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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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:

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

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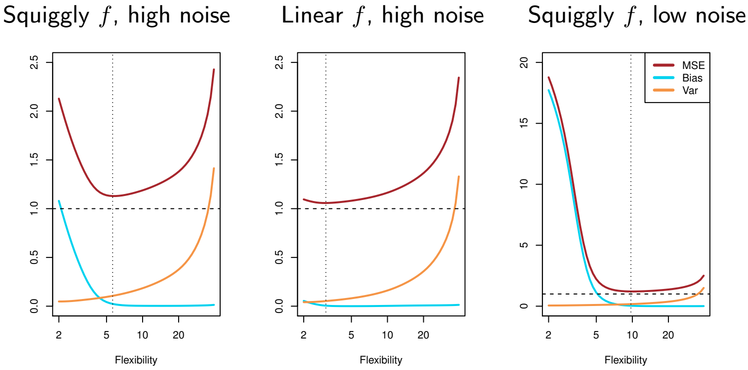
Both variance and squared bias are always positive, so to minimize the MSE, you must reach a tradeoff between bias and variance.



Squiggly f, high noise
Linear f, high noise
Squiggly f, low noise
MSE
Bias
Var
Flexibility
Flexibility
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$, \ldots\}$.

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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:

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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

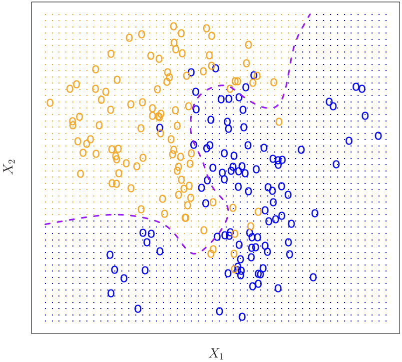

Figure 2.13

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

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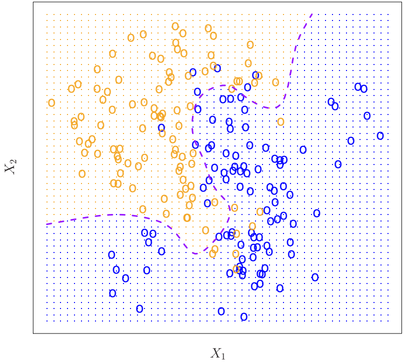

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The Bayes classifier assigns:

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

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

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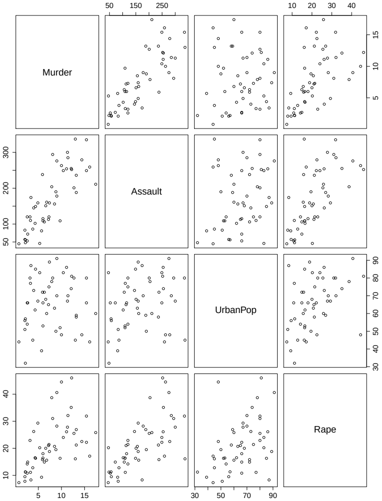
- **What does it do?** It provides a way to visualize high dimensional data, summarizing the most important information.

What is PCA good for?



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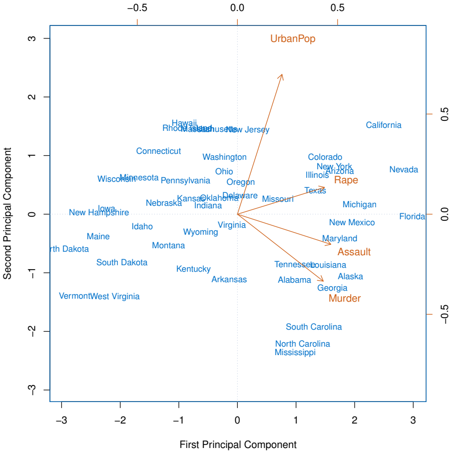
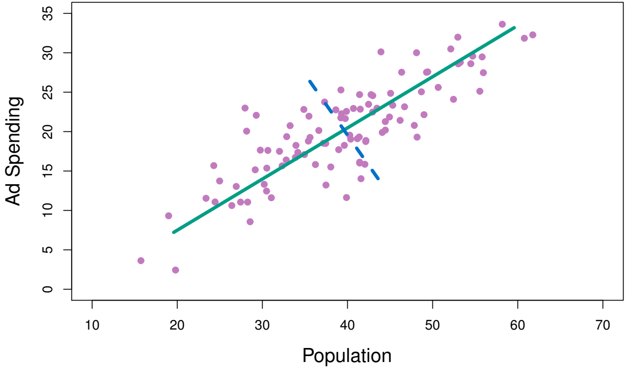


Figure 10.1

What is the first principal component?

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



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

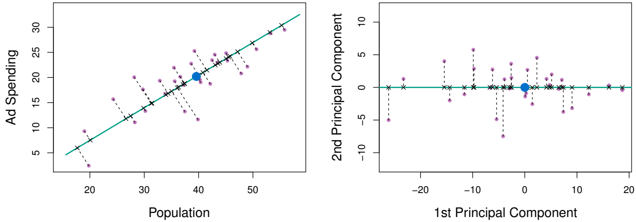


Figure 6.15

What does this look like with 3 variables?

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

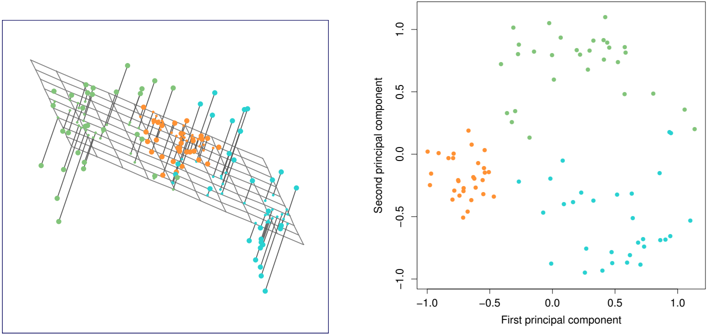
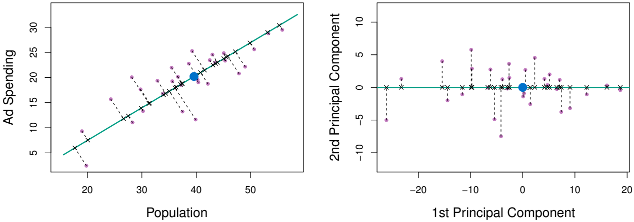


Figure 10.2

A second interpretation

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



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

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

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

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Variance of the n samples projected onto ϕ_1.

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

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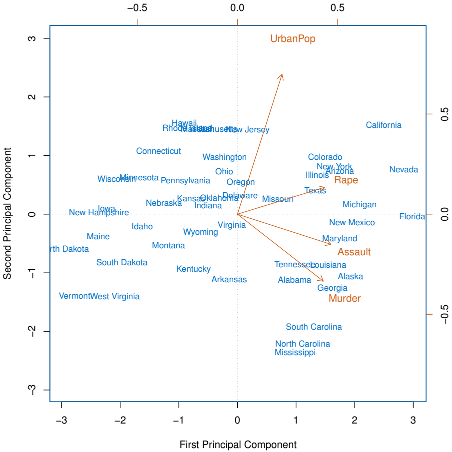
- The eigendecomposition of $\mathbf{X}^T\mathbf{X}$:

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

PCA in practice: The biplot



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Scaling the variables

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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

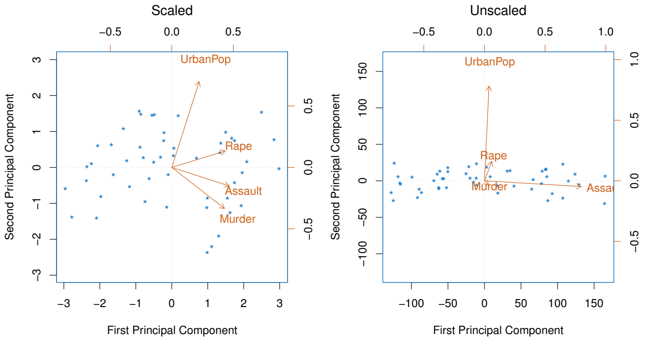

Figure 10.3

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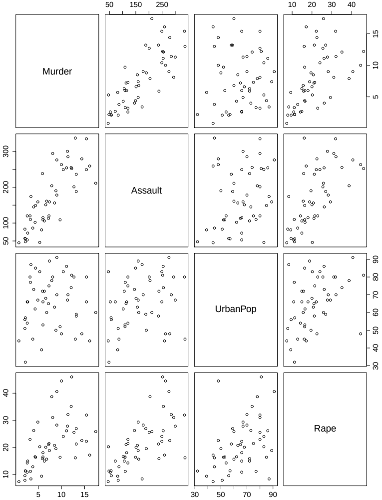
Therefore, we care about the absolute value of the variables and we can perform PCA without scaling.

How many principal components are enough?



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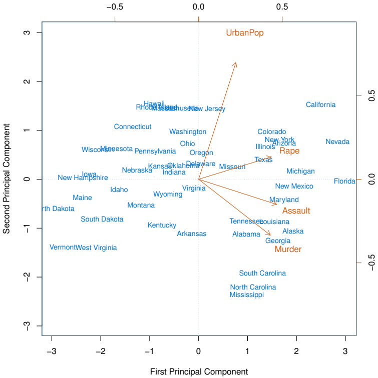

We said 2 principal components capture most of the relevant information. But how can we tell?

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

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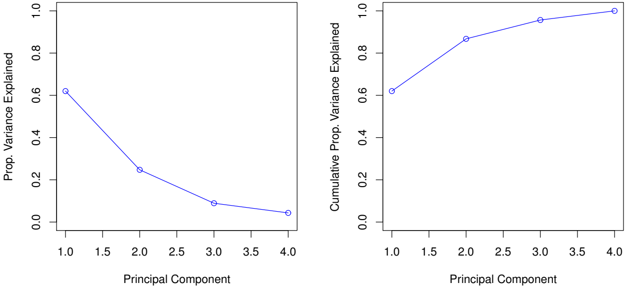

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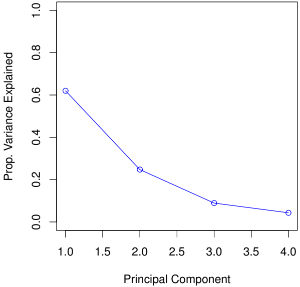

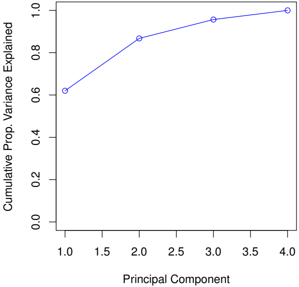

Scree plot

Generalizations of PCA

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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).