Introduction to Machine Learning

Session 3b: Principal Components Analysis

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Outline

Principal Components Analysis

Principal Components Analysis

- Suppose that we wish to visualize n observations with measurements on a set of p features, $X_1, X_2, \ldots, X_p$, as part of an exploratory data analysis.
- How can we achieve this goal?
- We could examine two-dimensional scatterplots of the data, each of which containing the n observations' measurements on two of the features.

Principal Components Analysis

- However, there would be $\binom{p}{2} = p(p-1)/2$ such scatterplots (e.g., 45 scatterplots for $p = 10$).
- Moreover, these scatterplots would not be informative since each would contain only a small fraction of the total information present in the data set.
- Clearly, a better method is required to visualize the n observations when p is large.

Principal Components Analysis

- Our goal is to find a low-dimensional representation of the data that captures as much of the information as possible.
- PCA is a method that allows us to do just this.
- It finds a low-dimensional representation of a data set that contains as much as possible of the variation.

Principal Components Analysis

The idea behind PCA is the following:

- Each of the n observations lives in a p-dimensional space, but not all of these dimensions are equally interesting.
- PCA seeks a small number of dimensions that are as interesting as possible.
- "Interesting" is determined by the amount that the observations vary along a dimension.
- Each of the dimensions found by PCA is a linear combination of the p features.

How Are the Principal Components Determined?

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- The first principal component of features $X_1, X_2, \ldots, X_p$ is the normalized linear combination

$$Z_1 = \phi_{11} X_1 + \phi_{21} X_2 + \ldots + \phi_{p1} X_p \tag{1}$$

  that has the largest variance.

- By normalized, we mean that $\sum_{j=1}^{p} \phi_{j1}^2 = 1$.

- The elements $\phi_{11}, \ldots, \phi_{p1}$ are called the loadings of the first principal component. Together, they make up the principal component loading vector, $\phi_1 = (\phi_{11} \;\; \phi_{21} \;\; \ldots \;\; \phi_{p1})^T$.

How Are the Principal Components Determined?

- Why do we constrain the loadings so that their sum of squares is equal to 1?
- Without this constraint, the loadings could be arbitrarily large in absolute value, resulting in an arbitrarily large variance.
- Given an $n \times p$ data set $\mathbf{X}$, how do we compute the first principal component?
- As we are only interested in variance, we center each variable in $\mathbf{X}$ to have mean 0.

How Are the Principal Components Determined?

- We then look for the linear combination of the feature values of the form

$$z_{i1} = \phi_{11} x_{i1} + \phi_{21} x_{i2} + \ldots + \phi_{p1} x_{ip} \tag{2}$$

  that has the largest sample variance, subject to the constraint that $\sum_{j=1}^{p} \phi_{j1}^2 = 1$.

- Hence, the first principal component loading vector solves the optimization problem

$$\underset{\phi_{11},\ldots,\phi_{p1}}{\arg\max} \left\{ \frac{1}{n} \sum_{i=1}^{n} \left(\sum_{j=1}^{p} \phi_{j1} x_{ij} \right)^2 \right\} \; s.t. \; \sum_{j=1}^{p} \phi_{j1}^2 = 1. \tag{3}$$

How Are the Principal Components Determined?

- Problem (3) can be solved via an eigen decomposition (for details, see Hastie et al. 2009, 534ff.).
- The $z_{11}, \ldots, z_{n1}$ are called the scores of the first principal component.
- After the first principal component Z_1 of the features has been determined, we can find the second principal component Z_2.

How Are the Principal Components Determined?

- The second principal component is the linear combination of $X_1, \ldots, X_p$ that has maximal variance out of all linear combinations that are uncorrelated with Z_1.
- The second principal component scores $z_{12}, z_{22}, \ldots, z_{n2}$ take the form

$$z_{i2} = \phi_{12} x_{i1} + \phi_{22} x_{i2} + \ldots + \phi_{p2} x_{ip}, \tag{4}$$

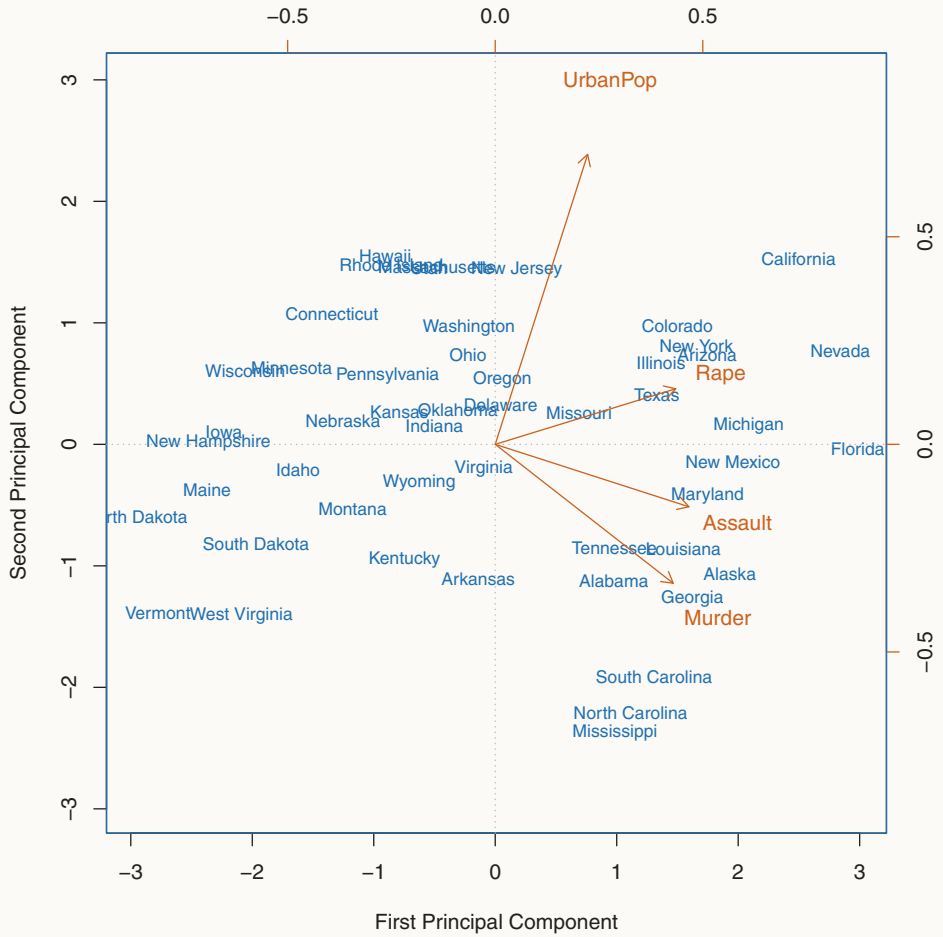
  where ϕ_2 is the second principal component loading vector, with elements $\phi_{12}, \phi_{22}, \ldots, \phi_{p2}$.
- It turns out that constraining Z_2 to be uncorrelated with Z_1 is equivalent to constraining the direction ϕ_2 to be orthogonal to the direction ϕ_1.

Example: USA Arrests Data

- For each of the 50 US states, the data set contains the number of arrests per $100{,}000$ residents for each of three crimes: `Assault`, `Murder`, and `Rape`.
- We also have for each state the population living in urban areas: `UrbanPop`.
- The principal component score vectors have length $n = 50$, and the principal component loading vectors have length $p = 4$.
- PCA was performed after standardizing each variable to have mean 0 and standard deviation 1.

Example: USA Arrests Data

Biplot (principal component scores and loading vectors for the first two principal components)



(Source: James et al. 2013, 378)

Example: USA Arrests Data

- In the figure, the blue state names represent the scores for the first two principal components (axes on the bottom and left).
- The orange arrows indicate the first two principal component loading vectors (axes on the top and right).
- For example, the loading for `Rape` on the first component is 0.54, and its loading on the second component 0.17 (the word `Rape` in the plot is centered at the point $(0.54, 0.17)$).

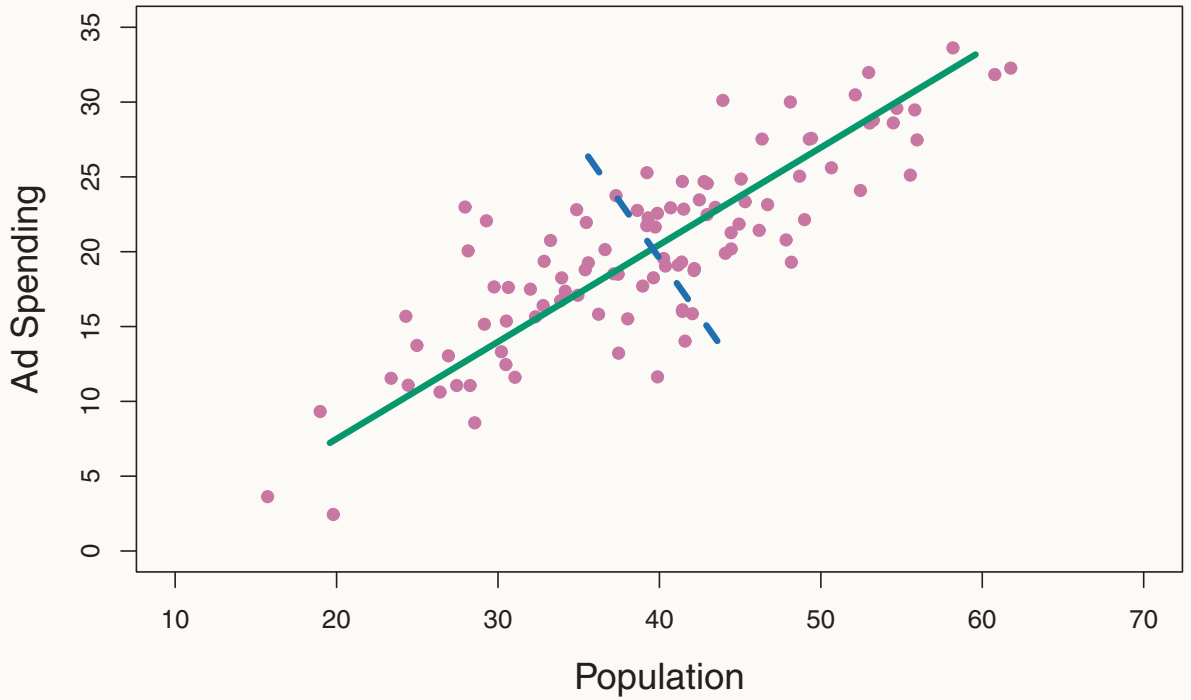
Example: USA Arrests Data

- The first loading vector places approximately equal weight on the crime-related variables, with much less weight on `UrbanPop`. Hence, this component roughly corresponds to a measure of overall crime rates.
- The second loading vector places most of its weight on `UrbanPop` and much less weight on the other three features. Hence, this component roughly corresponds to the level of urbanization of a state.

Interpretation of Principal Components

Interpretation I: Principal component loading vectors are the directions in feature space along which the data vary the most.

Population size (in $10{,}000$) and ad spending for a company (in $1{,}000$)

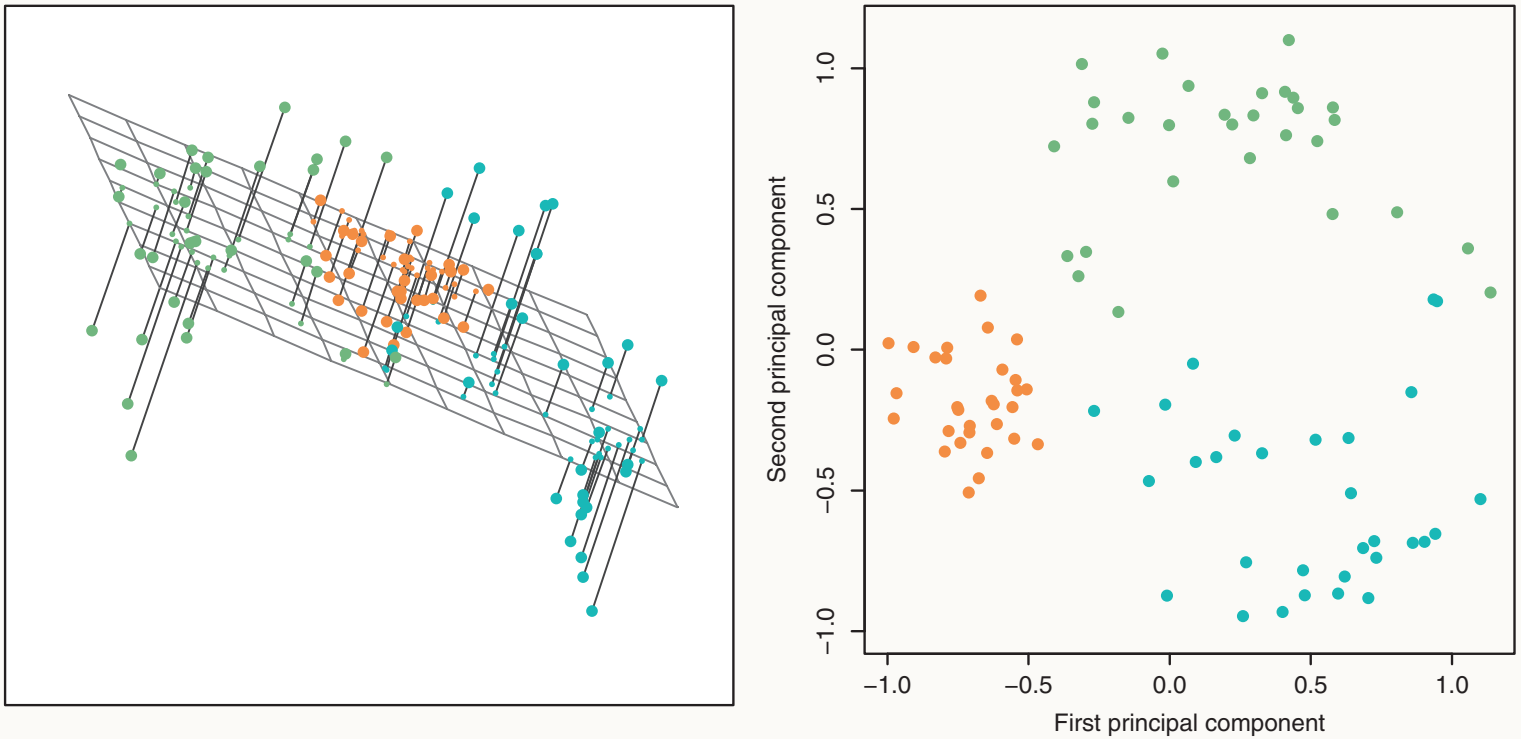


(Source: James et al. 2013, 230)

Interpretation of Principal Components

Interpretation II: The first M principal component loading vectors span the M-dimensional hyperplane that is closest to the n observations.

Simulated three-dimensional data set

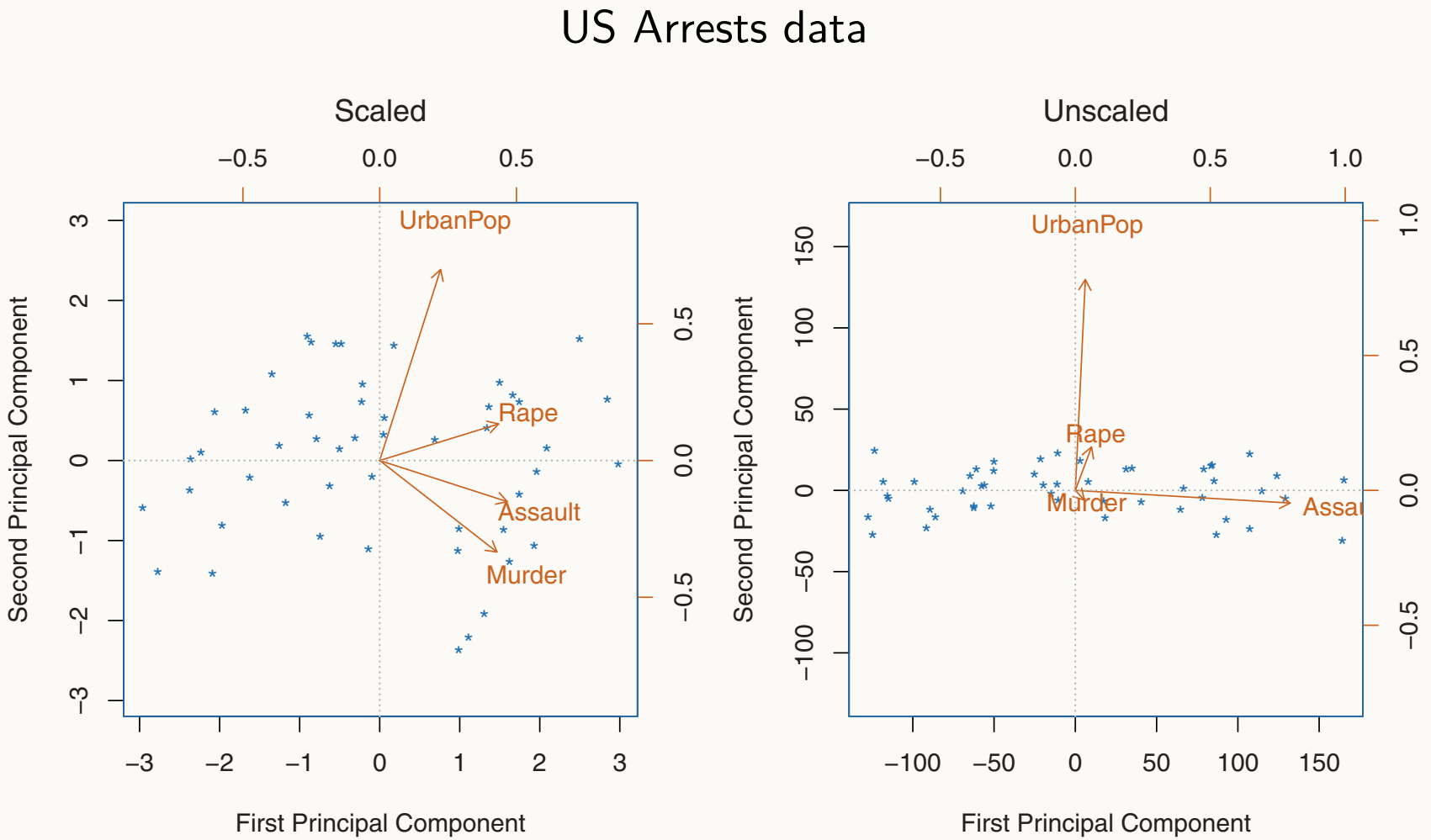


(Source: James et al. 2013, 380)

Scaling the Variables

- The results obtained by PCA depend on the scales of the variables.
- In the US Arrests data, the variables are measured in different units: `Murder`, `Rape`, and `Assault` are occurrences per $100{,}000$ people and `UrbanPop` is the percentage of a state's population that lives in an urban area.
- These variables have variance 18.97, 87.73, 6945.16, and 209.5, respectively.
- If we perform PCA on the unscaled variables, then the first principal component loading vector will have a very large loading for `Assault`.

Scaling the Variables



(Source: James et al. 2013, 381)

Scaling the Variables

- Suppose that `Assault` were measured in occurrences per 100 people rather than per $100{,}000$ people.
- In this case, the variance of the variable would be tiny, and so the first principal component loading vector would have a very small value for that variable.
- We typically scale each variable to have a standard deviation of 1 before we perform PCA, so that the principal components do not depend on the choice of scaling.
- However, if the variables are measured in the same units, we might choose not to scale the variables.

Uniqueness of the Principal Components

- Each principal component loading vector is unique, up to a sign flip.
- The reason is that a principal component loading vector specifies a direction in p-dimensional space. Flipping the sign has no effect as the direction does not change.
- Similarly, the score vectors are unique up to a sign flip, since the variance in Z is the same as the variance in $-Z$.

The Proportion of Variance Explained

- Above, we performed PCA on a simulated three-dimensional data set (left panel) and projected the data onto the first two principal component loading vectors (right panel).
- In this case, the two-dimensional representation of the three-dimensional data successfully captures the major pattern in the data.
- But how much of the information in a data set is lost by projecting the observations onto the first few principal components? Or, how much of the variance in the data is not contained in the first few principal components?

The Proportion of Variance Explained

- The total variance present in a data set is (assuming that the variables have been centered)

$$\sum_{j=1}^{p} Var(X_j) = \sum_{j=1}^{p} \frac{1}{n} \sum_{i=1}^{n} x_{ij}^2. \tag{5}$$

- The variance explained by the mth principal component is

$$\frac{1}{n} \sum_{i=1}^{n} z_{im}^2 = \frac{1}{n} \sum_{i=1}^{n} \left(\sum_{j=1}^{p} \phi_{jm} x_{ij} \right)^2. \tag{6}$$

The Proportion of Variance Explained

- Therefore, the Proportion of Variance Explained (PVE) by the mth principal component is

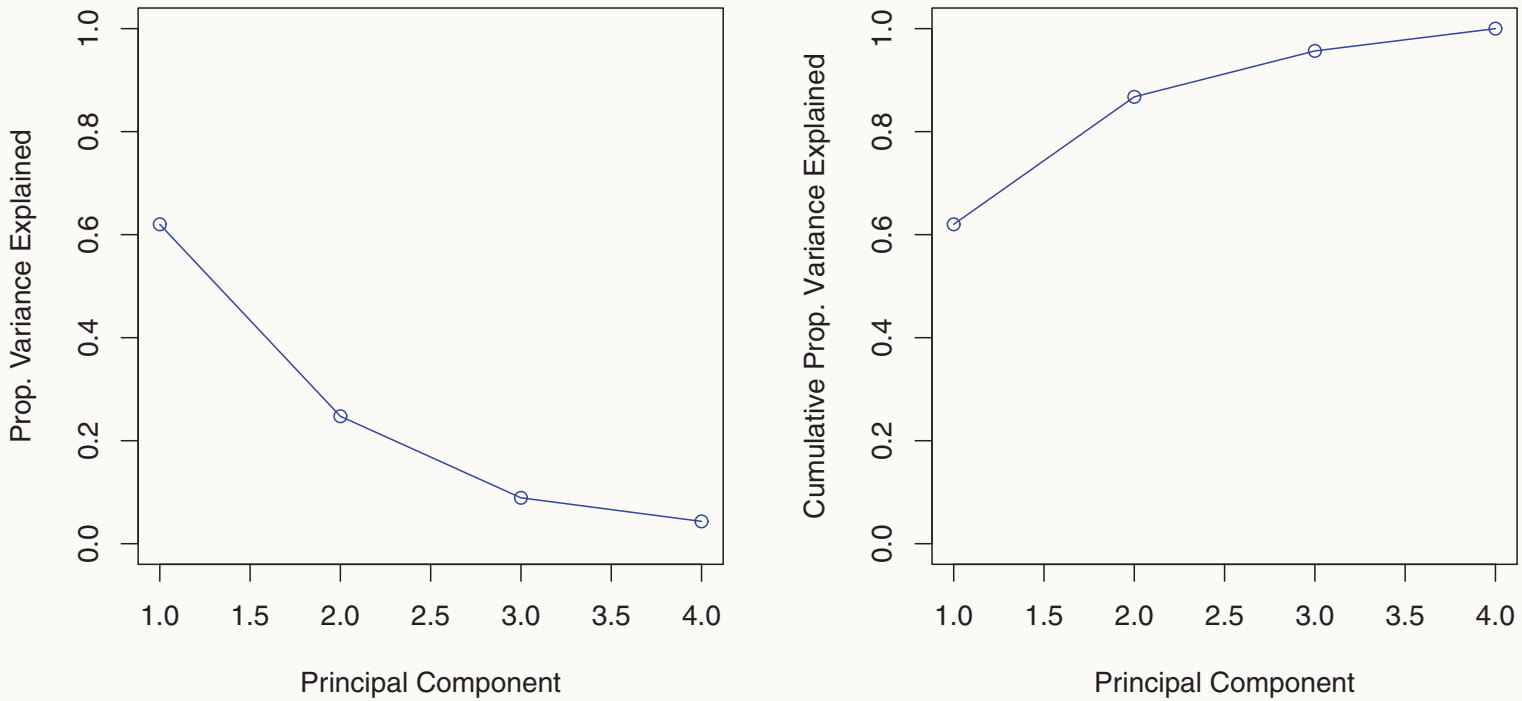
$$\frac{\sum_{i=1}^{n}\left(\sum_{j=1}^{p}\phi_{jm}x_{ij}\right)^2}{\sum_{j=1}^{p}\sum_{i=1}^{n}x_{ij}^2}. \tag{7}$$

- To compute the cumulative PVE of the first M principal components, we can sum (7) over each of the first M PVEs.
- In the US Arrests data, the first principal component explains 62.0% of the variance in the data and the second principal component explains 24.7% of the variance.

The Proportion of Variance Explained

- Together, the first two principal components explain $\approx 87\%$ of the variance and the last two principal components explain only $\approx 13\%$ of the variance.

PVE (scree plot) and cumulative PVE



(Source: James et al. 2013, 383)

How Many Principal Components Should We Use?

- A $n \times p$ data matrix $\mathbf{X}$ has $\min(n-1, p)$ principal components.
- Our goal is to use the smallest number of principal components required to get a good understanding of the data.
- We typically decide on the number of principal components by examining a scree plot (see above).
- We do so by eyeballing the scree plot and looking for an "elbow" in the plot (a point at which the PVE drops off).