Lecture 3: Principal Components Analysis (PCA)

Reading: Sections 6.3.1, 10.1, 10.2, 10.4

STATS 202: Data mining and analysis

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October 7, 2013

Announcements

- Kaggle invitations have been sent. You have to register + join the competition.
- If you want to form a team, you should do so before making any submissions.
- I'm extending my office hours on Monday for Python help.
- Warning: Some nodes on corn have a different version of IPython.

The bias variance decomposition

Let x_0 be fixed, $y_0 = f(x_0) + \varepsilon$, and $\hat{f}$ be estimated from n separate training samples $\{x_1, \ldots, x_n; y_1, \ldots, y_n\}$.

Let E denote the expectation over ε and the training samples. Then, the Mean Squared Error at x_0 can be decomposed:

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

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Irreducible error

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The variance of the estimate of Y: $E[\hat{f}(x_0) - E(\hat{f}(x_0))]^2$

This measures how much the estimate of $\hat{f}$ at x_0 changes when we sample new training data.

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The squared bias of the estimate of Y: $[E(\hat{f}(x_0) - f(x_0))]^2$

This measures the deviation of the average estimate $\hat{f}$ at x_0 from $f(x_0)$.

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Both variance and squared bias are always positive.

Higher variance $\iff$ More flexibility $\iff$ Lower bias.

We will aim to minimize both sources of error simultaneously.

Principal Components Analysis

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- Invented by Karl Pearson (1901).
- Developed by Harold Hotelling (1933).
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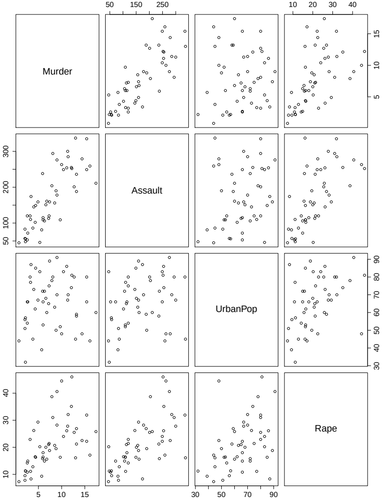
What is PCA good for?



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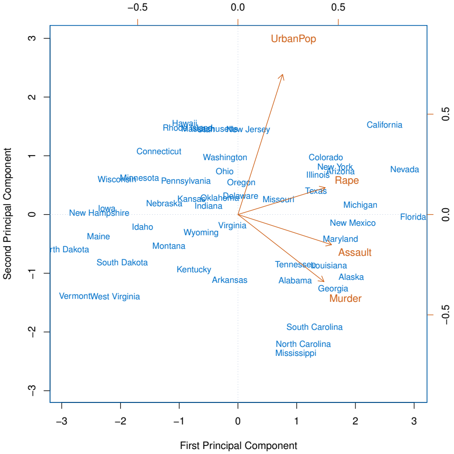
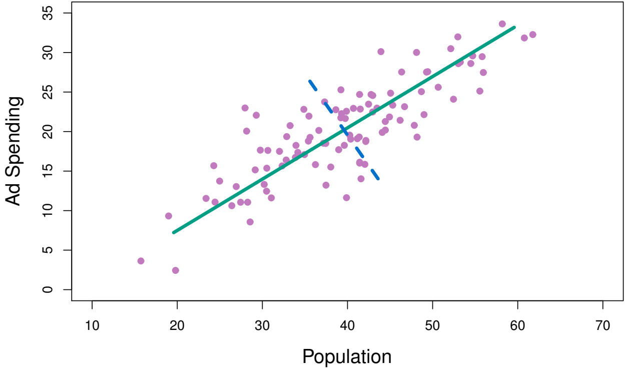


Figure 10.1

What is the first principal component?

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



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

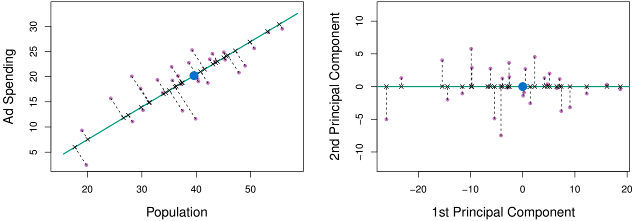


Figure 6.15

What does this look like with 3 variables?

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

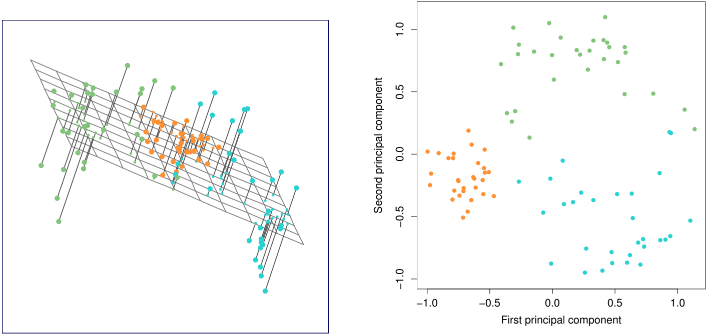


Figure 10.2

A second interpretation

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

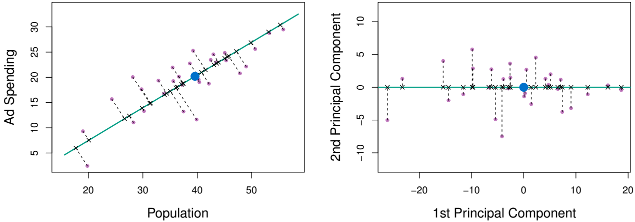


Figure 6.15

How do we say this in math?

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

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

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

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

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

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

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

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

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:

- 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

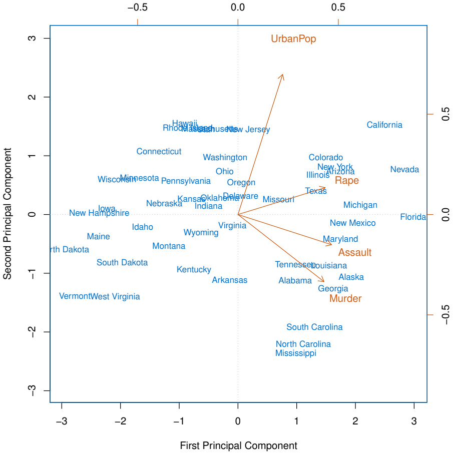


Figure 10.1

Scaling the variables

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

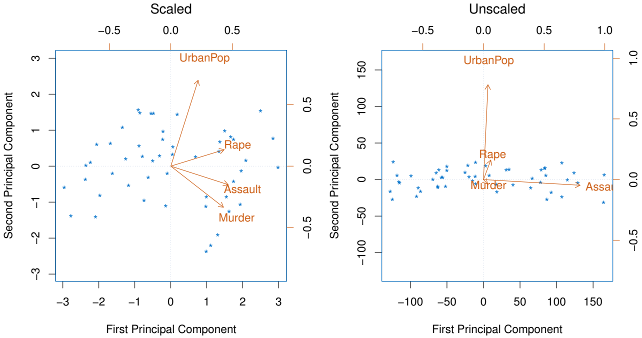


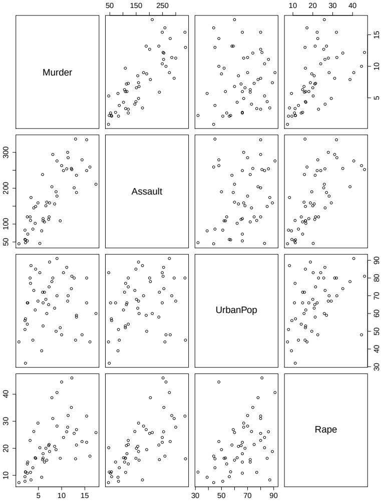
Figure 10.3

Scaling the variables

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

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

How many principal components are enough?



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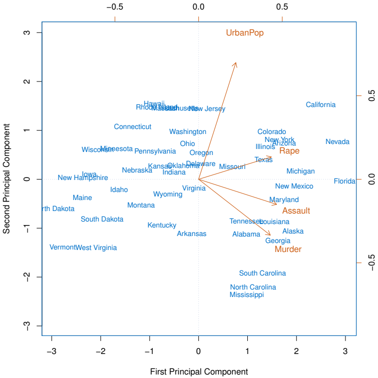


We said 2 principal components capture most of the relevant information. But how can we tell?

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 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:

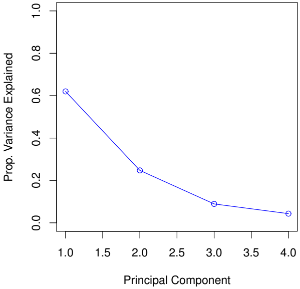
$$\sum_{k=1}^{p} \frac{1}{n} \sum_{j=1}^{n} x_{jk}^2.$$

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

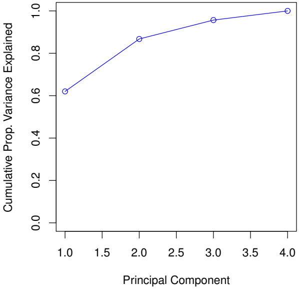
The proportion of variance explained

The variance of the mth score variable is:

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



Scree plot



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 counts for different gut bacteria, samples are different people. We expect bacteria that are close phylogenetically to be strongly correlated.

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 GuerryÕs data: Introducing spatial constraints in multivariate analysis.* (2011).
4. Genevera Allen, Logan Grosenick, and Jonathan Taylor. *A Generalized Least Squares Matrix Decomposition*. (2011).