Almost everything you need to know about PLS

Part 2: How to do PLS in Matlab and R

Jenny Rieck & Derek Beaton

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The BIG outline

- Part 1: Background & Examples

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  - It was on Oct. 24 (YOU MISSED IT).

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  - RIGHT NOW.
  - Put knowledge into practice

Part 2 outline

- Refresher

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  - Principal component analysis (PCA)

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- And beyond!

Principal Components Analysis

What is PCA?

- Visualize high dimensional data

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- Orthogonal transformation

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    - S. Wold et al., (1987)

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What is PCA?

- Find "components"

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    - Components are new variables that are combinations of old variables

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- Find “components”
  - Components are new variables that are combinations of old variables
- Components explain maximum possible variance
  - Conditional to orthogonality

Visual example

Visual example

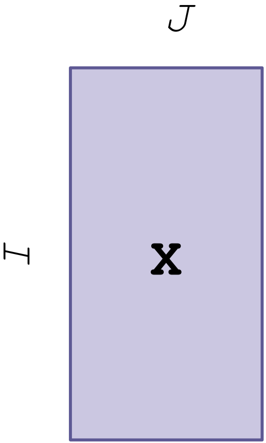
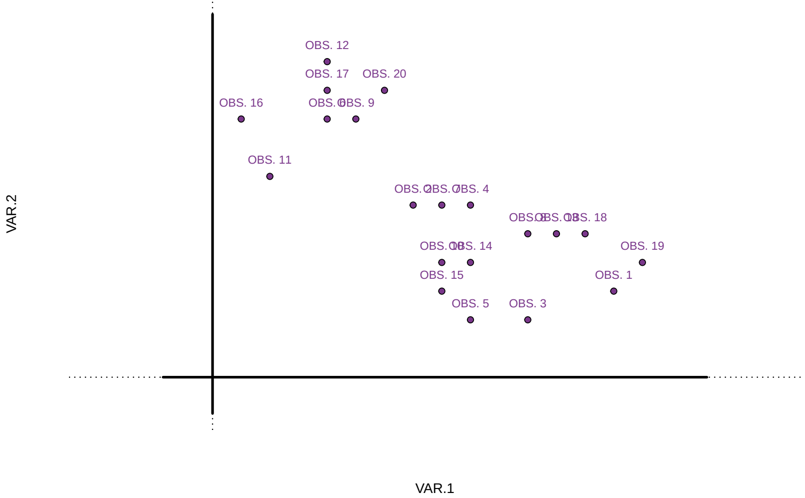


Figure 1: The kind of data we usually expect for PCA

Visual example



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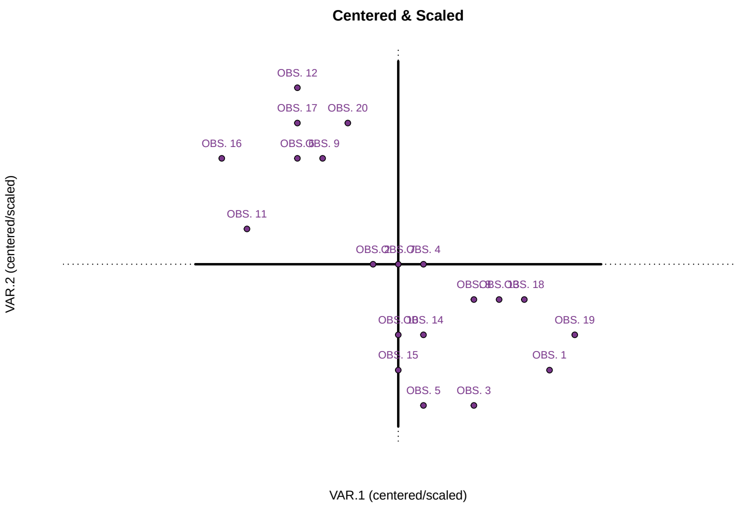

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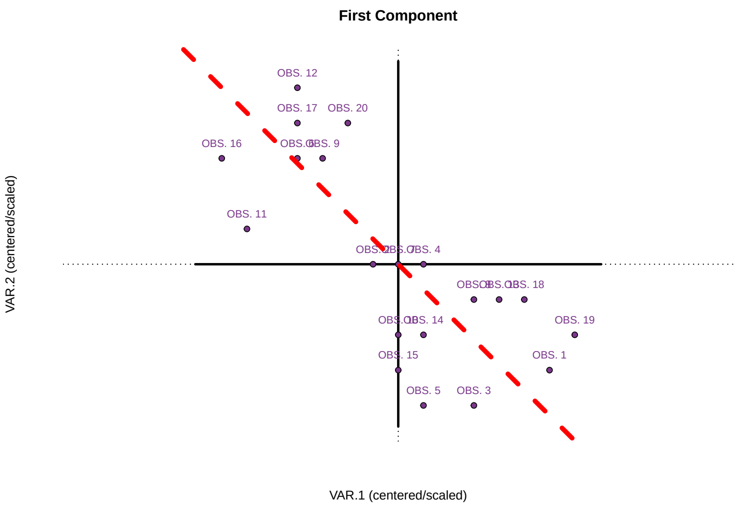

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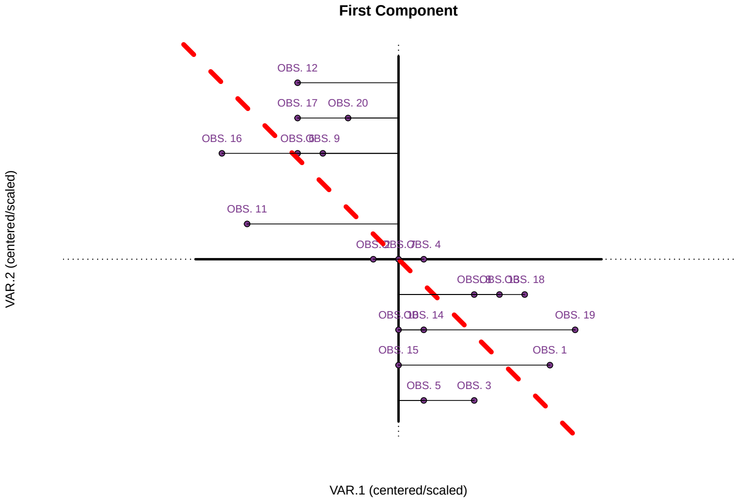

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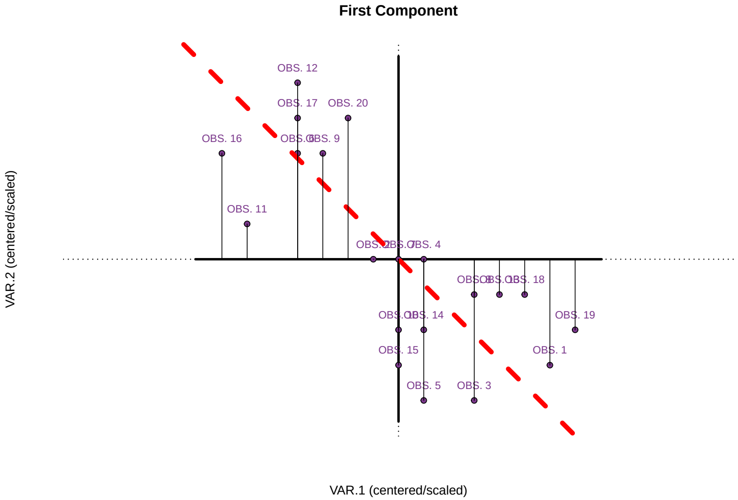

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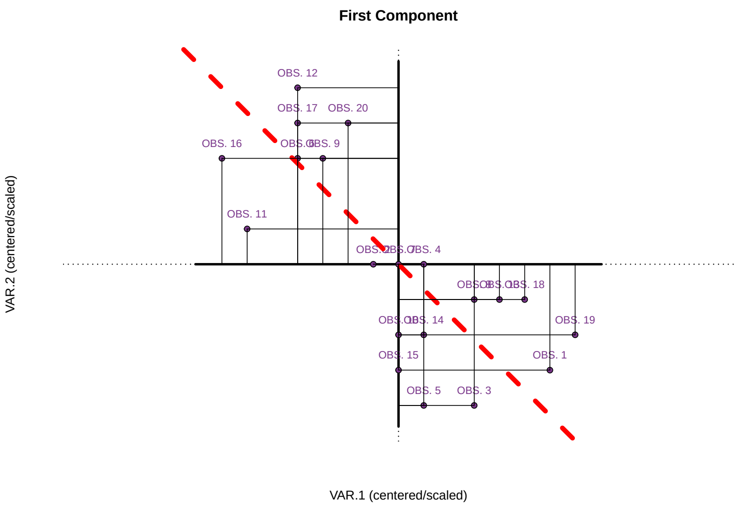

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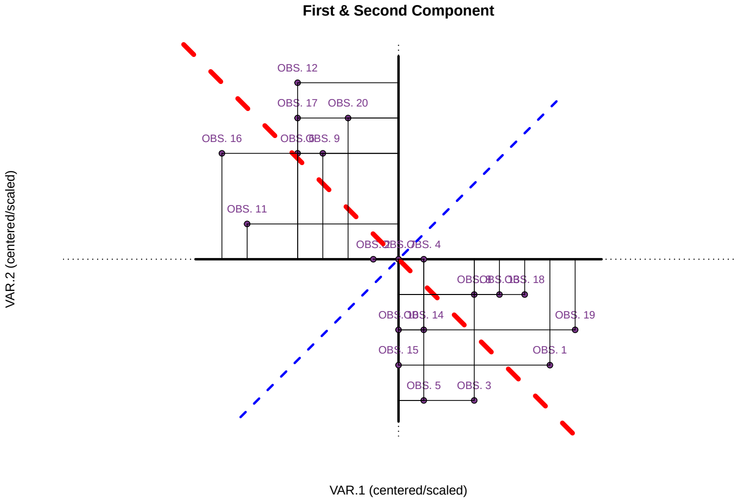

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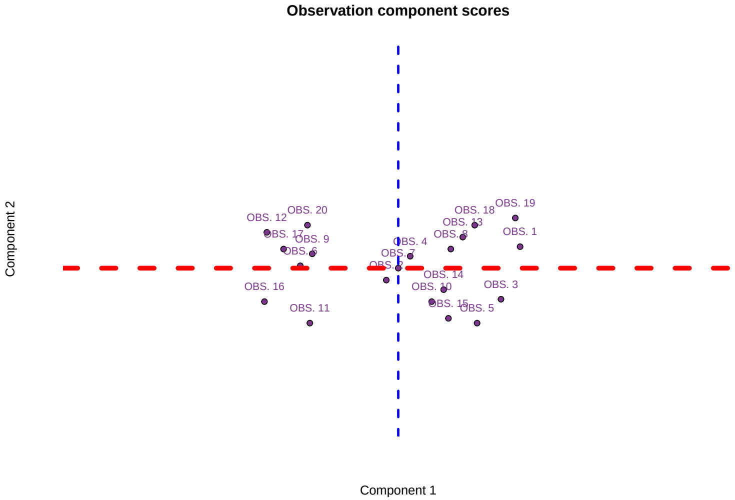

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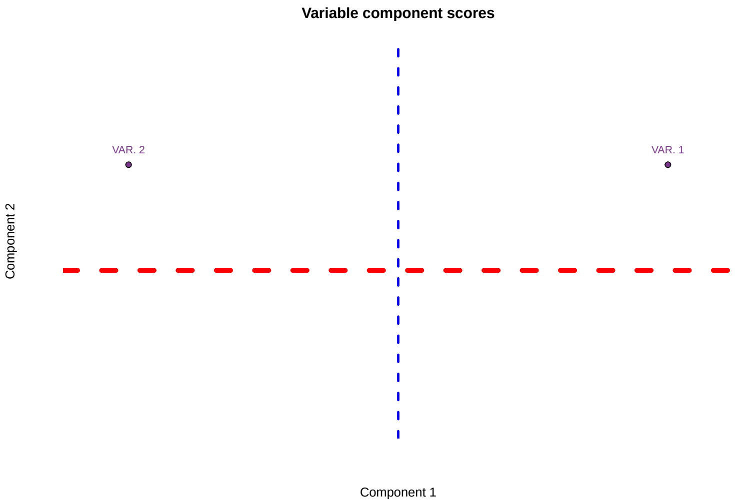

Background

What is PCA?

- The basis of modern techniques

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  - Factor analyses

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  - Independent components analysis

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    - Discriminant analyses

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  - Discriminant analyses
  - Multi-table (e.g., MFA, GCCA)

What is PCA?

- A special case of the singular value decomposition (SVD)

What is PCA?

- A special case of the singular value decomposition (SVD)
- Which means (almost) everything else is, too

Singular value decomposition

- The SVD is one of the most ubiquitous and important tools

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- If you want more:

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Singular value decomposition

- The SVD is one of the most ubiquitous and important tools
- If you want more:
  - S. Wold et al., (1987)
  - Jollife (2002)
  - Abdi & Williams (2010)
  - And many others...

Formalization

SVD

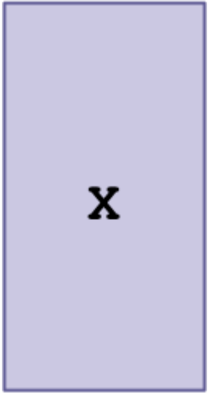

Figure 2: The shape of the data

SVD

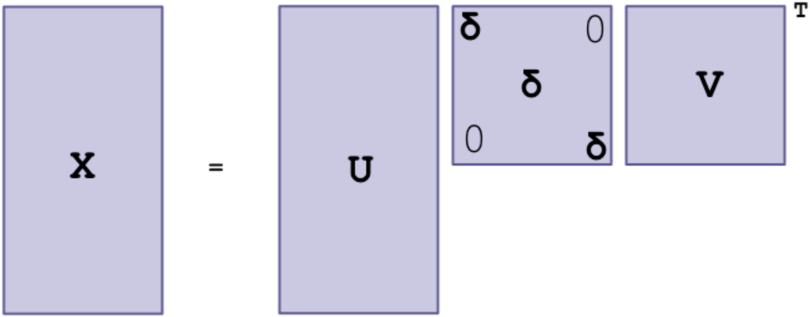

Figure 3: SVD breaks down the data

SVD

Notation

SVD

Notation

- x - a scalar

SVD

Notation

- x - a scalar
- $\mathbf{a}$ - a vector

SVD

Notation

- x - a scalar
- $\mathbf{a}$ - a vector
- $\mathbf{A}$ - a matrix

SVD

Notation

- x - a scalar
- $\mathbf{a}$ - a vector
- $\mathbf{A}$ - a matrix
- $\mathbf{A}^T$ - transpose

SVD

Notation

- x - a scalar
- $\mathbf{a}$ - a vector
- $\mathbf{A}$ - a matrix
- $\mathbf{A}^T$ - transpose
- $\mathbf{AB}$ - multiplication

SVD

Given a matrix $\mathbf{X}$ we generally assume that

SVD

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- column-wise centered

SVD

Given a matrix **X** we generally assume that

- column-wise centered
- column-wise scaled (e.g., z-scores or sums of squares $= 1$)

SVD

The SVD of $\mathbf{X}$ of size $I \times J$:

SVD

The SVD of $\mathbf{X}$ of size $I \times J$:

$$\mathbf{X} = \mathbf{U}\boldsymbol{\Delta}\mathbf{V}^{\mathbf{T}} \quad (1)$$

SVD

The SVD of $\mathbf{X}$ of size $I \times J$:

$$\mathbf{X} = \mathbf{U}\boldsymbol{\Delta}\mathbf{V}^{\mathbf{T}} \tag{1}$$

$\mathbf{U}$ and $\mathbf{V}$ are orthonormal such that

SVD

The SVD of $\mathbf{X}$ of size $I \times J$:

$$\mathbf{X} = \mathbf{U}\boldsymbol{\Delta}\mathbf{V}^{\mathbf{T}} \tag{1}$$

$\mathbf{U}$ and $\mathbf{V}$ are orthonormal such that

$$\mathbf{U}^{\mathbf{T}}\mathbf{U} = \mathbf{I} = \mathbf{V}^{\mathbf{T}}\mathbf{V} \tag{2}$$

SVD

$\mathbf{X} = \mathbf{U}\boldsymbol{\Delta}\mathbf{V}^{\mathsf{T}}$ such that $\mathbf{U}^{\mathsf{T}}\mathbf{U} = \mathbf{I} = \mathbf{V}^{\mathsf{T}}\mathbf{V}$

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$\mathbf{X} = \mathbf{U}\boldsymbol{\Delta}\mathbf{V}^{\mathbf{T}}$ such that $\mathbf{U}^{\mathbf{T}}\mathbf{U} = \mathbf{I} = \mathbf{V}^{\mathbf{T}}\mathbf{V}$

- where rank is L (i.e., number of extractable components)

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$\mathbf{X} = \mathbf{U}\boldsymbol{\Delta}\mathbf{V}^\mathsf{T}$ such that $\mathbf{U}^\mathsf{T}\mathbf{U} = \mathbf{I} = \mathbf{V}^\mathsf{T}\mathbf{V}$

- where rank is L (i.e., number of extractable components)
- $\mathbf{U}$ is $I \times L$ (left singular vectors; rows of $\mathbf{X}$)

SVD

$\mathbf{X} = \mathbf{U\Delta V^T}$ such that $\mathbf{U^TU} = \mathbf{I} = \mathbf{V^TV}$

- where rank is L (i.e., number of extractable components)
- $\mathbf{U}$ is $I \times L$ (left singular vectors; rows of $\mathbf{X}$)
- $\mathbf{V}$ is $J \times L$ (right singular vectors; columns of $\mathbf{X}$)

SVD

$$\mathbf{X} = \mathbf{U\Delta V^T} \text{ such that } \mathbf{U^TU} = \mathbf{I} = \mathbf{V^TV}$$

SVD

$\mathbf{X} = \mathbf{U}\boldsymbol{\Delta}\mathbf{V}^{\mathsf{T}}$ such that $\mathbf{U}^{\mathsf{T}}\mathbf{U} = \mathbf{I} = \mathbf{V}^{\mathsf{T}}\mathbf{V}$

- $\boldsymbol{\Delta}$ is $L \times L$ diagonal matrix

SVD

$\mathbf{X} = \mathbf{U\Delta V^T}$ such that $\mathbf{U^TU} = \mathbf{I} = \mathbf{V^TV}$

- $\mathbf{\Delta}$ is $L \times L$ diagonal matrix
- $\mathrm{diag}\{\mathbf{\Delta}\} = \boldsymbol{\delta}$ are singular values (decreasing)

SVD

$\mathbf{X} = \mathbf{U}\boldsymbol{\Delta}\mathbf{V}^{\mathbf{T}}$ such that $\mathbf{U}^{\mathbf{T}}\mathbf{U} = \mathbf{I} = \mathbf{V}^{\mathbf{T}}\mathbf{V}$

- $\boldsymbol{\Delta}$ is $L \times L$ diagonal matrix
- $\mathrm{diag}\{\boldsymbol{\Delta}\} = \boldsymbol{\delta}$ are singular values (decreasing)
- $\boldsymbol{\lambda} = \boldsymbol{\delta}^{2}$ are the eigenvalues (variance)

SVD

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- $\mathbf{F}_I = \mathbf{U}\mathbf{\Delta}$ (row component scores)

SVD

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- $\mathbf{F}_I = \mathbf{U}\boldsymbol{\Delta}$ (row component scores)
- $\mathbf{F}_J = \mathbf{V}\boldsymbol{\Delta}$ (column component scores)

SVD

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SVD

$\mathbf{X} = \mathbf{U \Delta V^T}$ such that $\mathbf{U^T U} = \mathbf{I} = \mathbf{V^T V}$

- $\mathbf{F}_I = \mathbf{U\Delta} = \mathbf{XV}$

SVD

$\mathbf{X} = \mathbf{U\Delta V^T}$ such that $\mathbf{U^TU} = \mathbf{I} = \mathbf{V^TV}$

- $\mathbf{F}_I = \mathbf{U\Delta} = \mathbf{XV}$
- $\mathbf{F}_J = \mathbf{V\Delta} = \mathbf{X}^T\mathbf{U}$

Partial Least Squares

Refresher

PLS means a lot of things

- Projection onto latent structures

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  - Probably the most accurate name

PLS means a lot of things

- Projection onto latent structures
  - Probably the most accurate name
  - But also probably too broad a definition

PLS means a lot of things

Partial least squares sounds like ordinary least squares

- When we have two matrices: **X** and **Y**

PLS means a lot of things

Partial least squares sounds like ordinary least squares

- When we have two matrices: $\mathbf{X}$ and $\mathbf{Y}$
- OLS: $(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$

PLS means a lot of things

Partial least squares sounds like ordinary least squares

- When we have two matrices: $\mathbf{X}$ and $\mathbf{Y}$
- OLS: $(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$
- PLS: $\mathbf{X}^T\mathbf{Y}$

PLS means a lot of things

- Partial least squares path modelling (PLS-PM)

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- Partial least squares path modelling (PLS-PM)
- Partial least squares regression (PLSR)

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- Partial least squares regression (PLSR)
- Partial least squares correlation (PLSC)

PLS means a lot of things

- Partial least squares path modelling (PLS-PM)
- Partial least squares regression (PLSR)
- Partial least squares correlation (PLSC)
  - This is the one we'll talk about today

PLSC has many. . .

Names

- Inter-battery (factor) analysis (Tucker, 1958)

PLSC has many...

Names

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PLSC has many. . .

Names

- Inter-battery (factor) analysis (Tucker, 1958)
- Covariance between two fields (Bretherton, Smith, & Wallace, 1992)
- PLS-SVD (Tenenhaus, 2005)
- Co-inertia analysis (Dray, 2014)

PLSC has many. . .

Friends

- Reduced Rank Regression (a.k.a. redundancy analysis)

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- Canonical Correlation Analysis

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- Canonical Correlation Analysis
- (Fisher's) Linear Discriminant Analysis

PLSC has many. . .

Friends

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- Canonical Correlation Analysis
- (Fisher's) Linear Discriminant Analysis
- PLS-correspondence analysis

PLSC

History

- McIntosh, Bookstein, Haxby, & Grady (1996)

PLSC

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PLSC

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- McIntosh, Bookstein, Haxby, & Grady (1996)
- Bookstein (1992)
- Tucker (1958)

PLSC

Modern overviews

- McIntosh & Lobaugh (2004)

PLSC

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- McIntosh & Lobaugh (2004)
- Krishnan et al., (2011)

PLSC

It's effectively just PCA applied to the cross product of two matrices measured on the same observations:

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PLSC

It's effectively just PCA applied to the cross product of two matrices measured on the same observations:

- $\mathbf{X}$ which is $I \times J$
- $\mathbf{Y}$ which is $I \times K$

PLSC via the SVD

Compute the relationship between $\mathbf{X}$ and $\mathbf{Y}$

$$\mathbf{R} = \mathbf{X}^{\mathsf{T}}\mathbf{Y} \tag{3}$$

PLSC via the SVD

Compute the relationship between **X** and **Y**

$$\mathbf{R} = \mathbf{X}^{\mathbf{T}}\mathbf{Y} \tag{3}$$

Compute the SVD of **R**

$$\mathbf{R} = \mathbf{U}\boldsymbol{\Delta}\mathbf{V}^{\mathbf{T}} \tag{4}$$

PLSC via the SVD

Compute the relationship between $\mathbf{X}$ and $\mathbf{Y}$

$$\mathbf{R} = \mathbf{X}^{\mathsf{T}}\mathbf{Y} \tag{3}$$

Compute the SVD of $\mathbf{R}$

$$\mathbf{R} = \mathbf{U}\boldsymbol{\Delta}\mathbf{V}^{\mathsf{T}} \tag{4}$$

Compute the latent variables

$$\mathbf{L}_{\mathbf{X}} = \mathbf{X}\mathbf{U} \text{ and } \mathbf{L}_{\mathbf{Y}} = \mathbf{Y}\mathbf{V} \tag{5}$$

PLSC via the SVD

Almost everything is the same:

- $\boldsymbol{\Delta}$ are singular values

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- $\mathbf{F}_J = \mathbf{U}\mathbf{\Delta}$ (component scores for variables of $\mathbf{X}$)

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Almost everything is the same:

- $\mathbf{\Delta}$ are singular values
- $\mathbf{F}_J = \mathbf{U\Delta}$ (component scores for variables of $\mathbf{X}$)
- $\mathbf{F}_K = \mathbf{V\Delta}$ (component scores for variables of $\mathbf{Y}$)
- So our nomeclature will align with PCA

PLSC via the SVD

The new-ness

- $\mathbf{L_X} = \mathbf{XU}$ express the individuals w.r.t. $\mathbf{X}$

PLSC via the SVD

The new-ness

- $\mathbf{L_X} = \mathbf{XU}$ express the individuals w.r.t. $\mathbf{X}$
- $\mathbf{L_Y} = \mathbf{YV}$ express the individuals w.r.t. $\mathbf{Y}$

PLSC via the SVD

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- $\mathbf{L_Y} = \mathbf{YV}$ express the individuals w.r.t. $\mathbf{Y}$
- Not in PCA

PLSC via the SVD

The new-ness

- $\mathbf{L_X} = \mathbf{XU}$ express the individuals w.r.t. $\mathbf{X}$
- $\mathbf{L_Y} = \mathbf{YV}$ express the individuals w.r.t. $\mathbf{Y}$
- Not in PCA
  - We'll call these "latent variable scores"

PLSC via the SVD

Maximizes the latent variables

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$$\mathbf{L}_{\mathbf{X}}^{T}\mathbf{L}_{\mathbf{Y}} = \boldsymbol{\Delta} \tag{6}$$

PLSC via the SVD

Maximizes the latent variables

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When expanded

$(\mathbf{XU})^{\mathbf{T}}(\mathbf{YV}) = \boldsymbol{\Delta}$

PLSC via the SVD

Maximizes the latent variables

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When expanded

$(\mathbf{XU})^{\mathbf{T}}(\mathbf{YV}) = \boldsymbol{\Delta}$

$\mathbf{U}^{\mathbf{T}}\mathbf{X}^{\mathbf{T}}\mathbf{YV} = \boldsymbol{\Delta}$

PLSC via the SVD

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When expanded

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$\mathbf{U}^{\mathbf{T}}\mathbf{X}^{\mathbf{T}}\mathbf{YV} = \boldsymbol{\Delta}$

$\mathbf{U}^{\mathbf{T}}\mathbf{RV} = \boldsymbol{\Delta}$

PLSC via the SVD

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$$\mathbf{L}_{\mathbf{X}}^{T}\mathbf{L}_{\mathbf{Y}} = \mathbf{\Delta} \tag{6}$$

When expanded

$(\mathbf{XU})^{\mathbf{T}}(\mathbf{YV}) = \mathbf{\Delta}$

$\mathbf{U}^{\mathbf{T}}\mathbf{X}^{\mathbf{T}}\mathbf{YV} = \mathbf{\Delta}$

$\mathbf{U}^{\mathbf{T}}\mathbf{RV} = \mathbf{\Delta}$

$\mathbf{U}^{\mathbf{T}}\mathbf{U\Delta V}^{\mathbf{T}}\mathbf{V} = \mathbf{\Delta}$

PLSC via the SVD

Maximizes the latent variables

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When expanded

$(\mathbf{XU})^{\mathbf{T}}(\mathbf{YV}) = \mathbf{\Delta}$

$\mathbf{U}^{\mathbf{T}}\mathbf{X}^{\mathbf{T}}\mathbf{YV} = \mathbf{\Delta}$

$\mathbf{U}^{\mathbf{T}}\mathbf{RV} = \mathbf{\Delta}$

$\mathbf{U}^{\mathbf{T}}\mathbf{U\Delta V}^{\mathbf{T}}\mathbf{V} = \mathbf{\Delta}$

because

$\mathbf{U}^{\mathbf{T}}\mathbf{U} = \mathbf{I} = \mathbf{V}^{\mathbf{T}}\mathbf{V}$

PLSC via the SVD

It's effectively just PCA with some new-ness:

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A Glossary

For PCA nomenclature and PLSGui:

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Example

PLSC dataset

Via ADNI ($N = 569$)

- 3 groups of participants

PLSC dataset

Via ADNI ($N = 569$)

- 3 groups of participants
    - $N = 178$ healthy control

PLSC dataset

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PLSC dataset

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- 8 neuropsych measures

PLSC dataset

Via ADNI ($N = 569$)

- 3 groups of participants
  - $N = 178$ healthy control
  - $N = 275$ late MCI
  - $N = 116$ AD
- 8 neuropsych measures
- 68 cortical thickness estimates (via Freesurfer)

Data matrices

$$\mathbf{X} = \begin{array}{cc} & \begin{array}{cccc} \text{BNT} & \text{Clock} & \ldots & \text{RAVLT} \end{array} \\ \begin{array}{c} \text{Subj}_1 \\ \text{Subj}_2 \\ \text{Subj}_3 \\ \vdots \\ \text{Subj}_{N\text{-}1} \\ \text{Subj}_N \end{array} & \begin{bmatrix} 10 & 5 & \ldots & 30 \\ 7 & 4 & \ldots & 26 \\ 3 & 0 & \ldots & 23 \\ \vdots & \vdots & & \vdots \\ 2 & 1 & \ldots & 18 \\ 8 & 4 & \ldots & 27 \end{bmatrix} \end{array} \qquad \mathbf{Y} = \begin{array}{cc} & \begin{array}{cccc} \text{R.IFG} & \text{L.IFG} & \ldots & \text{L.Fusi} \end{array} \\ \begin{array}{c} \text{Subj}_1 \\ \text{Subj}_2 \\ \text{Subj}_3 \\ \vdots \\ \text{Subj}_{N\text{-}1} \\ \text{Subj}_N \end{array} & \begin{bmatrix} 3.24 & 6.27 & \ldots & 2.32 \\ 5.89 & 0.26 & \ldots & 4.51 \\ 2.84 & 2.51 & \ldots & 1.17 \\ \vdots & \vdots & & \vdots \\ 1.96 & 8.9 & \ldots & 3.46 \\ 4.42 & 7.81 & \ldots & 1.96 \end{bmatrix} \end{array}$$

Figure 4: **X** and **Y** matrices in standard PLS

Standard PLSC scree

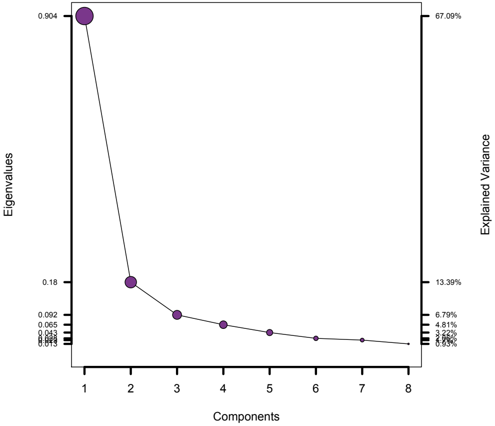

Figure 5:

How many components to interpret?

- A mix of art & science

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- Use tests, effects sizes, and heuristics

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  - Peres-Neto et al., (2005)
  - Dray (2008)
  - Josse and Husson (2011)
- We'll talk about the first 2

Two components

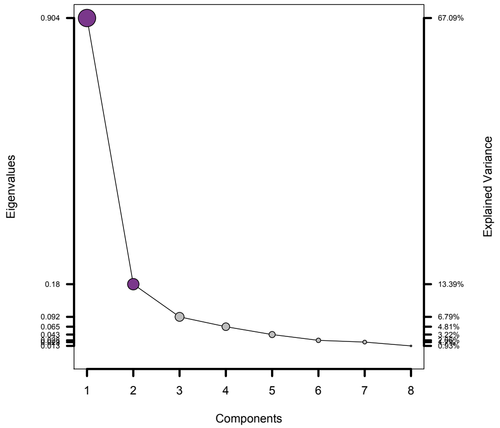

Figure 6:

Latent variables

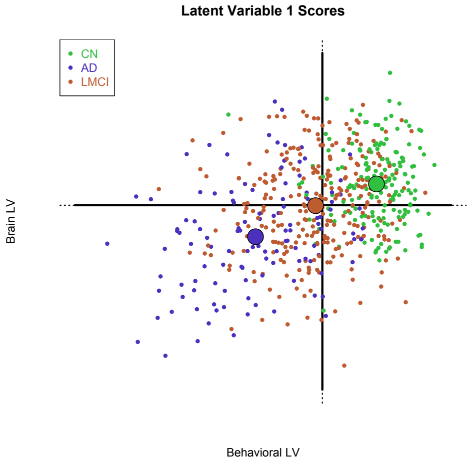

Figure 7:

Latent variables

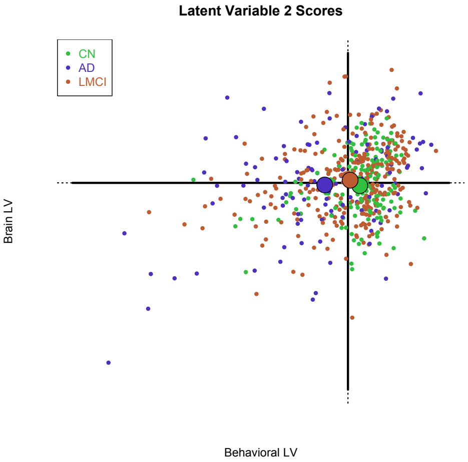

Figure 8:

Neuropsych component scores

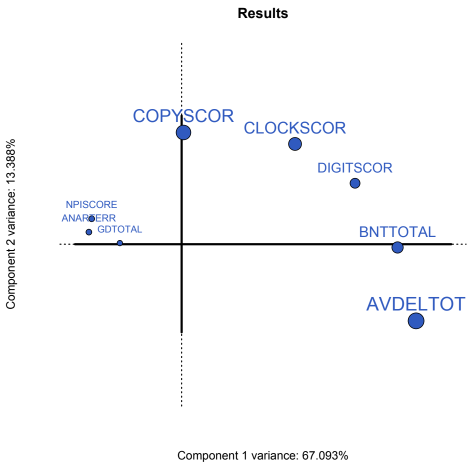

Figure 9:

Structural thickness component scores

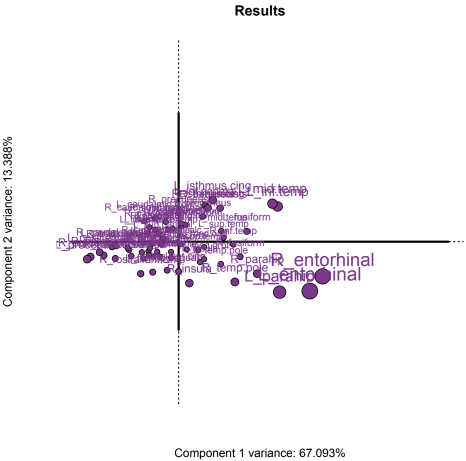

Figure 10:

LV1: Altogether now

- Let's focus on LV1

LV1: Altogether now

- Let's focus on LV1
- How can we put a story to the pictures?

LV1: Altogether now

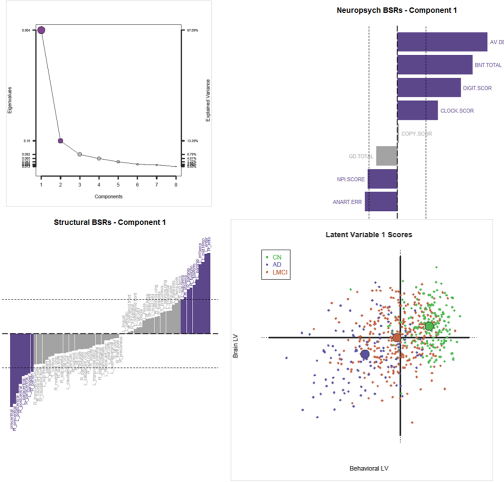

Figure 11: