Lecture 3: Principal Components Analysis (PCA)

Reading: Sections 6.3.1, 10.1, 10.2, 10.4

STATS 202: Data mining and analysis

Jonathan Taylor, 9/28
Slide credits: Sergio Bacallado

The bias variance decomposition

The inputs, $x_1, \ldots, x_n$ are fixed, a test point x_0 is also fixed.

$$y_i = f(x_i) + \varepsilon_i \qquad \varepsilon_i \text{ i.i.d, mean } 0.$$

A regression method fit to $(x_1, y_1), \ldots, (x_n, y_n)$ produces the estimate $\hat{f}$. Then, the Mean Squared Error at x_0 satisfies:

$$MSE(x_0) = E(y_0 - \hat{f}(x_0))^2 = \text{Var}(\hat{f}(x_0)) + [\text{Bias}(\hat{f}(x_0))]^2 + \text{Var}(\varepsilon).$$

The bias variance decomposition

The inputs, $x_1, \dots, x_n$ are fixed, a test point x_0 is also fixed.

$$y_i = f(x_i) + \varepsilon_i \qquad \varepsilon_i \text{ i.i.d, mean } 0.$$

A regression method fit to $(x_1, y_1), \dots, (x_n, y_n)$ produces the estimate $\hat{f}$. Then, the Mean Squared Error at x_0 satisfies:

$$MSE(x_0) = E(y_0 - \hat{f}(x_0))^2 = \text{Var}(\hat{f}(x_0)) + [\text{Bias}(\hat{f}(x_0))]^2 + \text{Var}(\varepsilon).$$

Both variance and squared bias are always positive, so to minimize the MSE, you must reach a tradeoff between bias and variance.

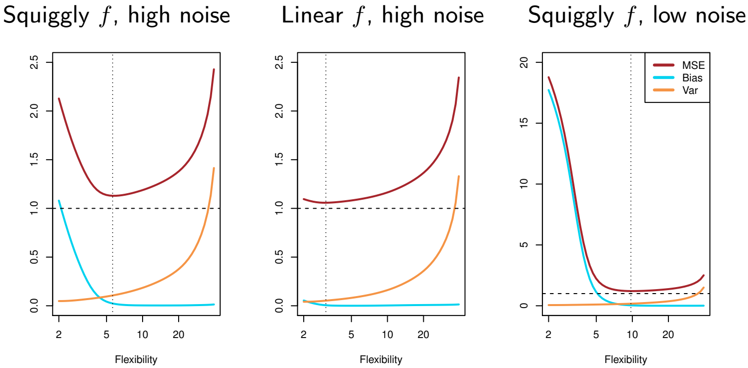

Squiggly f, high noise
Linear f, high noise
Squiggly f, low noise
MSE
Bias
Var
0.0
0.5
1.0
1.5
2.0
2.5
0
5
10
15
20
2
5
10
20
Flexibility

Figure 2.12

Classification problems

In a classification setting, the output takes values in a discrete set.

For example, if we are predicting the brand of a car based on a number of variables, the function f takes values in the set $\{$Ford, Toyota, Mercedes-Benz$, \dots\}$.

Classification problems

In a classification setting, the output takes values in a discrete set.

For example, if we are predicting the brand of a car based on a number of variables, the function f takes values in the set $\{$Ford, Toyota, Mercedes-Benz, $\ldots\}$.

The model:

$$Y = f(X) + \varepsilon$$

becomes insufficient, as X is not necessarily real-valued.

Classification problems

In a classification setting, the output takes values in a discrete set.

For example, if we are predicting the brand of a car based on a number of variables, the function f takes values in the set $\{$Ford, Toyota, Mercedes-Benz, $\ldots\}$.

The model:

$$\cancel{Y = f(X) + \varepsilon}$$

becomes insufficient, as X is not necessarily real-valued.

Classification problems

In a classification setting, the output takes values in a discrete set.

For example, if we are predicting the brand of a car based on a number of variables, the function f takes values in the set $\{$Ford, Toyota, Mercedes-Benz, $\ldots\}$.

We will use slightly different notation:

$$
\begin{aligned}
P(X, Y) &: \text{joint distribution of } (X, Y), \\
P(Y \mid X) &: \text{conditional distribution of } Y \text{ given } X, \\
\hat{y}_i &: \text{prediction for } x_i.
\end{aligned}
$$

Loss function for classification

There are many ways to measure the error of a classification prediction. One of the most common is the 0-1 loss:

$$E(\mathbf{1}(y_0 \neq \hat{y}_0))$$

Loss function for classification

There are many ways to measure the error of a classification prediction. One of the most common is the 0-1 loss:

$$E(\mathbf{1}(y_0 \neq \hat{y}_0))$$

Like the MSE, this quantity can be estimated from training and test data by taking a sample average:

$$\frac{1}{n}\sum_{i=1}^{n}\mathbf{1}(y_i \neq \hat{y}_i)$$

Bayes classifier

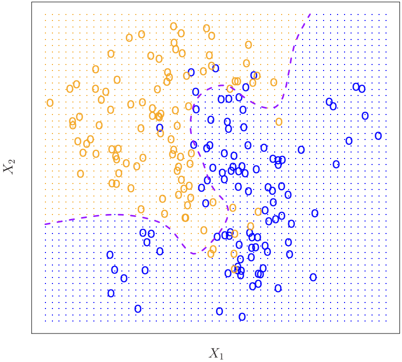


Figure 2.13

In practice, we never know the joint probability P. However, we can assume that it exists.

Bayes classifier

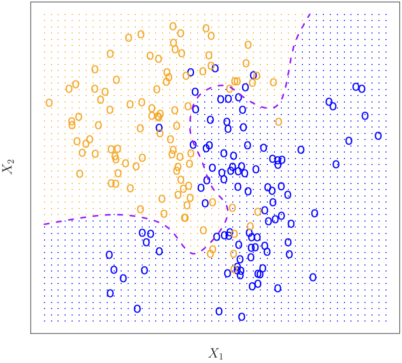


Figure 2.13

In practice, we never know the joint probability P. However, we can assume that it exists.

The Bayes classifier assigns:

$$\hat{y}_i = \text{argmax}_j \ \ P(Y = j \mid X = x_i)$$

It can be shown that this is the best classifier under the 0-1 loss.

Principal Components Analysis

- This is the most popular unsupervised procedure ever.
- Invented by Karl Pearson (1901).
- Developed by Harold Hotelling (1933).

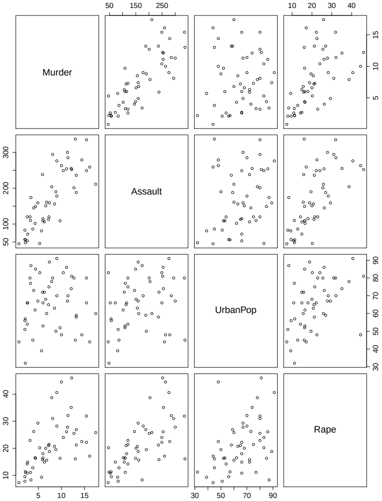
Principal Components Analysis

- This is the most popular unsupervised procedure ever.
- Invented by Karl Pearson (1901).
- Developed by Harold Hotelling (1933). $\leftarrow$ Stanford pride!

Principal Components Analysis

- This is the most popular unsupervised procedure ever.
- Invented by Karl Pearson (1901).
- Developed by Harold Hotelling (1933).
- **What does it do?** It provides a way to visualize high dimensional data, summarizing the most important information.

What is PCA good for?



What is PCA good for?

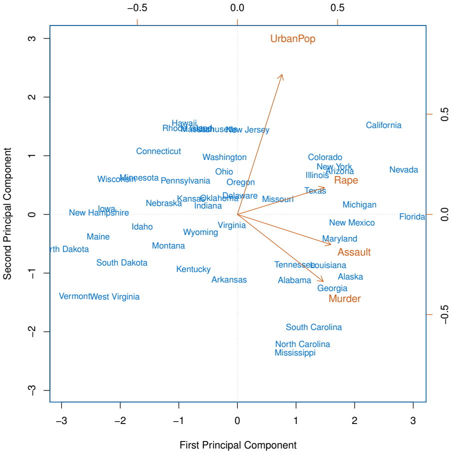
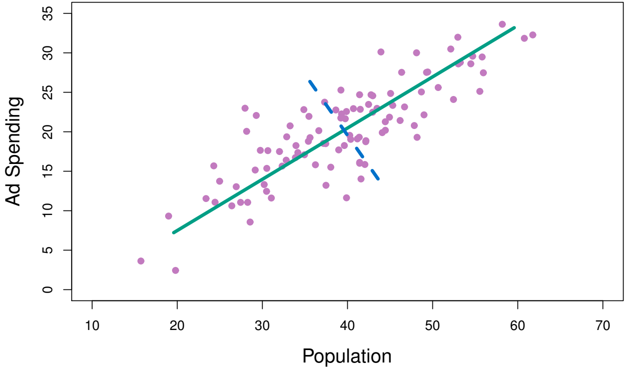


Figure 10.1

What is the first principal component?

It is the vector which passes the closest to a cloud of samples, in terms of squared Euclidean distance.



i.e. The green direction minimizes the average squared length of the dotted lines.

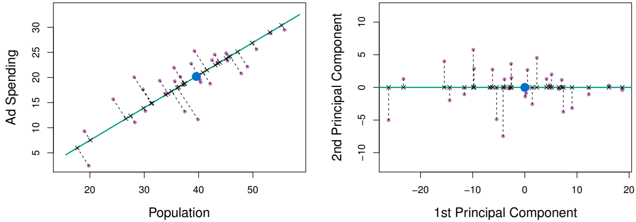


Figure 6.15

What does this look like with 3 variables?

The first two principal components span a plane which is closest to the data.

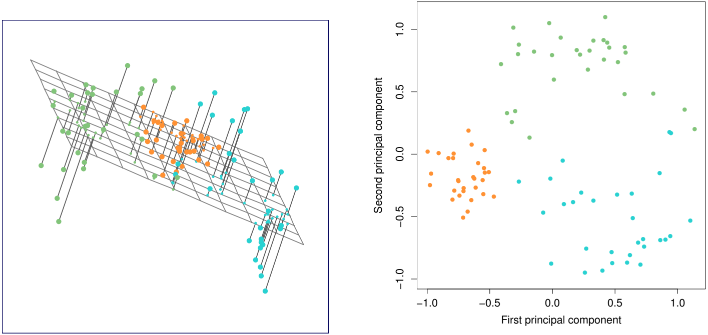


Figure 10.2

A second interpretation

The projection onto the first principal component is the one with the **highest variance**.

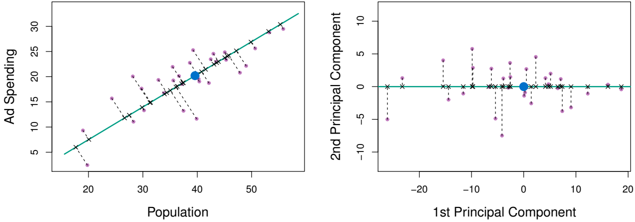


Figure 6.15

How do we say this in math?

Let $\mathbf{X}$ be a data matrix with n samples, and p variables.

How do we say this in math?

Let $\mathbf{X}$ be a data matrix with n samples, and p variables. From each variable, we subtract the mean of the column; i.e. we **center** the variables.

How do we say this in math?

Let $\mathbf{X}$ be a data matrix with n samples, and p variables. From each variable, we subtract the mean of the column; i.e. we **center** the variables.

To find the first principal component $\phi_1 = (\phi_{11}, \ldots, \phi_{p1})$, we solve the following optimization

How do we say this in math?

Let $\mathbf{X}$ be a data matrix with n samples, and p variables. From each variable, we subtract the mean of the column; i.e. we **center** the variables.

To find the first principal component $\phi_1 = (\phi_{11}, \ldots, \phi_{p1})$, we solve the following optimization

$$\max_{\phi_{11},\ldots,\phi_{p1}} \left\{ \frac{1}{n} \sum_{i=1}^{n} \left(\sum_{j=1}^{p} \phi_{j1} x_{ij} \right)^2 \right\}$$

$$\text{subject to} \sum_{j=1}^{p} \phi_{j1}^2 = 1.$$

How do we say this in math?

Let $\mathbf{X}$ be a data matrix with n samples, and p variables. From each variable, we subtract the mean of the column; i.e. we **center** the variables.

To find the first principal component $\phi_1 = (\phi_{11}, \ldots, \phi_{p1})$, we solve the following optimization

$$\max_{\phi_{11},\ldots,\phi_{p1}} \left\{ \frac{1}{n} \sum_{i=1}^{n} \left(\sum_{j=1}^{p} \phi_{j1} x_{ij} \right)^2 \right\}$$

$$\text{subject to} \sum_{j=1}^{p} \phi_{j1}^2 = 1.$$

Projection of the ith sample onto ϕ_1. Also known as **the score** z_{i1}

How do we say this in math?

Let $\mathbf{X}$ be a data matrix with n samples, and p variables. From each variable, we subtract the mean of the column; i.e. we **center** the variables.

To find the first principal component $\phi_1 = (\phi_{11}, \ldots, \phi_{p1})$, we solve the following optimization

$$\max_{\phi_{11},\ldots,\phi_{p1}} \left\{ \frac{1}{n} \sum_{i=1}^{n} \left(\sum_{j=1}^{p} \phi_{j1} x_{ij} \right)^2 \right\}$$

$$\text{subject to} \sum_{j=1}^{p} \phi_{j1}^2 = 1.$$

Variance of the n samples projected onto ϕ_1.

How do we say this in math?

To find the second principal component $\phi_2 = (\phi_{12}, \ldots, \phi_{p2})$, we solve the following optimization

How do we say this in math?

To find the second principal component $\phi_2 = (\phi_{12}, \ldots, \phi_{p2})$, we solve the following optimization

$$\max_{\phi_{12},\ldots,\phi_{p2}} \left\{ \frac{1}{n} \sum_{i=1}^{n} \left(\sum_{j=1}^{p} \phi_{j2} x_{ij} \right)^2 \right\}$$

$$\text{subject to} \quad \sum_{j=1}^{p} \phi_{j2}^2 = 1 \quad \text{and} \quad \sum_{j=1}^{p} \phi_{j1}\phi_{j2} = 0.$$

How do we say this in math?

To find the second principal component $\phi_2 = (\phi_{12}, \ldots, \phi_{p2})$, we solve the following optimization

$$\max_{\phi_{12},\ldots,\phi_{p2}} \left\{ \frac{1}{n} \sum_{i=1}^{n} \left(\sum_{j=1}^{p} \phi_{j2} x_{ij} \right)^2 \right\}$$

$$\text{subject to } \sum_{j=1}^{p} \phi_{j2}^2 = 1 \quad \text{and} \quad \sum_{j=1}^{p} \phi_{j1}\phi_{j2} = 0.$$

First and second principal components must be orthogonal.

How do we say this in math?

To find the second principal component $\phi_2 = (\phi_{12}, \ldots, \phi_{p2})$, we solve the following optimization

$$\max_{\phi_{12},\ldots,\phi_{p2}} \left\{ \frac{1}{n} \sum_{i=1}^{n} \left(\sum_{j=1}^{p} \phi_{j2} x_{ij} \right)^2 \right\}$$

$$\text{subject to } \sum_{j=1}^{p} \phi_{j2}^2 = 1 \quad \text{and} \quad \sum_{j=1}^{p} \phi_{j1}\phi_{j2} = 0.$$

First and second principal components must be orthogonal.

Equivalent to saying that the scores $(z_{11}, \ldots, z_{n1})$ and $(z_{12}, \ldots, z_{n2})$ are uncorrelated.

Solving the optimization

This optimization is fundamental in linear algebra. It is satisfied by either:

Solving the optimization

This optimization is fundamental in linear algebra. It is satisfied by either:

- The singular value decomposition (SVD) of $\mathbf{X}$:

$$\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{\Phi}^T$$

  where the ith column of $\mathbf{\Phi}$ is the ith principal component ϕ_i, and the ith column of $\mathbf{U}\mathbf{\Sigma}$ is the ith vector of scores $(z_{1i}, \ldots, z_{ni})$.

Solving the optimization

This optimization is fundamental in linear algebra. It is satisfied by either:

- The singular value decomposition (SVD) of $\mathbf{X}$:

  $$\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{\Phi}^T$$

  where the ith column of $\mathbf{\Phi}$ is the ith principal component ϕ_i, and the ith column of $\mathbf{U}\mathbf{\Sigma}$ is the ith vector of scores $(z_{1i}, \ldots, z_{ni})$.

- The eigendecomposition of $\mathbf{X}^T\mathbf{X}$:

  $$\mathbf{X}^T\mathbf{X} = \mathbf{\Phi}\mathbf{\Sigma}^2\mathbf{\Phi}^T$$

PCA in practice: The biplot

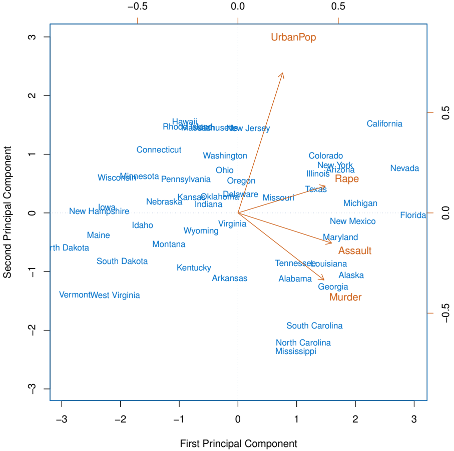


Figure 10.1

Scaling the variables

Most of the time, we don't care about the absolute numerical value of a variable.

Scaling the variables

Most of the time, we don't care about the absolute numerical value of a variable. We care about the value relative to the spread observed in the sample.

Before PCA, in addition to **centering** each variable, we also multiply it times a constant to make its variance equal to 1.

Example: scaled vs. unscaled PCA

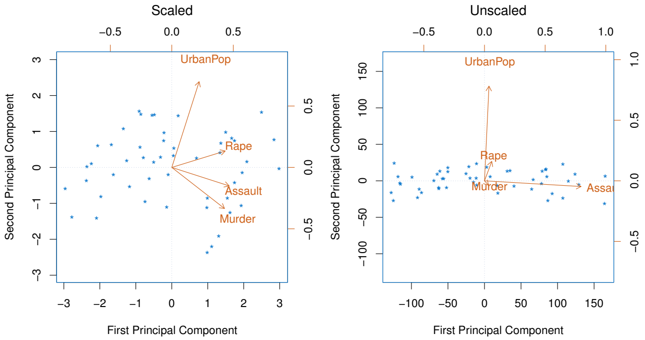


Figure 10.3

Scaling the variables

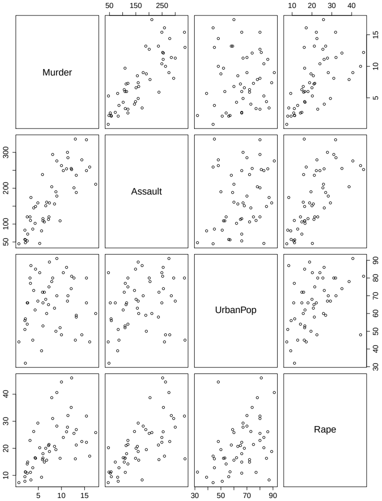
In special cases, we have variables measured in the same unit; e.g. gene expression levels for different genes.

Scaling the variables

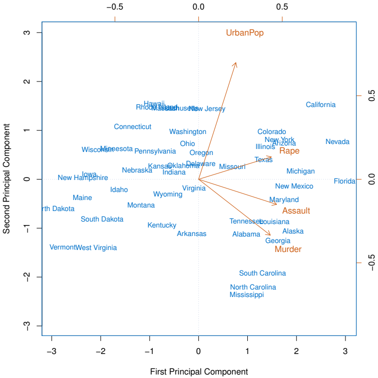
In special cases, we have variables measured in the same unit; e.g. gene expression levels for different genes.

Therefore, we care about the absolute value of the variables and we can perform PCA without scaling.

How many principal components are enough?



How many principal components are enough?



We said 2 principal components capture most of the relevant information. But how can we tell?

The proportion of variance explained

We can think of the top **principal components** as directions in space in which the data vary the most.

The proportion of variance explained

We can think of the top **principal components** as directions in space in which the data vary the most.

The ith **score vector** $(z_{1i}, \ldots, z_{ni})$ can be interpreted as a *new* variable. The variance of this variable decreases as we take i from 1 to p.

The proportion of variance explained

We can think of the top **principal components** as directions in space in which the data vary the most.

The ith **score vector** $(z_{1i}, \ldots, z_{ni})$ can be interpreted as a *new* variable. The variance of this variable decreases as we take i from 1 to p. However, the total variance of the score vectors is the same as the total variance of the original variables:

$$\sum_{i=1}^{p} \frac{1}{n} \sum_{j=1}^{n} z_{ji}^2 = \sum_{k=1}^{p} \mathsf{Var}(x_k).$$

The proportion of variance explained

We can think of the top **principal components** as directions in space in which the data vary the most.

The ith **score vector** $(z_{1i}, \ldots, z_{ni})$ can be interpreted as a *new* variable. The variance of this variable decreases as we take i from 1 to p. However, the total variance of the score vectors is the same as the total variance of the original variables:

$$\sum_{i=1}^{p} \frac{1}{n} \sum_{j=1}^{n} z_{ji}^2 = \sum_{k=1}^{p} \mathrm{Var}(x_k).$$

We can quantify how much of the variance is captured by the first m principal components/score variables.

The proportion of variance explained

The variance of the mth score variable is:

$$\frac{1}{n}\sum_{i=1}^{n} z_{im}^2$$

The proportion of variance explained

The variance of the mth score variable is:

$$\frac{1}{n}\sum_{i=1}^{n} z_{im}^2 = \frac{1}{n}\sum_{i=1}^{n}\left(\sum_{j=1}^{p}\phi_{jm}x_{ij}\right)^2$$

The proportion of variance explained

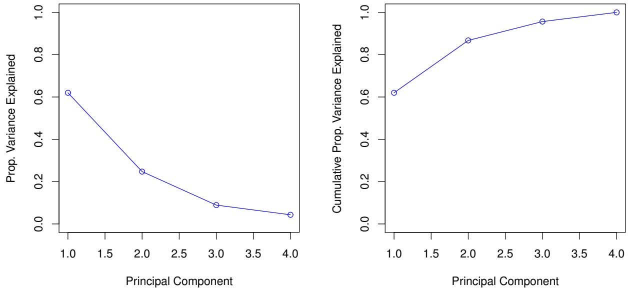
The variance of the mth score variable is:

$$\frac{1}{n}\sum_{i=1}^{n} z_{im}^2 = \frac{1}{n}\sum_{i=1}^{n}\left(\sum_{j=1}^{p}\phi_{jm}x_{ij}\right)^2 = \frac{1}{n}\mathbf{\Sigma}_{mm}^2.$$

The proportion of variance explained

The variance of the mth score variable is:

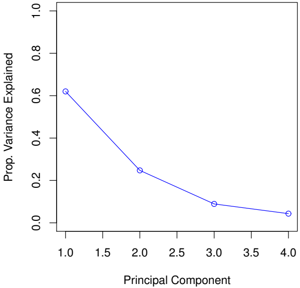
$$\frac{1}{n}\sum_{i=1}^{n} z_{im}^2 = \frac{1}{n}\sum_{i=1}^{n}\left(\sum_{j=1}^{p}\phi_{jm}x_{ij}\right)^2 = \frac{1}{n}\boldsymbol{\Sigma}_{mm}^2.$$



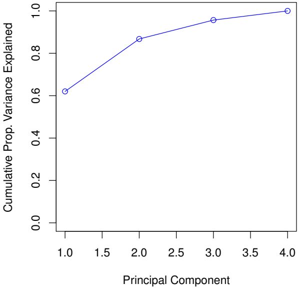
The proportion of variance explained

The variance of the mth score variable is:

$$\frac{1}{n}\sum_{i=1}^{n} z_{im}^2 = \frac{1}{n}\sum_{i=1}^{n}\left(\sum_{j=1}^{p}\phi_{jm}x_{ij}\right)^2 = \frac{1}{n}\Sigma_{mm}^2.$$



Scree plot



Generalizations of PCA

PCA works under a Euclidean geometry in the space of variables.
Often, the natural geometry is different:

Generalizations of PCA

PCA works under a Euclidean geometry in the space of variables. Often, the natural geometry is different:

- We expect some variables to be "closer" to each other that to other variables.

Generalizations of PCA

PCA works under a Euclidean geometry in the space of variables. Often, the natural geometry is different:

- We expect some variables to be "closer" to each other that to other variables.
- Some correlations between variables would be more surprising than others.

Generalizations of PCA

PCA works under a Euclidean geometry in the space of variables. Often, the natural geometry is different:

- We expect some variables to be "closer" to each other that to other variables.
- Some correlations between variables would be more surprising than others.

Examples:

- Variables are pixel values, samples are different images of the brain. We expect neighboring pixels to have stronger correlations.

Generalizations of PCA

PCA works under a Euclidean geometry in the space of variables. Often, the natural geometry is different:

- We expect some variables to be "closer" to each other that to other variables.
- Some correlations between variables would be more surprising than others.

Examples:

- Variables are pixel values, samples are different images of the brain. We expect neighboring pixels to have stronger correlations.
- Variables are rainfall measurements at different regions. We expect neighboring regions to have higher correlations.

Generalizations of PCA

There are ways to include this knowledge in a PCA. See:

1. Susan Holmes. *Multivariate Analysis, the French way.* (2006).
2. Omar de la Cruz and Susan Holmes. *An introduction to the duality diagram*. (2011).
3. Stéphane Dray and Thibaut Jombart. *Revisiting Guerry's data: Introducing spatial constraints in multivariate analysis.* (2011).
4. Genevera Allen, Logan Grosenick, and Jonathan Taylor. *A Generalized Least Squares Matrix Decomposition*. (2011).