Lecture 3: Principal Components Analysis (PCA)

Reading: Sections 6.3.1, 10.1, 10.2, 10.4

STATS 202: Data mining and analysis

September 29, 2017
Recap: The bias variance decomposition

Training data \((x_1, y_1), \ldots, (x_n, y_n)\), a fixed test point \(x_0\).

\[
y_i = f(x_i) + \varepsilon_i \quad \text{for } \varepsilon_i \text{ independent, mean 0.}
\]

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

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

Squiggly $f$, low noise  

Linear $f$, high noise  

Figure 2.12
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 \( \{ \text{Ford, Toyota, Mercedes-Benz, \ldots} \} \).
Classification problems

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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, ... \}.

Instead, we will adopt the notation:

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

\[ E(\mathbf{1}(y_0 \neq \hat{y}_0)) \]
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As with squared error, we can compute average test prediction error (called test error rate under 0-1 loss) using previously unseen test data \{\(x'_i, y'_i\); \(i = 1, \ldots, m\)}:

\[ \frac{1}{m} \sum_{i=1}^{m} \mathbf{1}(y'_i \neq \hat{y}'_i) \]

Similarly, we can compute the (usually optimistic) training error rate

\[ \frac{1}{n} \sum_{i=1}^{n} \mathbf{1}(y_i \neq \hat{y}_i) \]
Bayes classifier

If we knew the conditional probability $P(Y \mid X)$, we could compute the optimal classifier under the 0-1 loss.

Figure 2.13
Bayes classifier

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The Bayes classifier predicts

$$\hat{y}_i = \arg\max_j P(Y = j \mid X = x_i)$$

In practice we don’t know $P(Y \mid X)$, but many classification methods operate by estimating these conditional probabilities.
K-nearest neighbors

To assign a color to an input $x$, we look at its $K = 3$ nearest neighbors and predict the color of the majority of the neighbors.
K-nearest neighbors gives a similar decision boundary

Figure 2.15
Higher $K$ results in a smoother decision boundary.
Principal Components Analysis

- This is the most popular unsupervised procedure ever.
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- This is the most popular unsupervised procedure ever.
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- **What does it do?** It provides a way to visualize high dimensional data, summarizing the most important information.
Scatterplot matrix
Figure 10.1
What is the first principal component?

It is the direction of the line that is closest to the datapoints, in terms of squared Euclidean distance.
That is, the PC 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

Intuition: High variance directions are often interesting directions.
How do we say this in math?

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

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

subject to

$$
\sum_{j=1}^{p} \phi_{2j1} = 1
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Projection of the $i$th sample onto $\phi_1$. Also known as the score $z_{i1}$.
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Sample variance of the scores $Z_{i1}$
(i.e. sample variance of projections of datapoints onto $\phi_1$.)
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

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

subject to

$$\sum_{j=1}^{p} \phi_{2j}^2 = 1$$

and

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

\[ X = U \Sigma \Phi^T \]

where the \( i \)th column of \( \Phi \) is the \( i \)th principal component \( \phi_i \), and the \( i \)th column of \( U \Sigma \) is the \( i \)th vector of scores \((z_1, ..., z_n)\).

\[ X^T X = \Phi \Sigma^2 \Phi^T \]
Solving the optimization

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- The singular value decomposition (SVD) of $X$:

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- The eigendecomposition of $X^TX$:

  $X^TX = ΦΣ^2Φ^T$
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.
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In that case, before PCA, in addition to centering each variable, we also multiply it times a constant to make its variance equal to 1, i.e. we standardize each variable.
Example: scaled vs. unscaled PCA

Figure 10.3
Scaling the variables

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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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How can we tell if 2 principal components capture most of the relevant information?
The proportion of variance explained

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The $i$th 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 $p$. 
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\sum_{i=1}^{p} \frac{1}{n} \sum_{j=1}^{n} z_{ji}^2 = \sum_{k=1}^{p} \text{Var}(x_k).
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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 $m$th score variable is:

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$$

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