

Almost everything you need to know about PLS

Part 1: Background, Theory, and Examples

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The BIG outline

- Part 1: Background & Examples

The BIG outline

- Part 1: Background & Examples
 - RIGHT NOW

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 - Introduce everything we need

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 - Tuesday November 21, 10:00-12:00 Worstman Hall

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- Part 2: PLS in Matlab & R
 - Tuesday November 21, 10:00-12:00 Worstman Hall
 - Put knowledge into practice

Part 1 outline

- Theory & Background

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 - Principal component analysis (PCA)

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 - Discriminant PLS
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- And beyond!

Principal Component Analysis

Background

Where did PCA come from?

- Modern form

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What is PCA?

- Visualize high dimensional data

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- Orthogonal transformation

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- Dimensionality reduction

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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

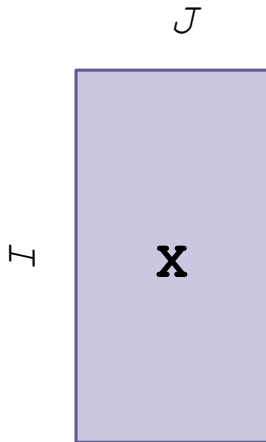
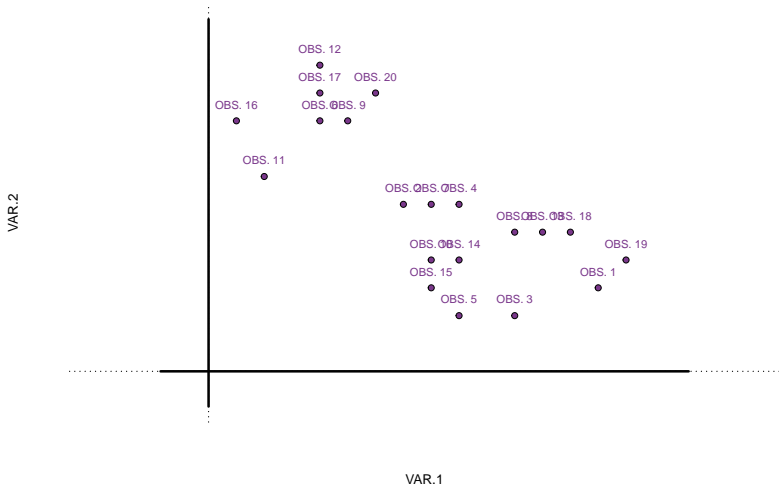
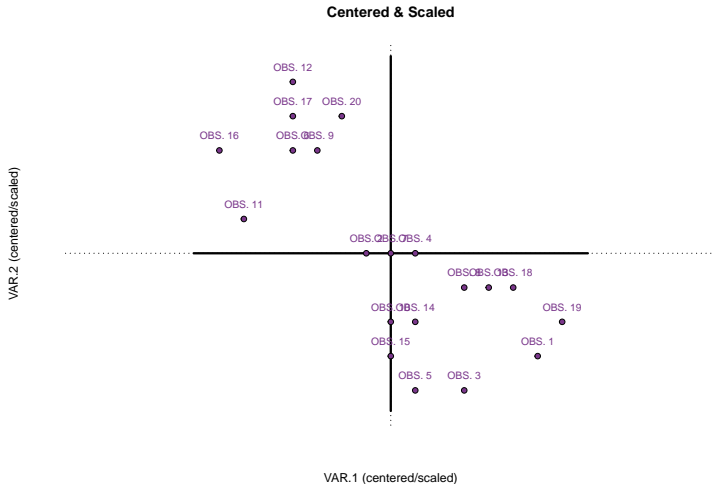


Figure 1: The kind of data we usually expect for PCA

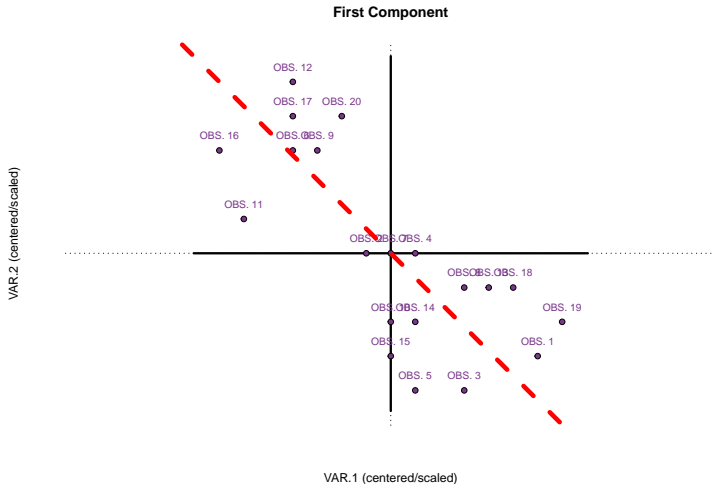
Visual example



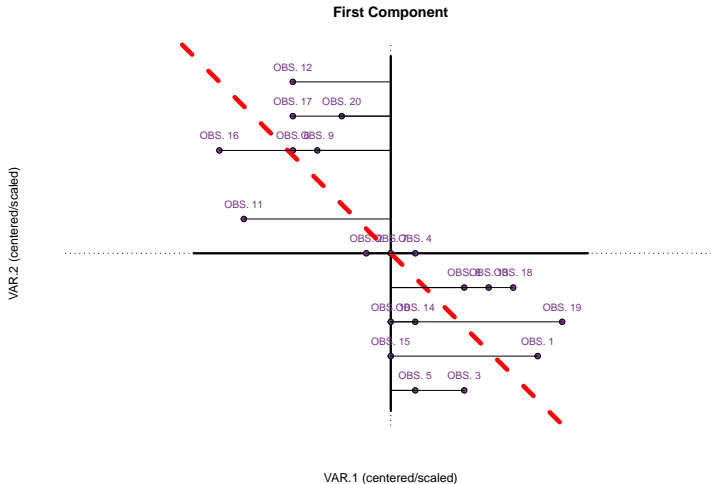
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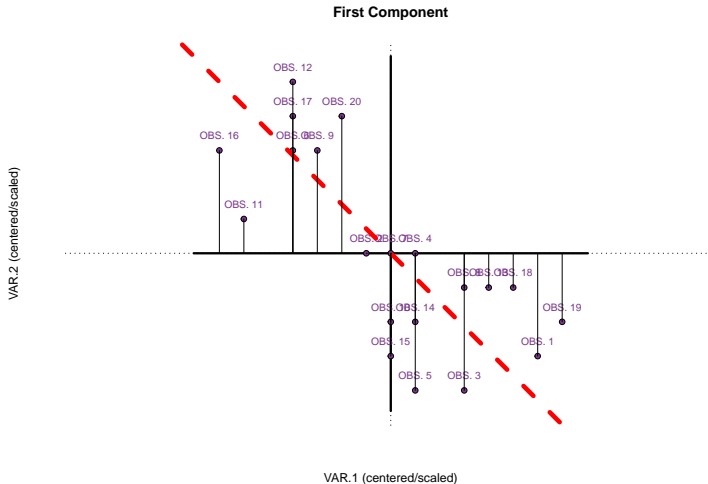
Visual example



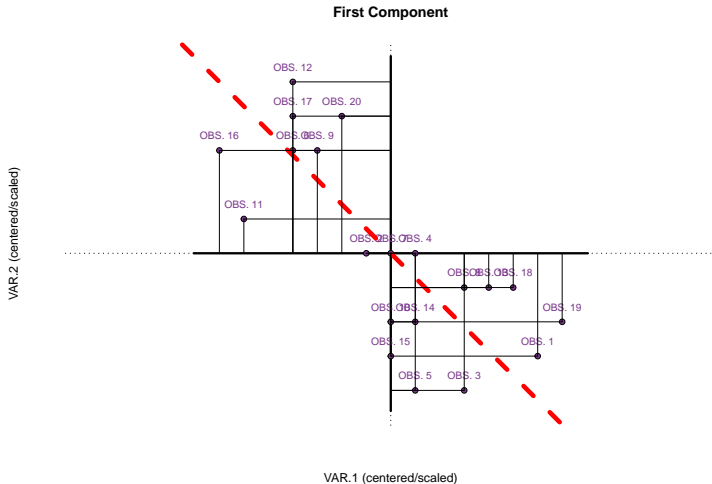
Visual example



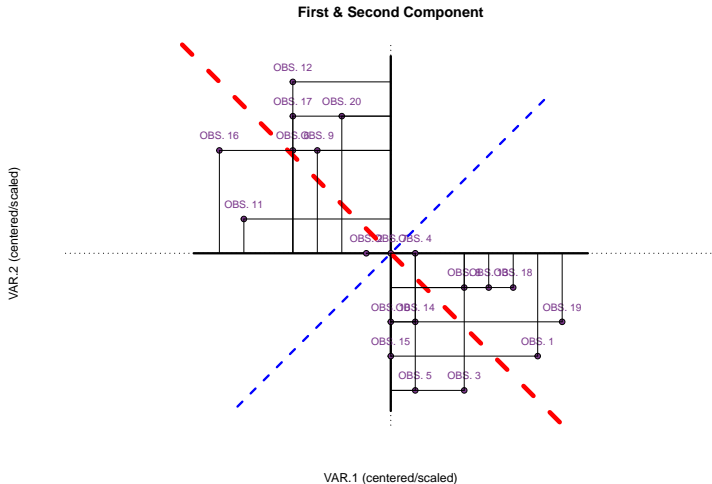
Visual example



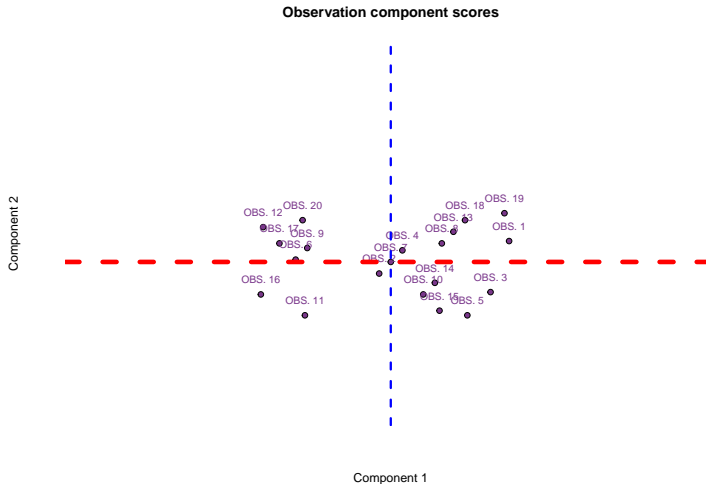
Visual example



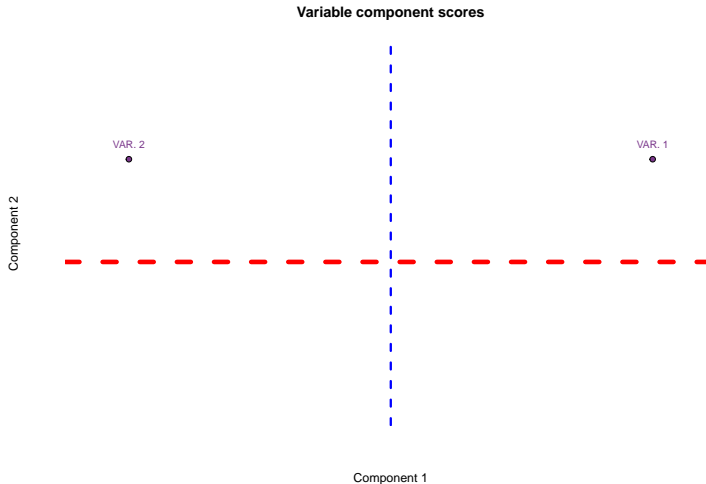
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 - Factor analyses

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What is PCA?

- The basis of modern techniques
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 - Independent components analysis
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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

Formalization

Singular value decomposition

The SVD is one of the most ubiquitous and important tools

SVD

- We'll go into *enough* formalization

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- If you want more:

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SVD

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- If you want more:
 - S. Wold et al., (1987)
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 - And many others...

SVD



Figure 2: The shape of the data

SVD

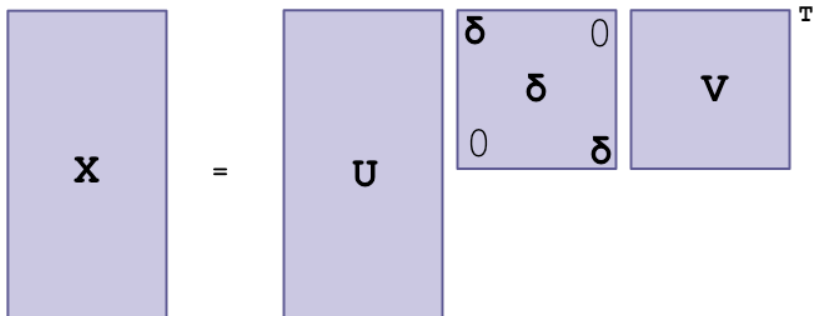


Figure 3: SVD breaks down the data

SVD

Notation

SVD

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- x - a scalar

SVD

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

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

SVD

- Think back to PCA

SVD

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- We want to find *the* principal component

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- We want to find *the* principal component
 - a.k.a. maximum source of variance

SVD

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

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- column-wise centered

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

SVD

Given \mathbf{X} of size $I \times J$

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We want to find vectors

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Given \mathbf{X} of size $I \times J$

We want to find vectors

- \mathbf{u} of size $I \times 1$
- \mathbf{v} of size $J \times 1$

SVD

Given \mathbf{X} of size $I \times J$

We want to find vectors

- \mathbf{u} of size $I \times 1$
- \mathbf{v} of size $J \times 1$

such that

$$\underset{\mathbf{u}, \mathbf{v}}{\operatorname{argmax}} \delta = \mathbf{u}^T \mathbf{X} \mathbf{v} \text{ conditional to } \mathbf{u}^T \mathbf{u} = 1 = \mathbf{v}^T \mathbf{v}$$

SVD

Which gives us the following equivalencies:

- $\mathbf{X}\mathbf{v} = \mathbf{u}\delta$
- $\mathbf{X}^T \mathbf{u} = \mathbf{v}\delta$

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- $\mathbf{X}_1 = \delta\mathbf{u}\mathbf{v}^T$

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where

- $\mathbf{X}_1 = \delta\mathbf{u}\mathbf{v}^T$
 - \mathbf{X}_1 is \mathbf{X} as represented by *source of maximum variance*

SVD

Given $\mathbf{X}_1 = \delta \mathbf{p} \mathbf{q}^T$ we can find the other components

SVD

Given $\mathbf{X}_1 = \delta \mathbf{p} \mathbf{q}^T$ we can find the other components

- $\mathbf{X}_{2:L} = \mathbf{X} - \mathbf{X}_1$
- $\mathbf{X}_{2:L}$ is orthogonal to \mathbf{X}_1

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- \mathbf{V} is $J \times L$ (right singular vectors; columns of \mathbf{X})

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

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

SVD

- Phew.

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- Let's get back to PCA

Toy example

- In R with ExPosition packages

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PCA Toy Dataset - Wine

- 36 different wines (e.g., USA red cab., CAN rose syrah)

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 - We’ll use both for PLS

PCA Subjective Measures

	fruity	floral	vegetal	spicy
Chili_red_merlot	6	2	1	4
Chili_red_cabernet	5	3	2	3
Chili_red_shiraz	7	1	2	6
Canada_red_pinot	4	2	3	1
Canada_white_chardonnay	4	3	2	1
Canada_white_sauvignon	8	4	3	2
USA_rose_cabernet	8	3	3	3
USA_rose_pinot	6	1	1	2
USA_rose_syrah	9	3	2	5

PCA - Wine

```
pca.res <- epPCA(  
  wine.subjective,  
  scale = T,  
  center = T,  
  graphs = F)
```

PCA - Wine

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 - Use the eigenvalues

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 - "Scree plot"

PCA - Wine

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- PCA is half

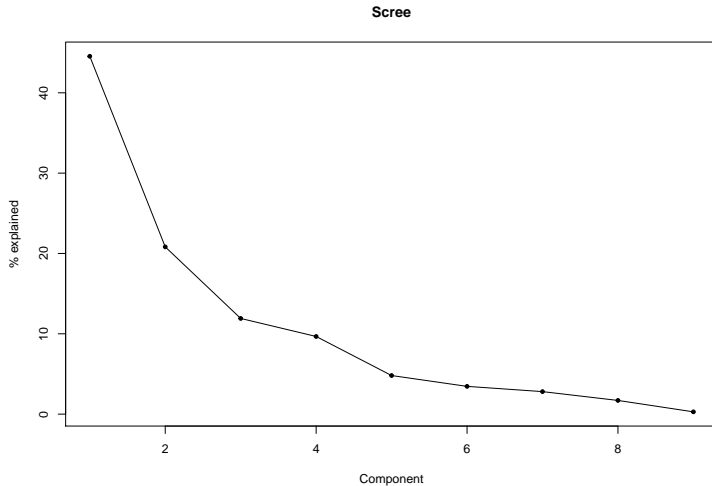
PCA - Wine

- Many ways to present the results
- We prioritize visualization
 - Use numbers and tables when needed
- PCA is half
 - Stats

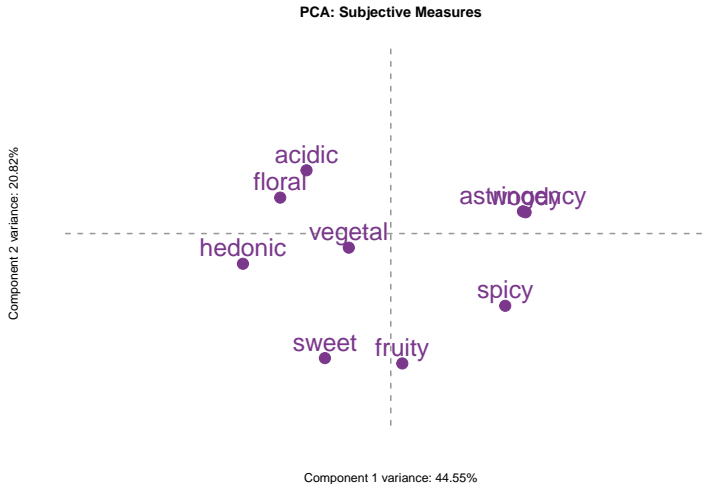
PCA - Wine

- Many ways to present the results
- We prioritize visualization
 - Use numbers and tables when needed
- PCA is half
 - Stats
 - Art

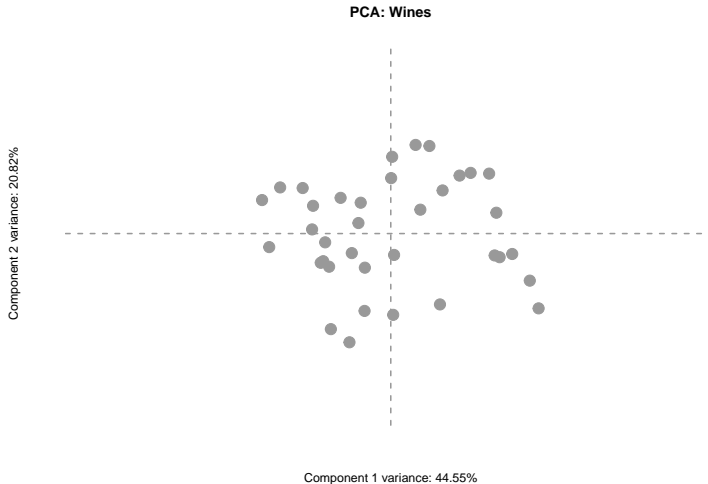
PCA - Wine



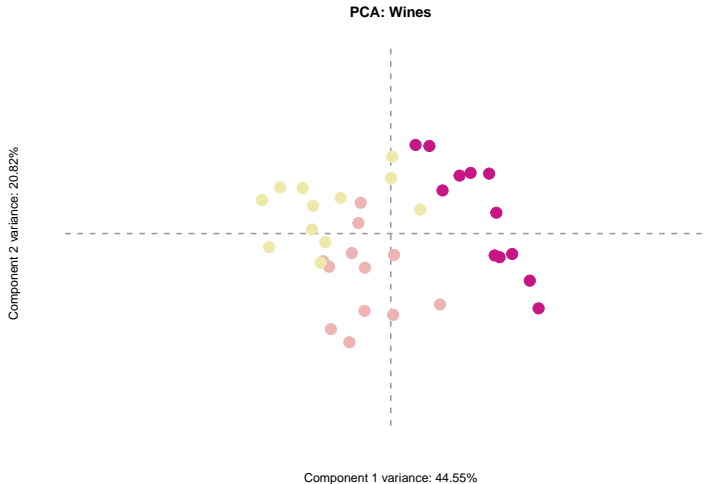
PCA - Wine



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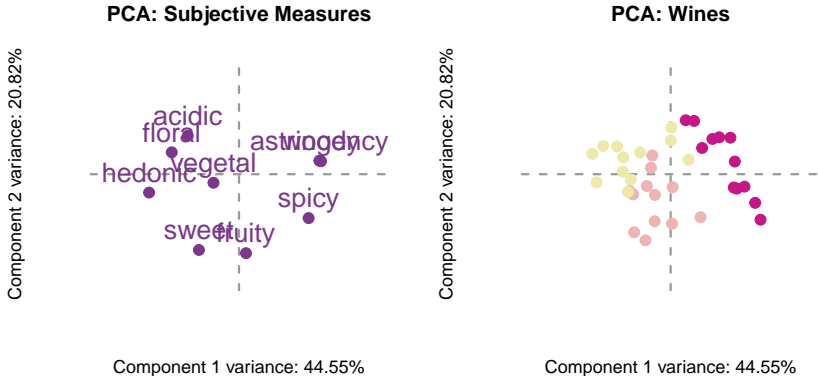


Figure 4: Variables & Observations

PCA

- If you know PCA you know about 90% of the multivariate stats in use

Partial least squares

Background

PLS means a lot of things

- Projection onto latent structures

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- Projection onto latent structures
 - 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: \mathbf{X} and \mathbf{Y}

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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)
- 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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- Covariance between two fields (Bretherton, Smith, & Wallace, 1992)

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- PLS-SVD (Tenenhaus, 2005)

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- PLS-SVD (Tenenhaus, 2005)
- co-inertia analysis (Dray, 2014)

PLSC has many...

Friends

- Reduced Rank Regression

PLSC has many...

Friends

- Reduced Rank Regression
- Canonical Correlation Analysis

PLSC has many...

Friends

- Reduced Rank Regression
- Canonical Correlation Analysis
- (Fisher's) Linear Discriminant Analysis

PLSC has many...

Friends

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

PLSC

History

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

PLSC

History

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

PLSC

History

- 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

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- **X** which is $I \times J$
- **Y** which is $I \times K$

Formalization

PLSC via the SVD

Given \mathbf{X} of size $I \times J$ and \mathbf{Y} of size $I \times K$

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- \mathbf{u} of size $J \times 1$
- \mathbf{v} of size $K \times 1$

To define latent variables

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such that

$$\operatorname{argmax}_{\mathbf{u}, \mathbf{v}} \delta = \mathbf{u}^T \mathbf{X}^T \mathbf{Y} \mathbf{v} \text{ conditional to } \mathbf{u}^T \mathbf{u} = 1 = \mathbf{v}^T \mathbf{v}$$

PLSC via the SVD

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

$$\mathbf{R} = \mathbf{X}^T \mathbf{Y} \quad (3)$$

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Compute the latent variables

$$\mathbf{L}_\mathbf{X} = \mathbf{X} \mathbf{U} \text{ and } \mathbf{L}_\mathbf{Y} = \mathbf{Y} \mathbf{V} \quad (5)$$

PLSC via the SVD

Almost everything is the same:

- Δ are singular values

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- So our nomenclature will align with PCA

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The new-ness

- $\mathbf{L}_X = \mathbf{X}\mathbf{U}$ express the individuals w.r.t. \mathbf{X}

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 - We'll call these "latent variable scores"

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Maximizes the latent variables

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because

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

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Example

PLS Toy Dataset - Wine

- 36 different wines (e.g., USA red cab., CAN rose syrah)

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- 4 objective measures (e.g., “Alcohol”, “Acidity”)
- 9 subjective measures (e.g., “sweet”, “acidic”)

PLS Subjective Measures

	fruity	floral	vegetal	spicy
Chili_red_merlot	6	2	1	4
Chili_red_cabernet	5	3	2	3
Chili_red_shiraz	7	1	2	6
Canada_red_pinot	4	2	3	1
Canada_white_chardonnay	4	3	2	1
Canada_white_sauvignon	8	4	3	2
USA_rose_cabernet	8	3	3	3
USA_rose_pinot	6	1	1	2
USA_rose_syrah	9	3	2	5

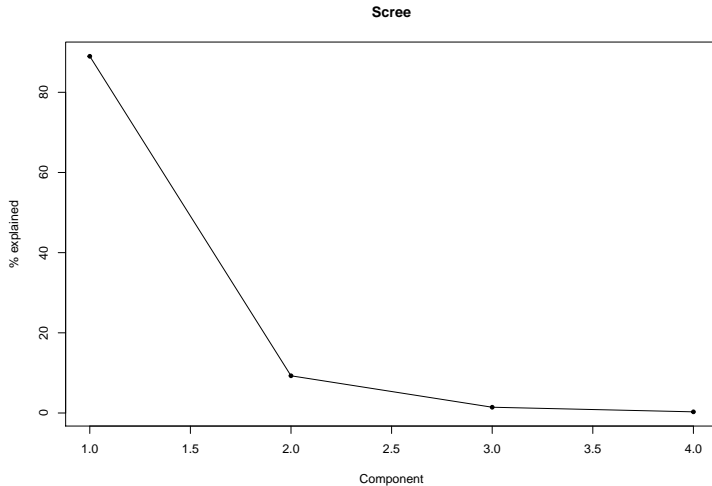
PLS Objective Measures

	Acidity	Alcohol	Sugar	Tanin
Chili_red_merlot	5.33	13.8	2.75	559
Chili_red_cabernet	5.14	13.9	2.41	672
Chili_red_shiraz	5.16	14.3	2.20	455
Canada_red_pinot	5.70	13.3	1.70	320
Canada_white_chardonnay	6.00	13.5	3.00	35
Canada_white_sauvignon	7.50	12.0	3.50	40
USA_rose_cabernet	5.71	12.5	4.30	93
USA_rose_pinot	5.40	13.0	3.10	79
USA_rose_syrah	6.50	13.5	3.00	89

PLS - Wine

```
pls.res <- tepPLS(  
  DATA1 = wine.objective,  
  center1 = T, scale1 = T,  
  DATA2 = wine.subjective,  
  center2 = T, scale2 = T,  
  graphs=F  
)
```

PLS - Wine



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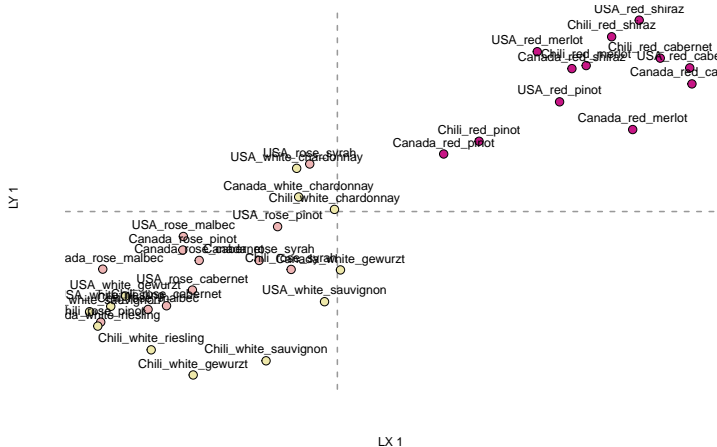
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So we'll start with the latent variable scores

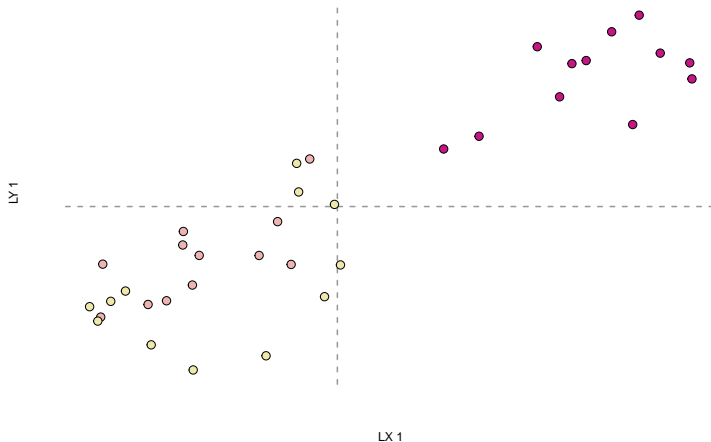
PLS - Wine

PLS Wine Latent Variable Scores: LV1

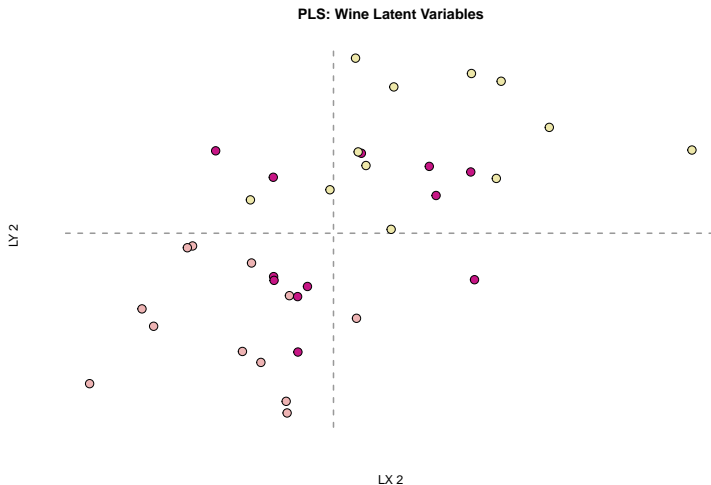


PLS - Wine

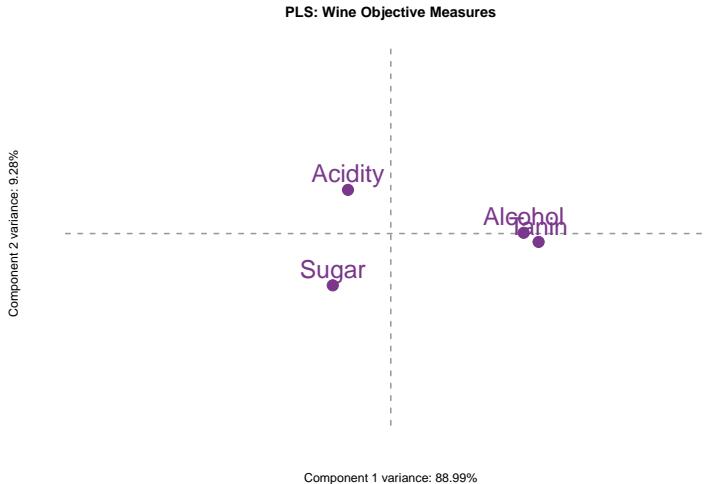
PLS Wine Latent Variable Scores: LV1



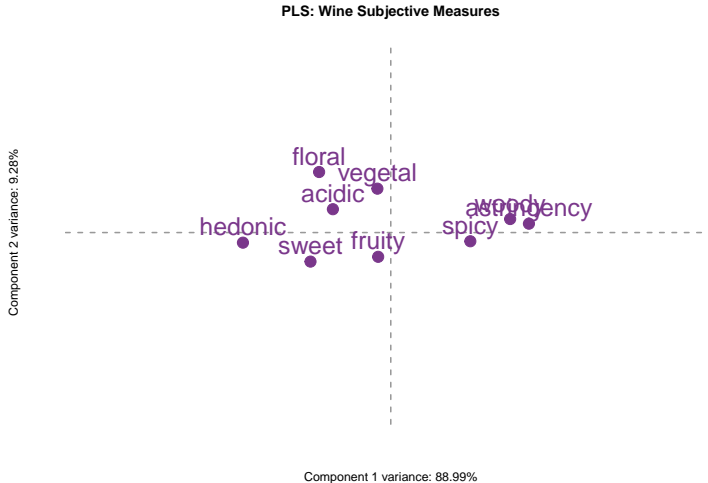
PLS - Wine



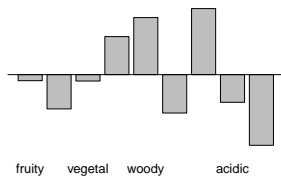
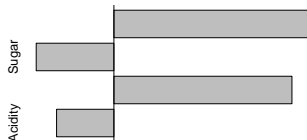
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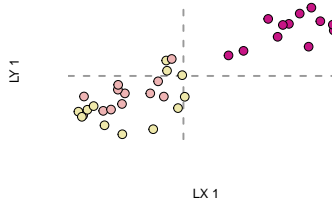
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Overview

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- PCA is the core of PLS

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- PLS generalizes PCA
 - If your two matrices are both the same, e.g., \mathbf{X}
 - PLS gives same results as PCA

We're experts now

- Visualize first

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- Visualize first
- Use what you know to help construct the story from the numbers

We're experts now

- Visualize first
- Use what you know to help construct the story from the numbers
 - We'll see some additional helpers in next part today

Break!

We covered a lot!

- And we're not even at the good part yet!

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- 7 ± 2 break

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 - Pressing questions