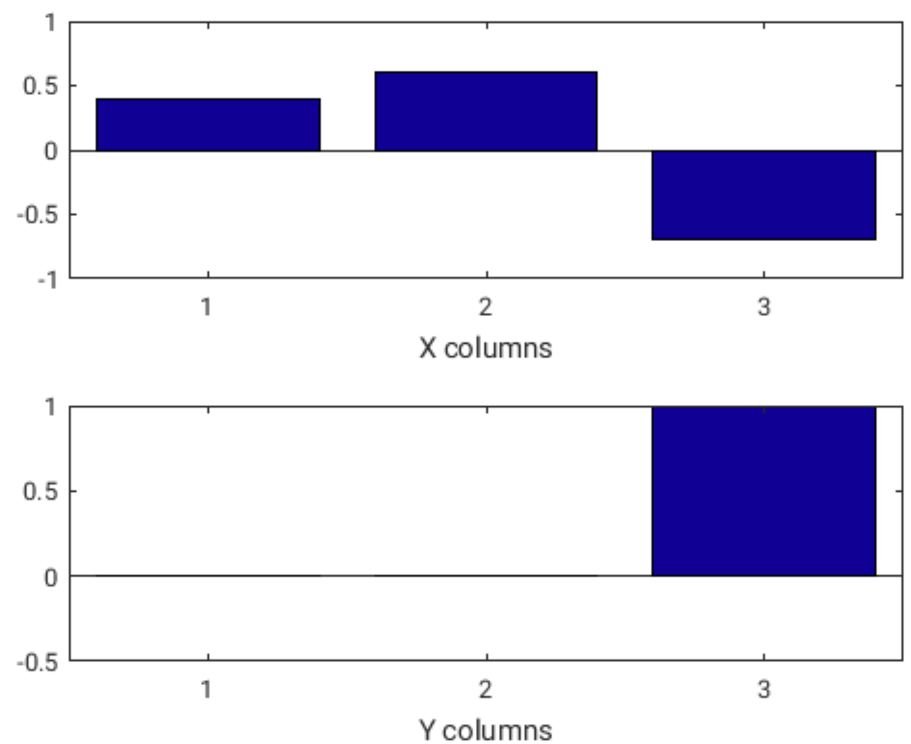
r =

1.0000 0.5194 0.0910





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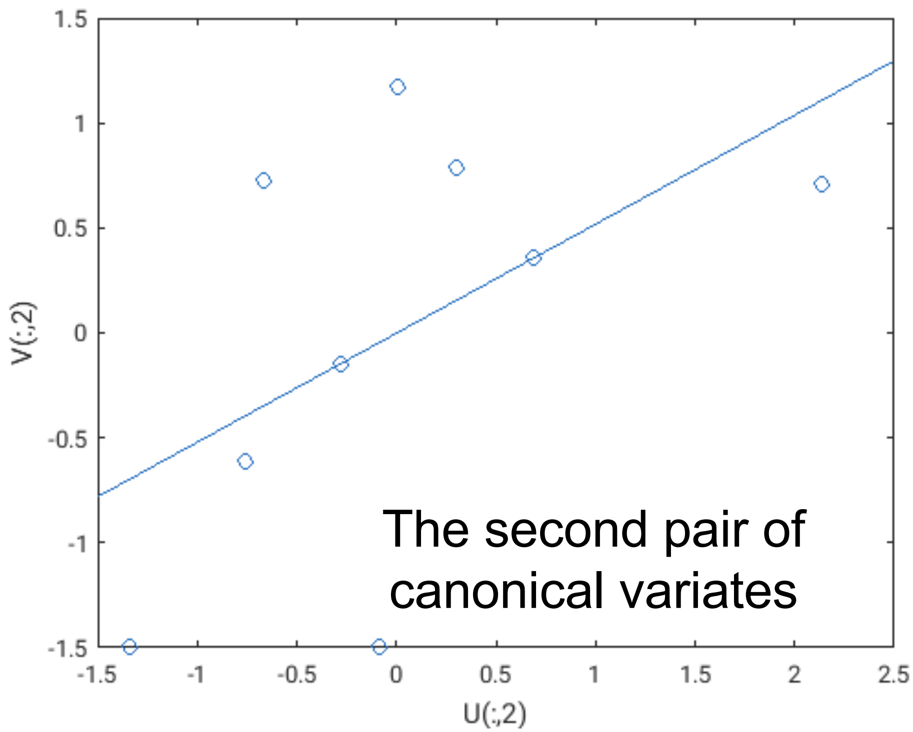

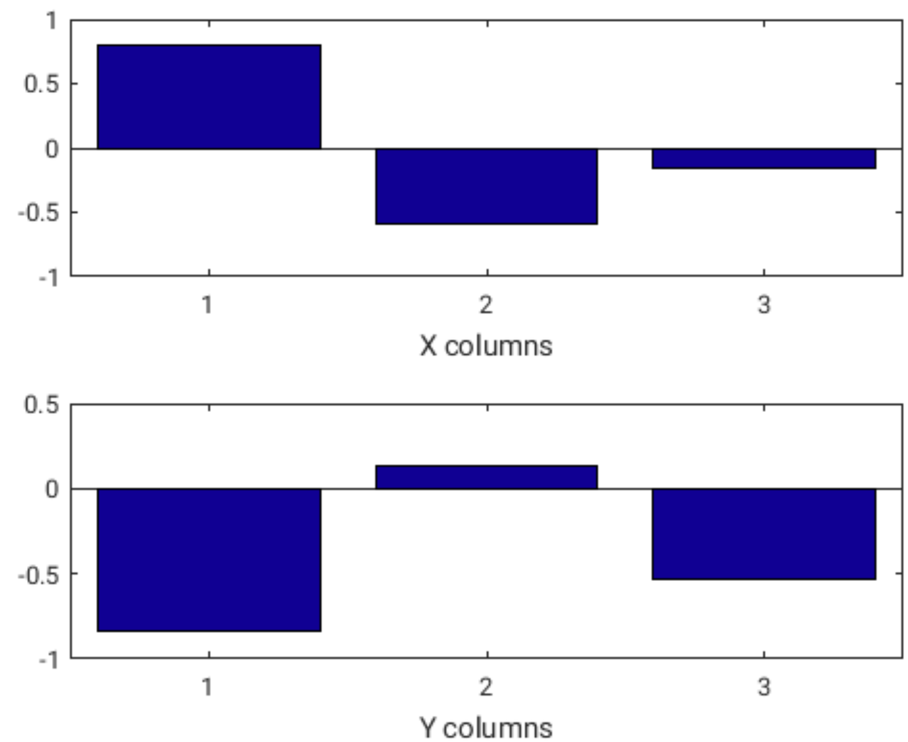

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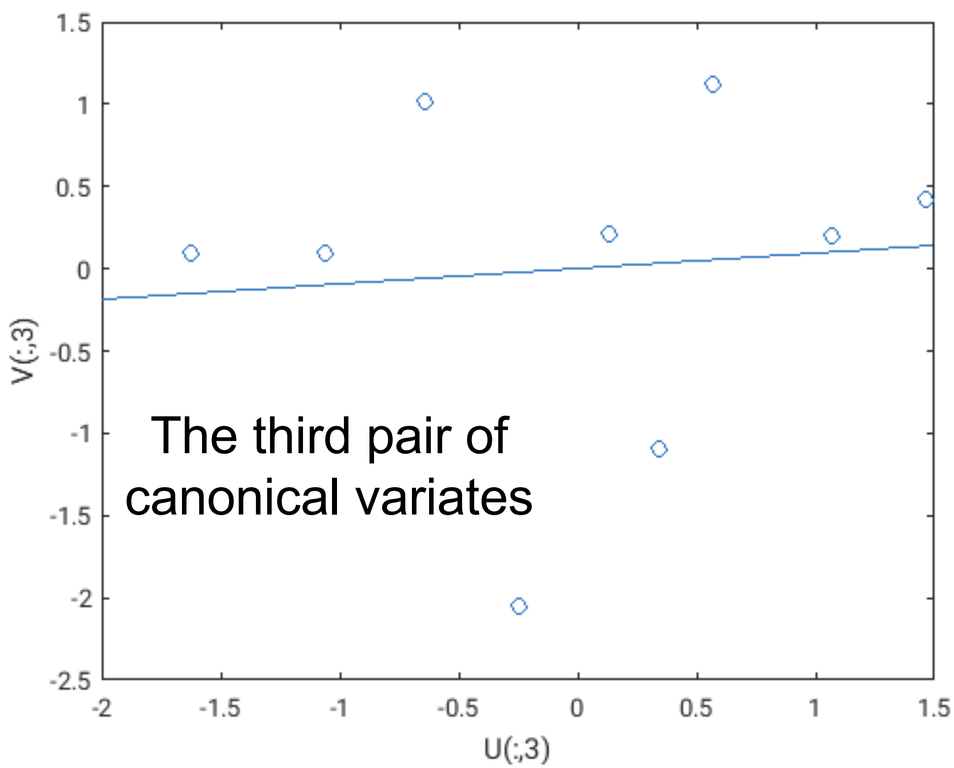

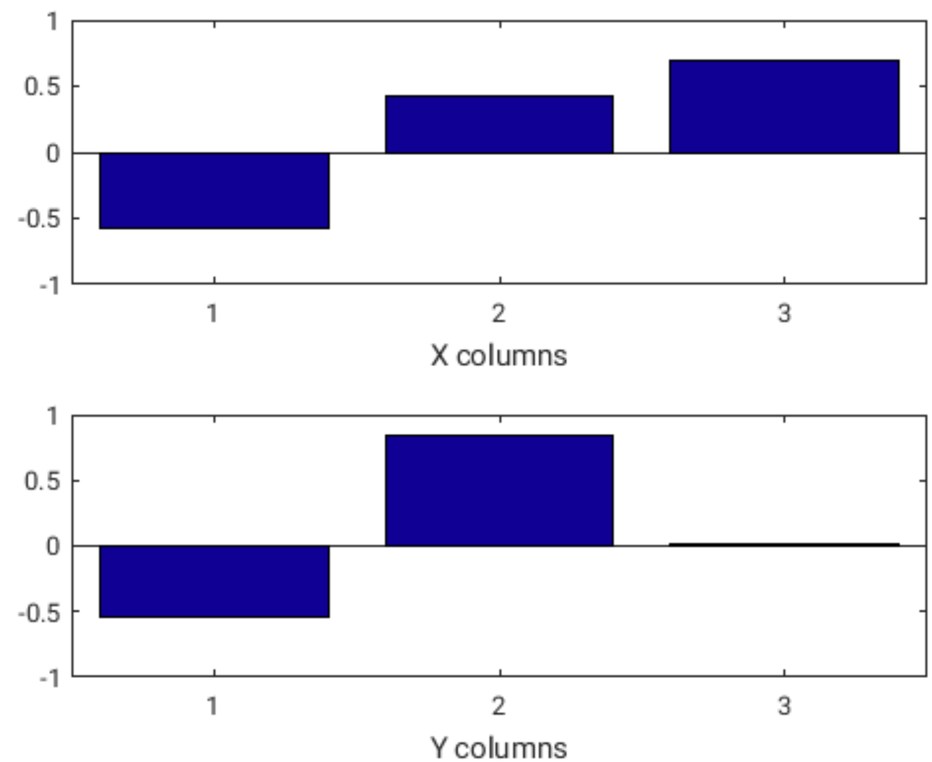

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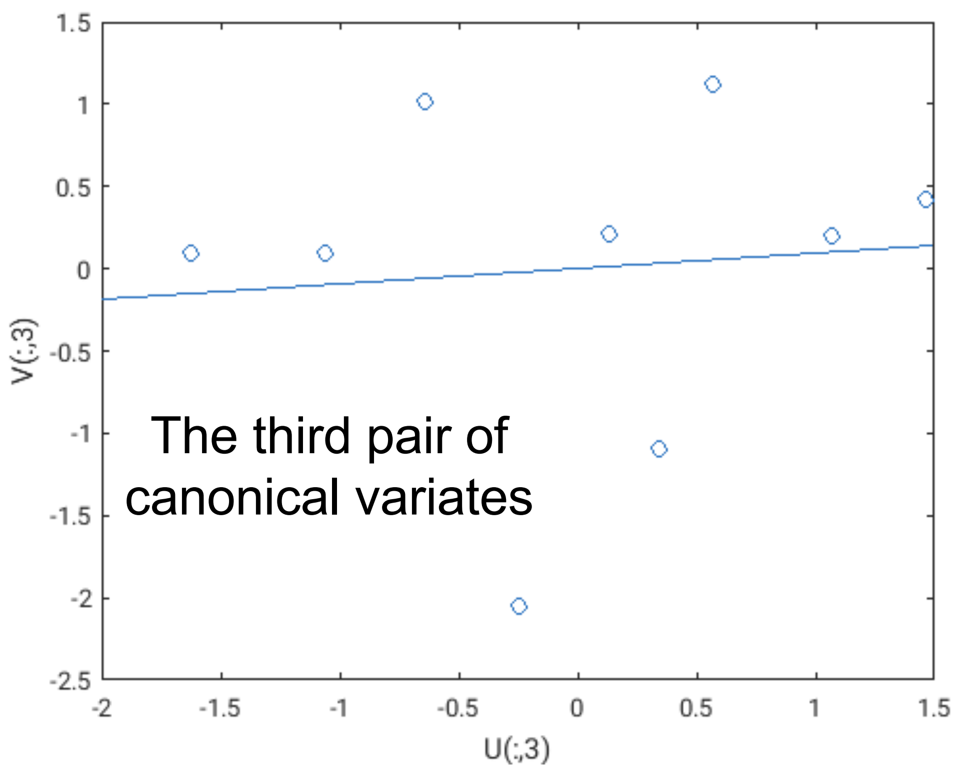

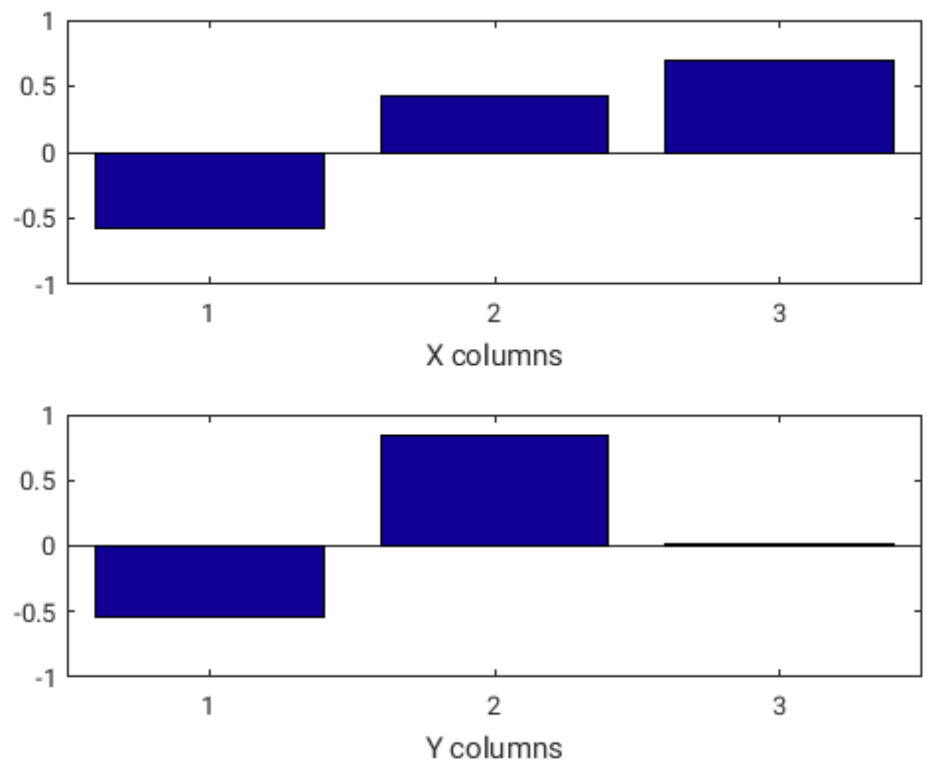

Example

[A, B, r, U, V, stat] = canoncorr(X, Y);

```
struct with fields:

   Wilks: [2.0261e-13 0.7242 0.9917]
     df1: [9 4 1]
     df2: [7.4518 8 5]
       F: [1.3602e+05 0.3502 0.0418]
      pF: [1.5799e-18 0.8370 0.8461]
   chisq: [131.5237 1.4522 0.0600]
  pChisq: [5.7628e-24 0.8351 0.8065]
     dfe: [9 4 1]
       p: [5.7628e-24 0.8351 0.8065]
```

About Final Project

- You will be asked to present a paper that uses one of methods talked in the class
- 20% Grade!
- Start from April 11th
- The presentation will be 10 minutes, followed by a 2-minute question session. You’re expected to prepare some PPT slides for the presentation!
- Be clear about
  - What is the major goal of the paper?
  - How did it use the method we talked about to achieve its goal?

About Final Project

- Let me know before next Tuesday (3/21) if you want to find a paper by yourself that is more relevant to your area of research

- Otherwise, I will randomly assign a paper to you next Tuesday, as well as the time of your presentation.

CCA: Examples