Lecture 14: The End

Dimensionality Reduction, Wrapping up

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95-791: Data Mining

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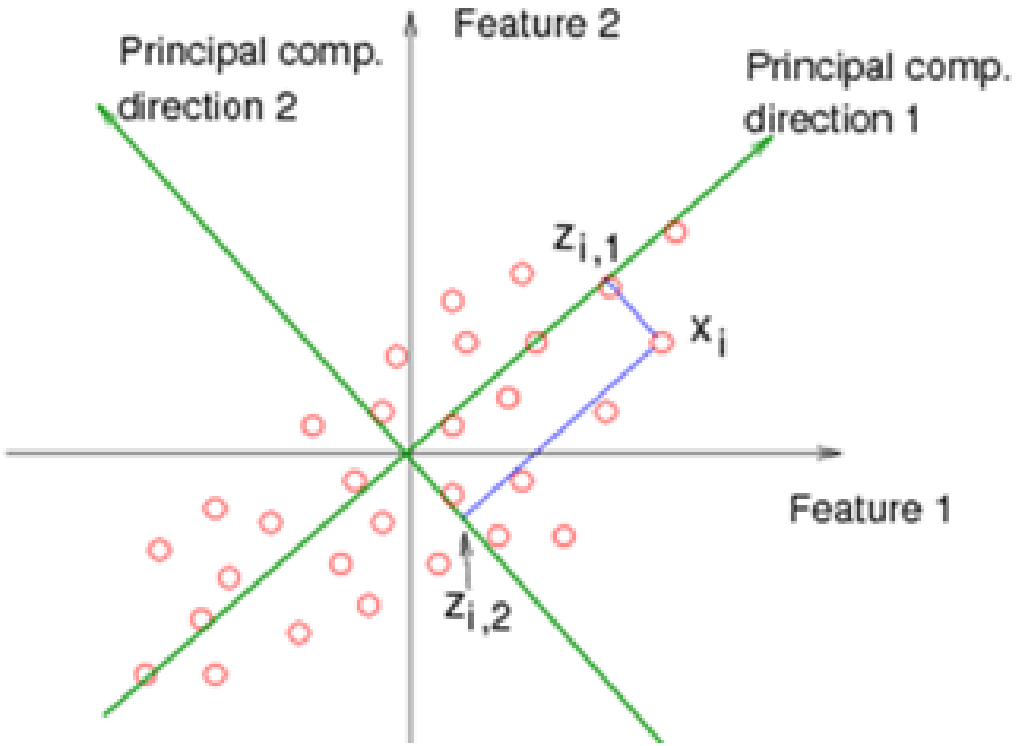
Agenda

- **Dimensionality reduction**
  - Principal Components Analysis [incl limitations]
  - Correspondence analysis
  - Multidimensional scaling
- **Cross-validation pitfalls**
- **Classification with imbalanced data**

A picture



[source: https://onlinecourses.science.psu.edu/stat857]

- This Figure shows an observation $x_i = (x_{i1}, x_{i2})$ along with z_{i1}, its projection onto the first principal component direction, and z_{i2}, its projection onto the second principal component direction

Example: USArrests Data

- `USArrests data`: For each of the $n = 50$ states in the United States, the data set contains the number of arrests per $100{,}000$ residents for each of three crimes: `Assault`, `Murder`, and `Rape`.

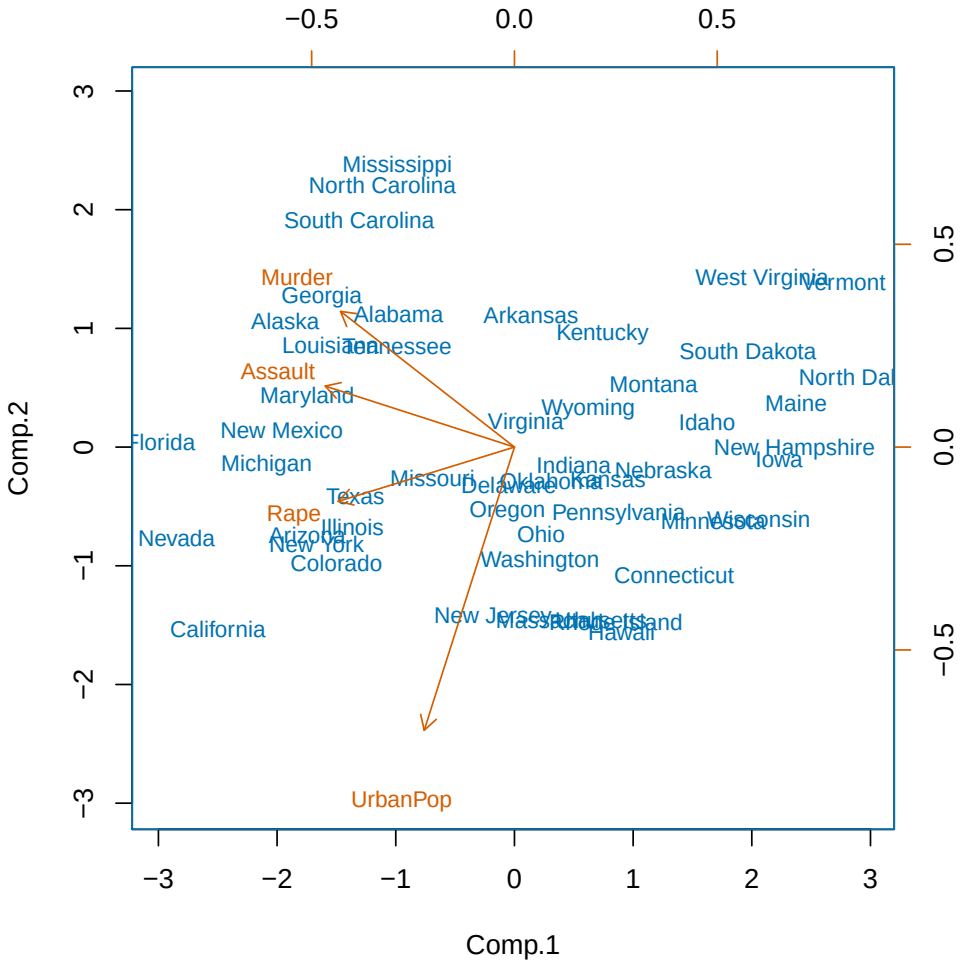
- We also record `UrbanPop`, the percent of the population in each state living in urban areas.

- The principal component score vectors have length $n = 50$, and the principal component loading vectors (directions) have length $p = 4$.

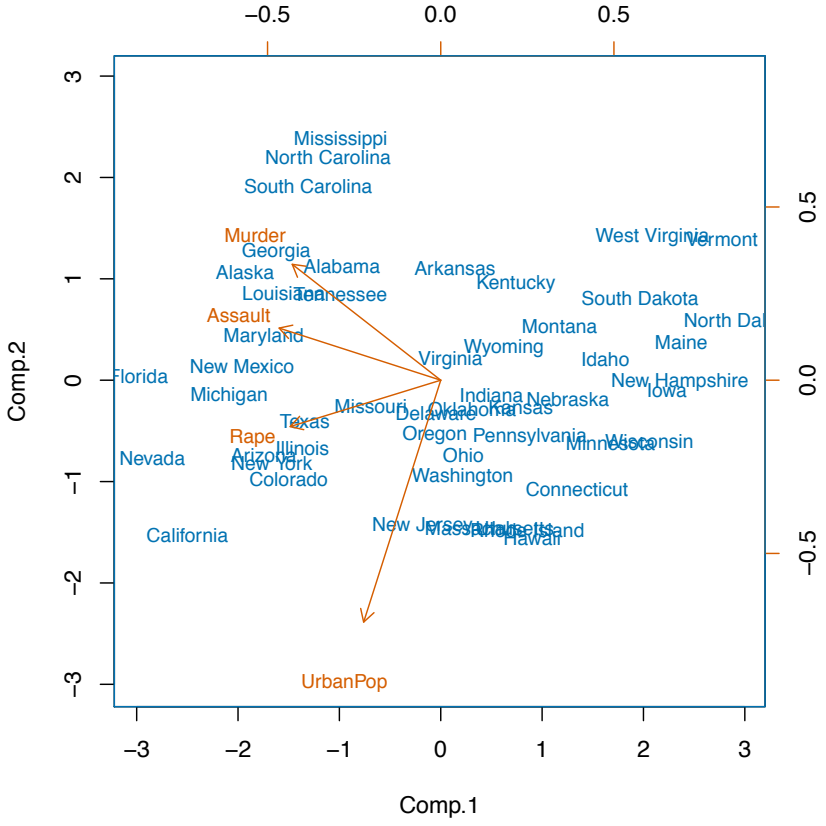
- PCA was performed after standardizing each variable to have mean zero and standard deviation one.
  - Normalization is very important!

USArrests biplot

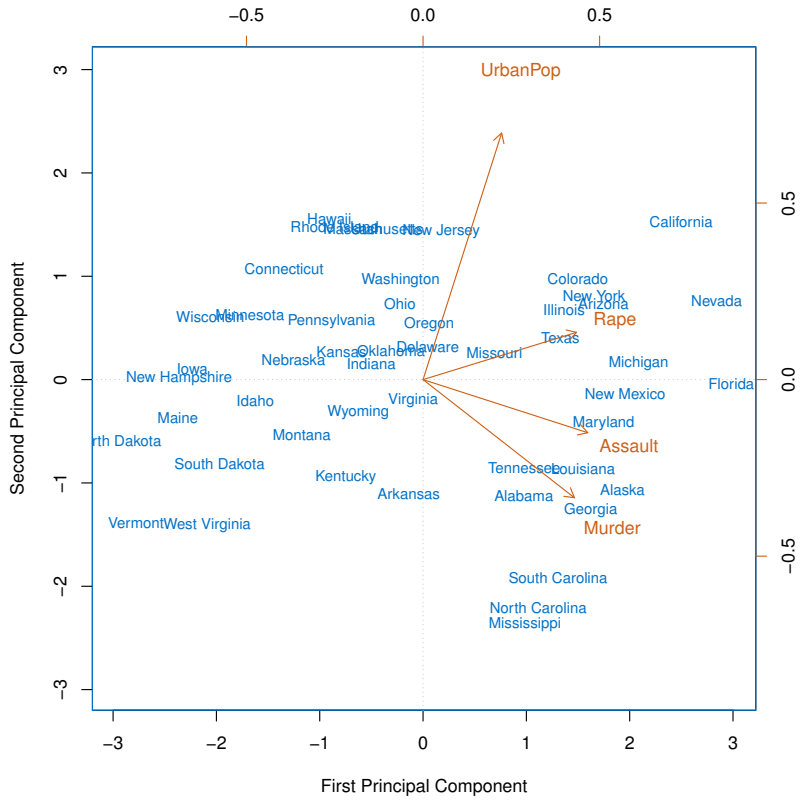
```
arrests.scaled <- scale(USArrests) # Normalize the data
arrests.pca <- princomp(arrests.scaled) # Perform PCA
biplot(arrests.pca, scale = 0) # Construct biplot
```



What happened?



Our biplot



ISL Figure 10.1

- The direction of the arrows and location of the points is now flipped...
- The PCA solution is *non-unique* in this sense: Loading vectors ϕ_1 and $-\phi_1$ will produce the same variance for the scores z_{i1}, but will result in opposite signs.

Let's look at the loadings

Here's what ISL reports for the loadings ϕ_1, ϕ_2:

	PC1	PC2
Murder	0.5358995	-0.4181809
Assault	0.5831836	-0.1879856
UrbanPop	0.2781909	0.8728062
Rape	0.5434321	0.1673186

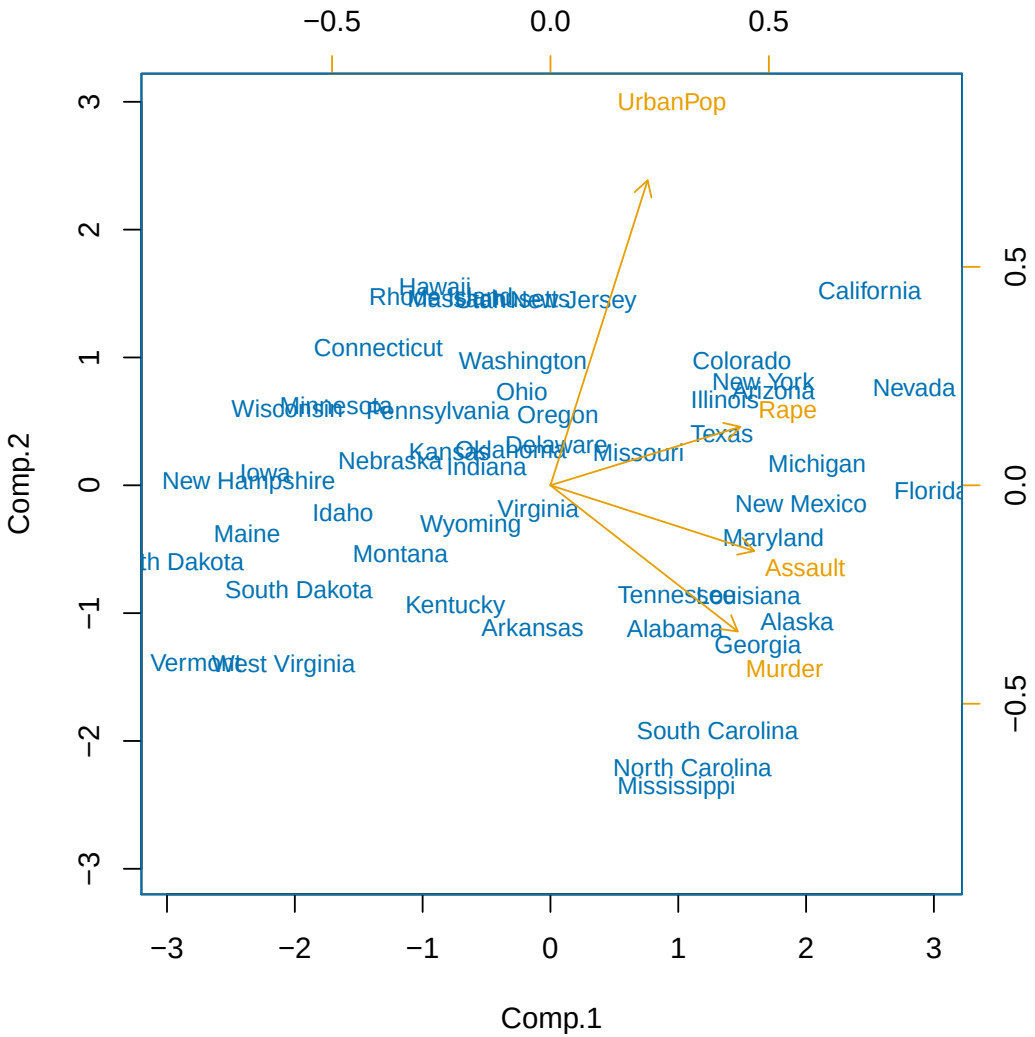
Here's what we got (all 4 loading vectors are shown):

	Comp.1	Comp.2	Comp.3	Comp.4
Murder	-0.53590	0.41818	-0.34123	0.64923
Assault	-0.58318	0.18799	-0.26815	-0.74341
UrbanPop	-0.27819	-0.87281	-0.37802	0.13388
Rape	-0.54343	-0.16732	0.81778	0.08902

- If we flip the sign of all the values in our table, we'll get the same answer as ISL.
- We'll want to flip the signs on the loadings ϕ_j and the scores z_j

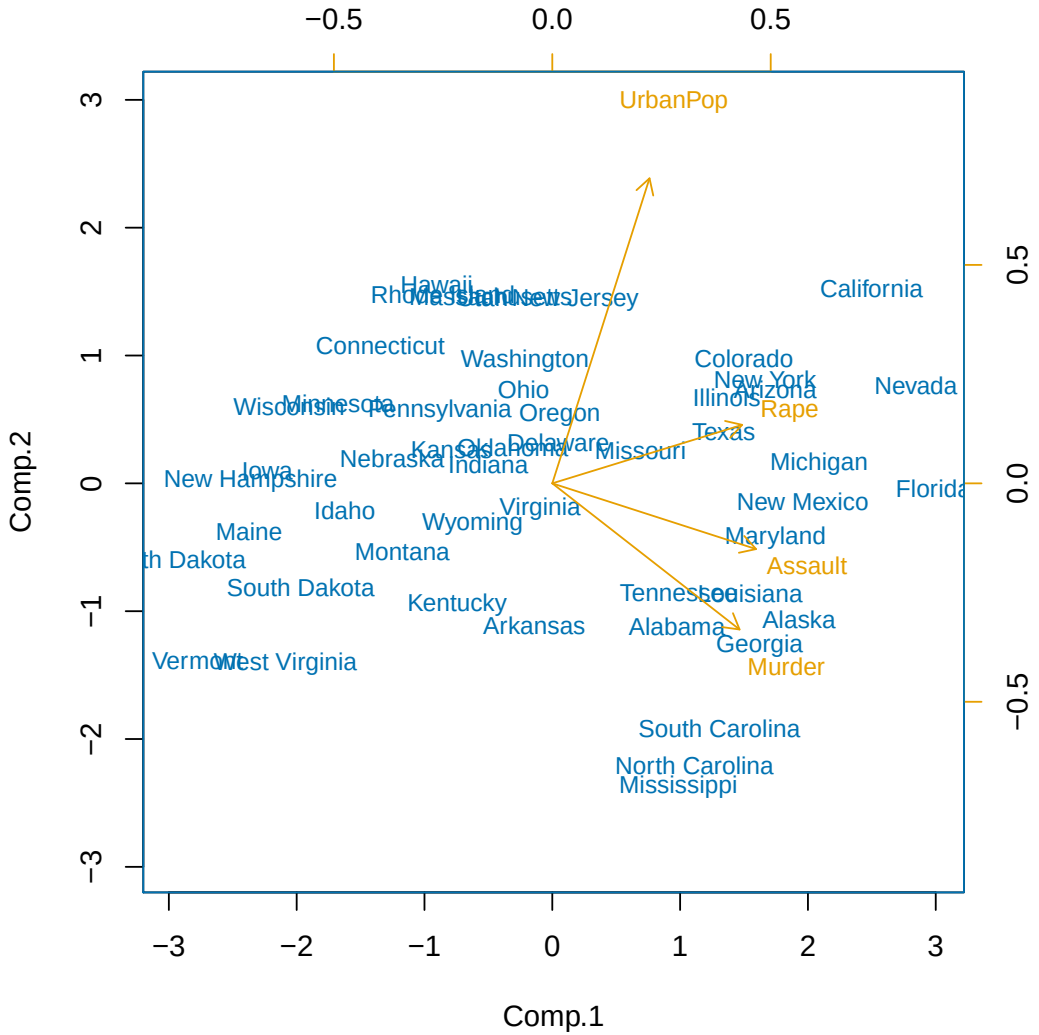
Here's our new biplot

```
arrests.pca$loadings = -arrests.pca$loadings # Flip loadings (phi's)
arrests.pca$scores = -arrests.pca$scores # Flip scores (z's)
biplot(arrests.pca, scale = 0) # Construct biplot
```



Loadings

	ϕ_1	ϕ_2
Murder	0.54	-0.42
Assault	0.58	-0.19
UrbanPop	0.28	0.87
Rape	0.54	0.17



- The word UrbanPop is centered at $(0.28, 0.87)$ (in terms of the top and right side coordinate axes)

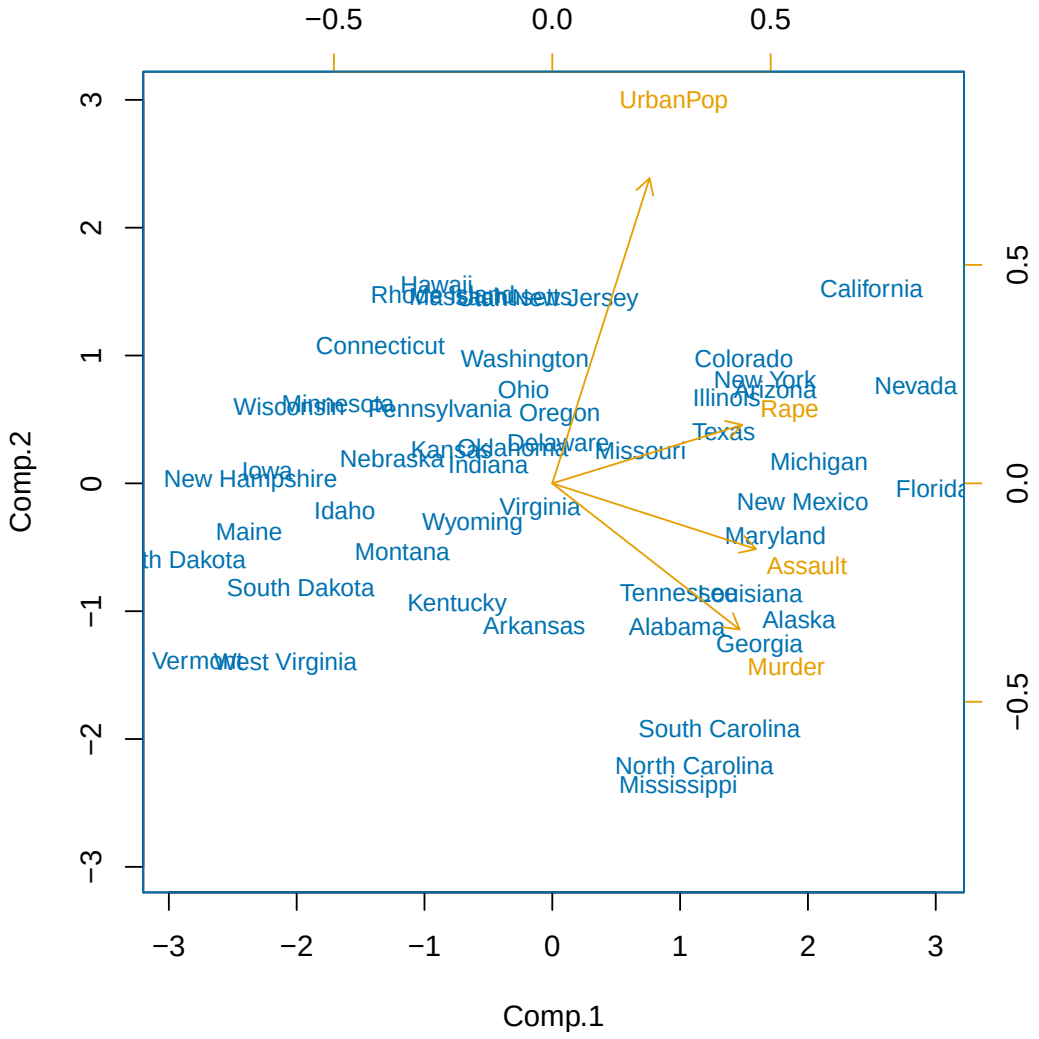
Let's look at the scores (z's)

	Comp.1	Comp.2	Comp.3	Comp.4
Alabama	0.98	-1.12	0.44	-0.15
Alaska	1.93	-1.06	-2.02	0.43
Arizona	1.75	0.74	-0.05	0.83
Arkansas	-0.14	-1.11	-0.11	0.18
California	2.50	1.53	-0.59	0.34
Colorado	1.50	0.98	-1.08	-0.00

- Just like we get 4 loading vectors, we get 4 score vectors.
- The table above shows the scores for all 4 principal components
- The biplot is constructed by plotting the points with Comp.1 on the x-axis and Comp.2 on the y-axis

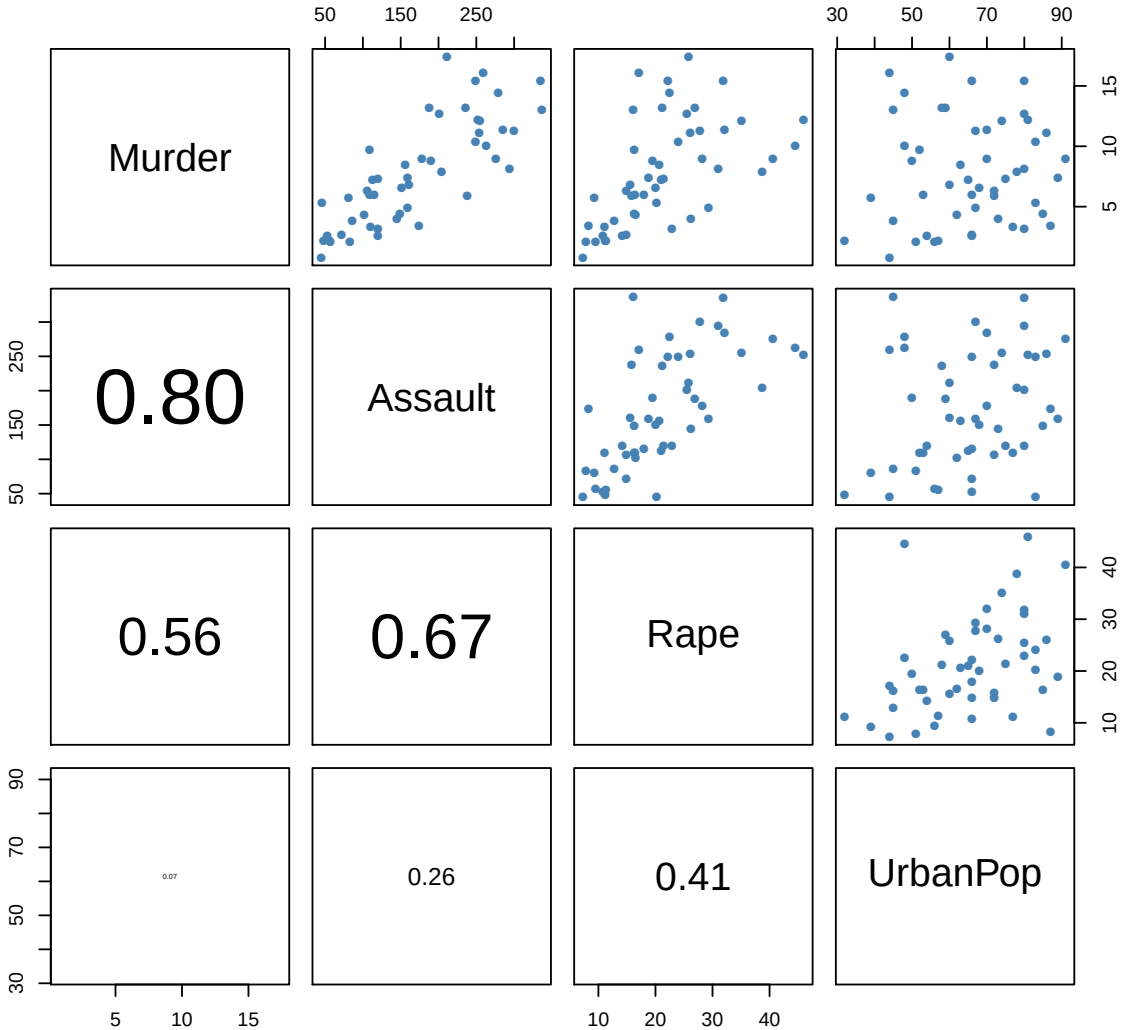
Scores

	Comp.1	Comp.2
Alabama	0.98	-1.12
Alaska	1.93	-1.06
Arizona	1.75	0.74
Arkansas	-0.14	-1.11
California	2.50	1.53
Colorado	1.50	0.98
⋮	⋮	⋮



- The word California is centered at $(2.5, 1.53)$ (in terms of the bottom and left side coordinate axes)

Why does PCA work well on this data?



In this pairs plot we can clearly see that the crime rate variables---`Murder`, `Assault`, and `Rape`---are highly correlated with one another. They provide redundant information. The first loading vector winds up forming a combination of these three features, essentially compressing 3 features into 1.

Proportion Variance Explained

- Dimensionality reduction techniques such as PCA work well when the data is essentially low dimensional
  - i.e., when there are many groups of highly correlated features

- i.e., We may have p features, but we might be able to describe the data with just $k \ll p$ linear combinations of them
  - For instance, if we have data on children, `height`, `weight` and `age` will all be highly correlated
  - PCA will be able to identify a linear combination of these features that we we'll roughly be able to interpret as the child's size

- In general, to understand how well PCA is doing, we look at the proportion of variance explained (PVE) of each principal component.

Proportion Variance Explained

- Assume as usual that all the variables have been centered to have mean 0.
- The total variance present in the data is defined as

$$\sum_{j=1}^{p} \mathrm{var}(X_j) = \sum_{j=1}^{p} \frac{1}{n} \sum_{i=1}^{n} x_{ij}^2$$

  and the variance explained by the mth principal component is

$$\mathrm{var}(Z_m) = \frac{1}{n} \sum_{i=1}^{n} z_{im}^2$$

- The PVE of the mth component is the ratio of these quantities:

$$\mathrm{PVE}(Z_m) = \frac{\mathrm{var}(Z_m)}{\text{total variance}}$$

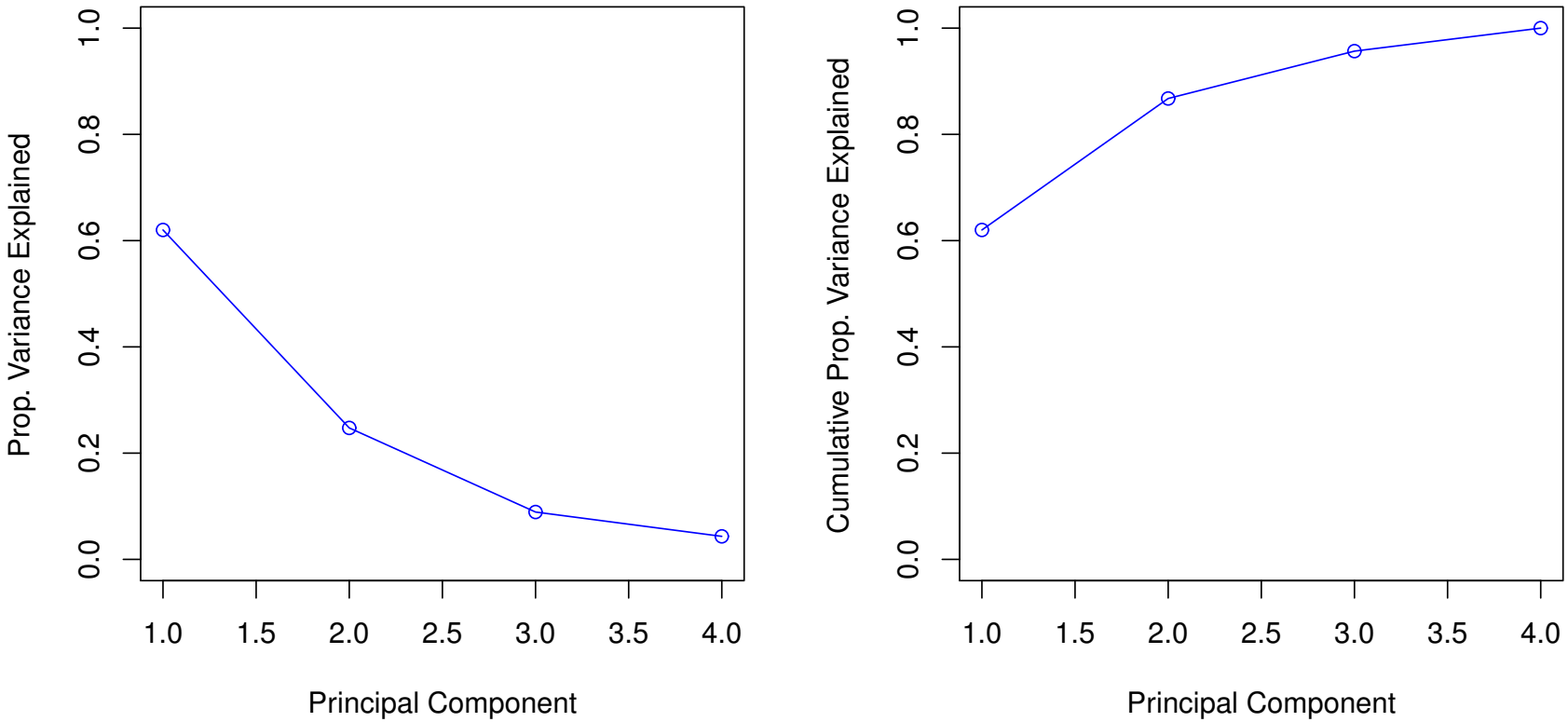


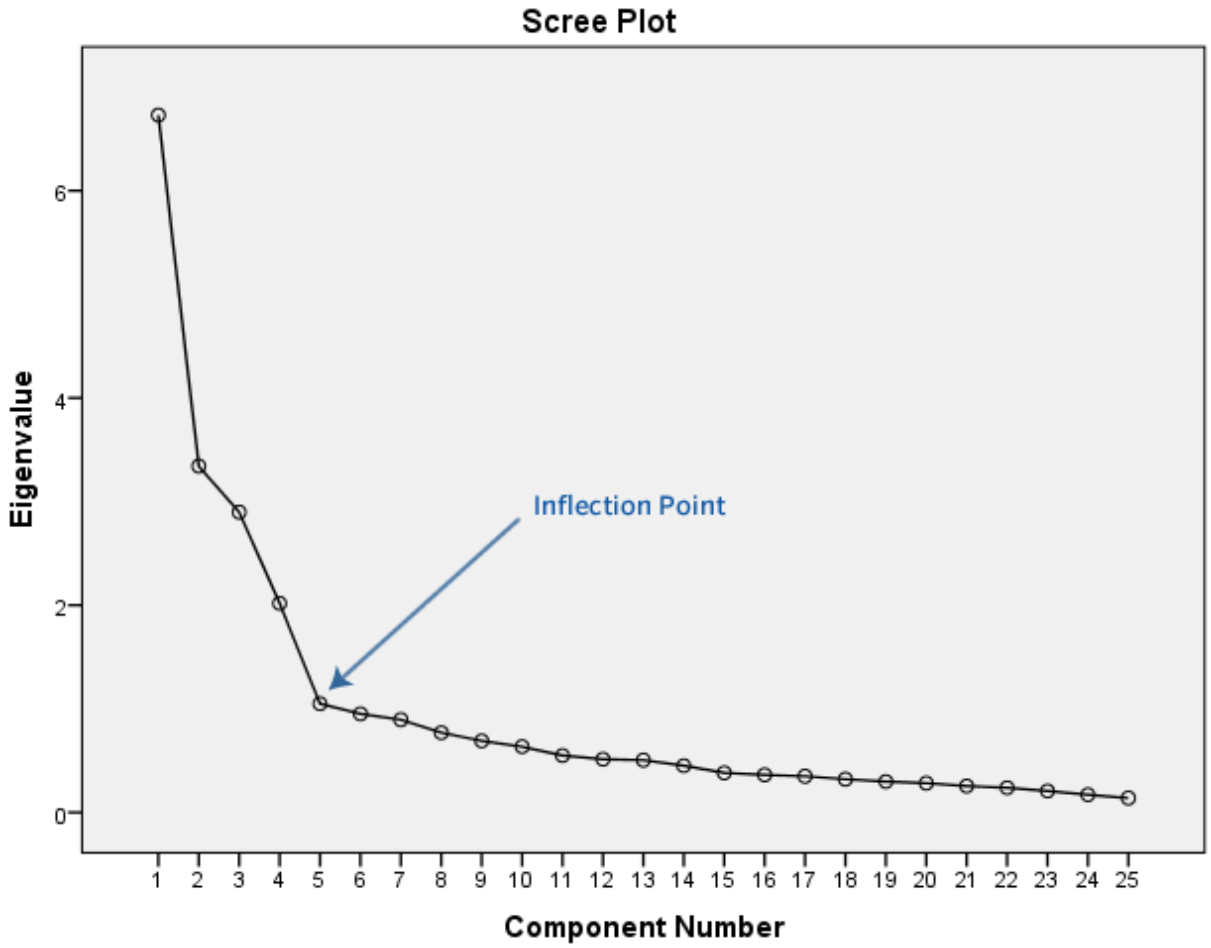
Figure 10.4 from ISL

- Left panel shows $\mathrm{PVE}(Z_m)$ for all 4 principal components in the `USArrests` data
- Right panel shows cumulative PVE: i.e., values of $\sum_{m \leq k} \mathrm{PVE}(Z_m)$ for $k = 1, 2, 3, 4$

How many principal components should we use?

- There's no simple answer to this question
- Cross-validation is not available for this problem
  - CV allows us to estimate test error... but we're doing unsupervised learning here and we don't really have a notion of *test error* to work with
  - If we treated our principal components as *derived features* in a regression or classification task, we could certainly run Cross-validation in that setting
- Often, people like to look at so-called scree plots, which is what we showed on the previous slide

Finding elbows in scree plots



[source: https://gugginotes.wordpress.com/]

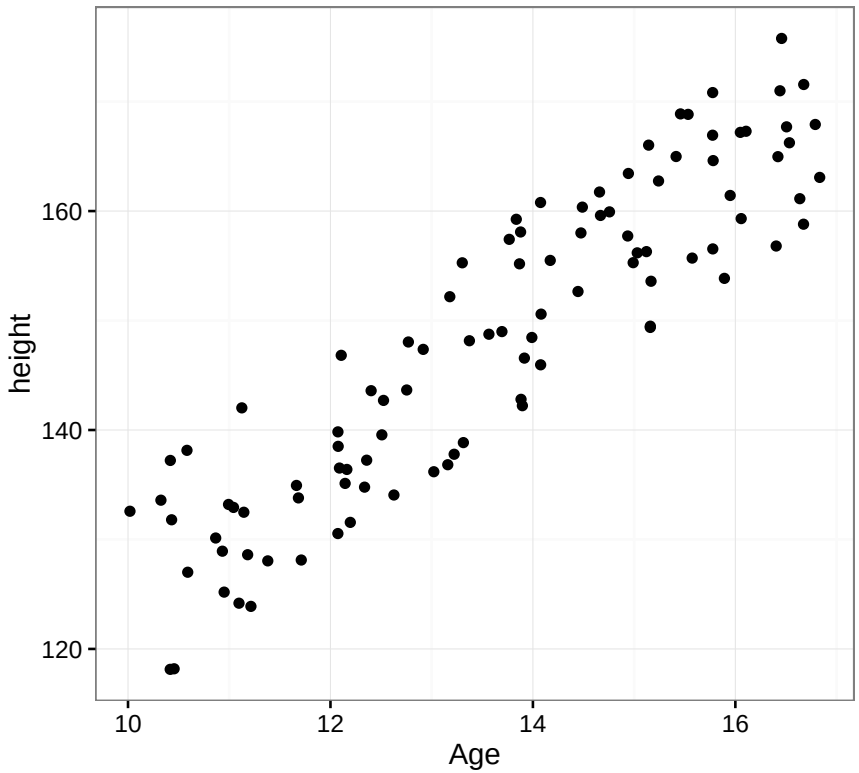
- *Eigenvalue* y-axis label should be interpreted as PVE
- Rule-of-thumb: Stop at the *elbow* in the Scree plot. ($k = 5$ here)

Principal Components Regression

- Suppose we're back in the supervised learning setting where we have observations (x_i, y_i)
- We have a lot of feature (p is large), and we suspect that many of them may be redundant/highly correlated
- We can perform PCA on the data matrix $\mathbf{X}$, treating this as a feature engineering step
- This will give us $k < p$ new features $z_1, \ldots, z_k$, corresponding to the top k principal components
- Then we can model y on $z_1, \ldots, z_k$ instead of on the x_j
- This method is called Principal Components Regression (PCR)
  - Of course, there's a classification version of PCR as well

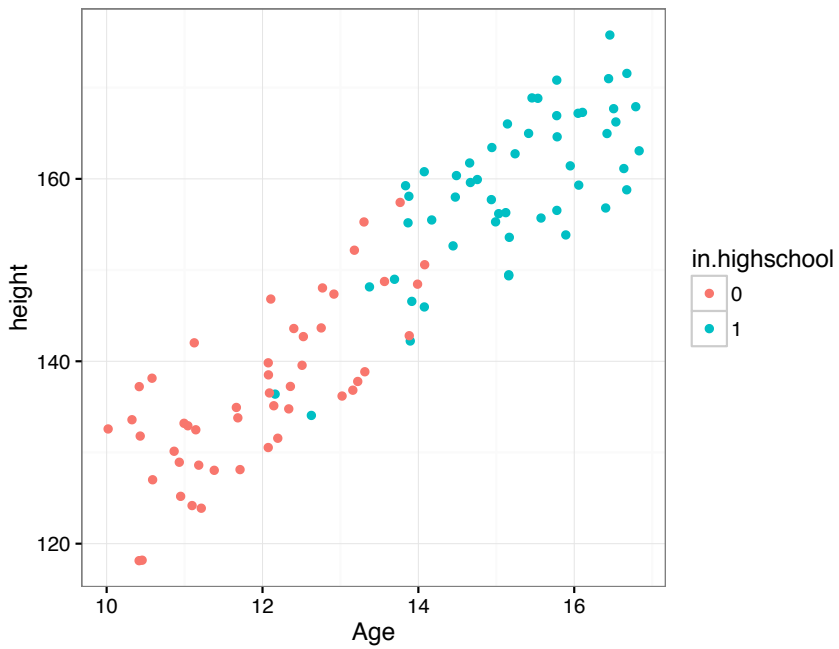
Simple PCR example

- Suppose that we have two features: `age` and `height`
- Everyone in our sample is between 10 and 17 years old, so these features are highly correlated
- Instead of using both features in our models, we could just use the 1st principal component.



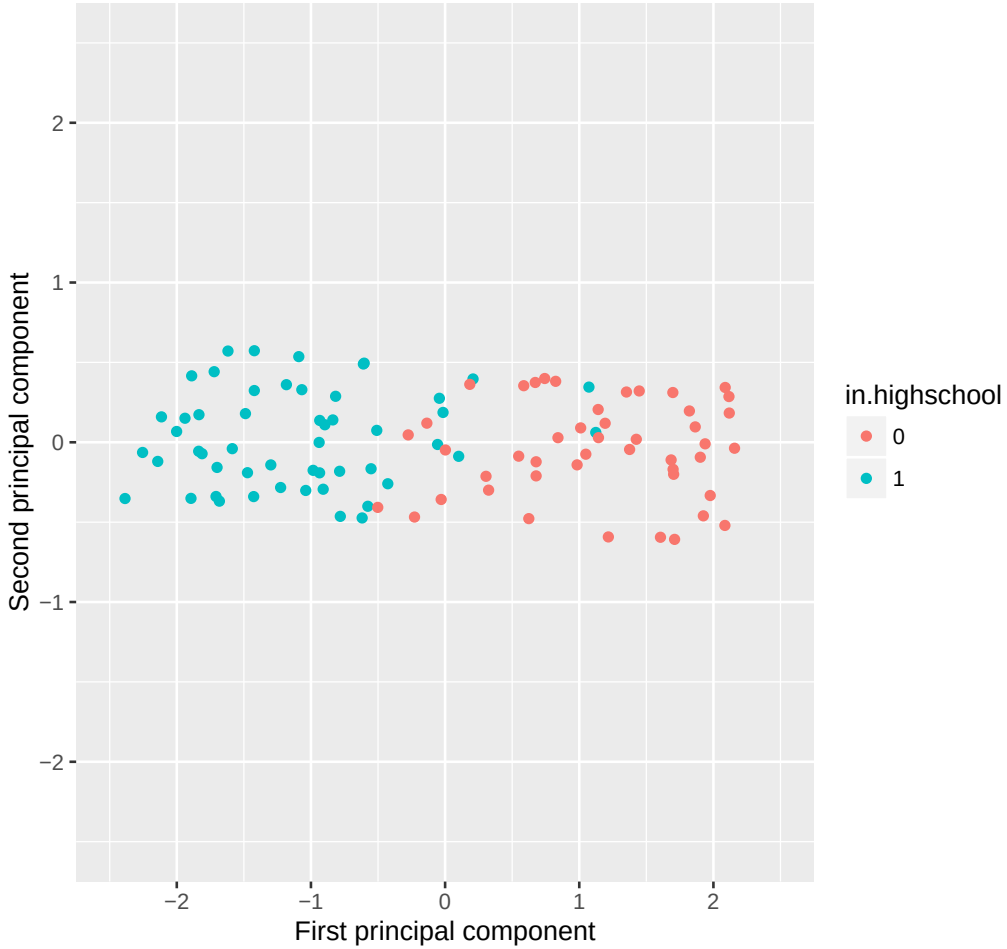
PCR Success case

- Will PCR work? This depends on the outcome, y
- Let's look at a classification setting where $y = 1$ if the individual is in high school, and 0 otherwise.



- Using just the first principal component for classification will work really well here!

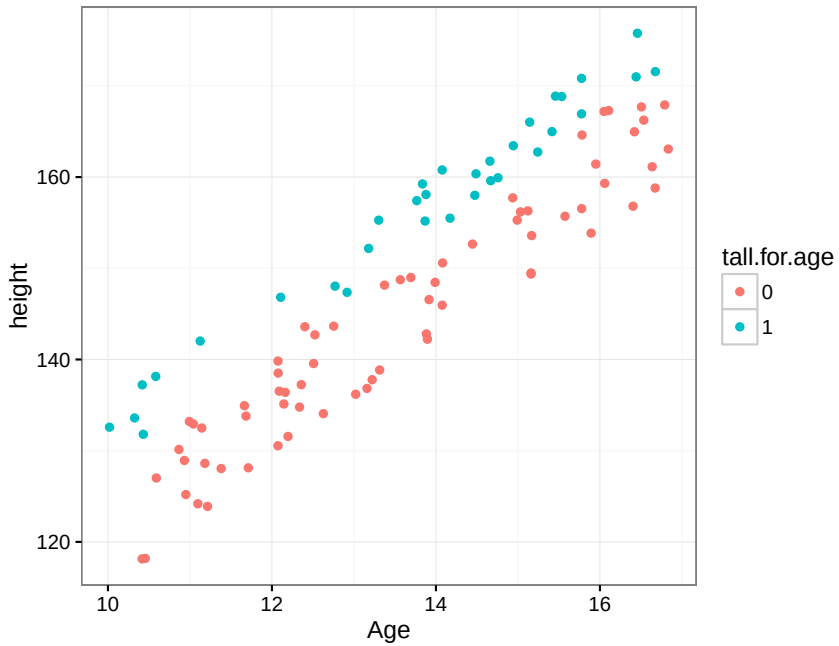
PCR Success case



- This is what the data looks like when plotted in terms of the two principal components
- We can clearly see that a logistic model with $y \sim z_1$ will classify really well

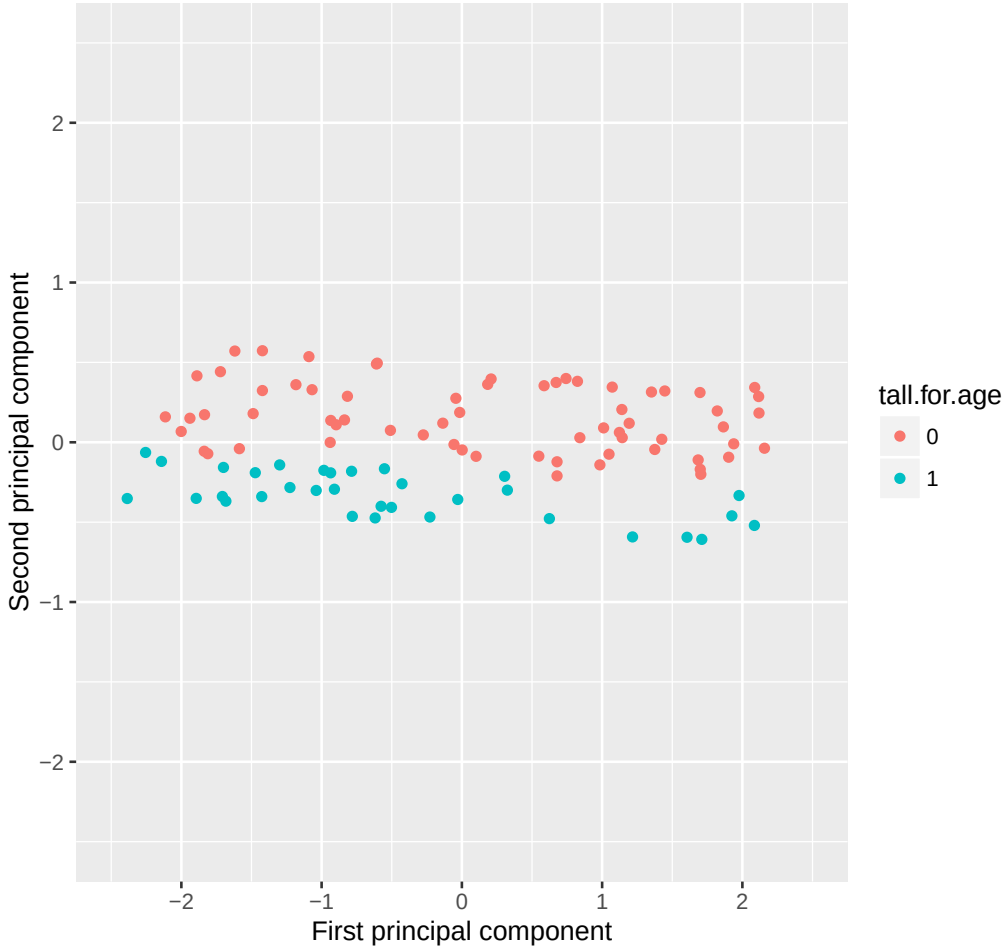
PCR Failure case

- Now what if our outcome was instead $y = 1$ if the person is *tall for their age*, and 0 otherwise.
- Here's a scatterplot of the data, colour-coded by outcome.



- The first principal component is going to be entirely orthogonal to the interesting direction for classification!

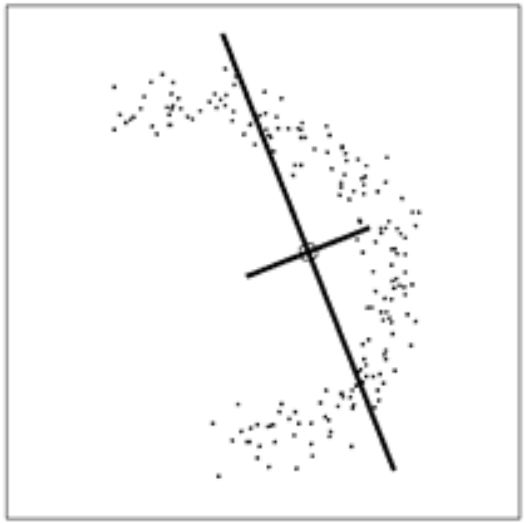
PCR Failure case



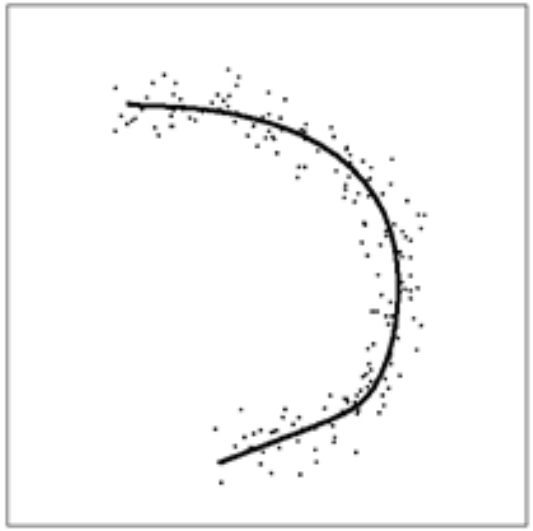
- A logistic model with $\mathrm{y} \sim z_1$ will fail completely!
- Take-away: PCR will work well when the leading principal components define directions that capture variation in the outcome y

PCA captures linear directions of variation

- PCA works well when the relationships between the features are linear (e.g., when features are linearly correlated)
- Shown below is an example where the two axes are clearly strongly associated, but the association is non-linear
- The PCA directions are reasonable... but don't *really* capture the key trend in the data
- Principal curves can be applied in such settings: This method generalizes PCA by fitting 1-dimensional *curves* instead of *lines*



PCA

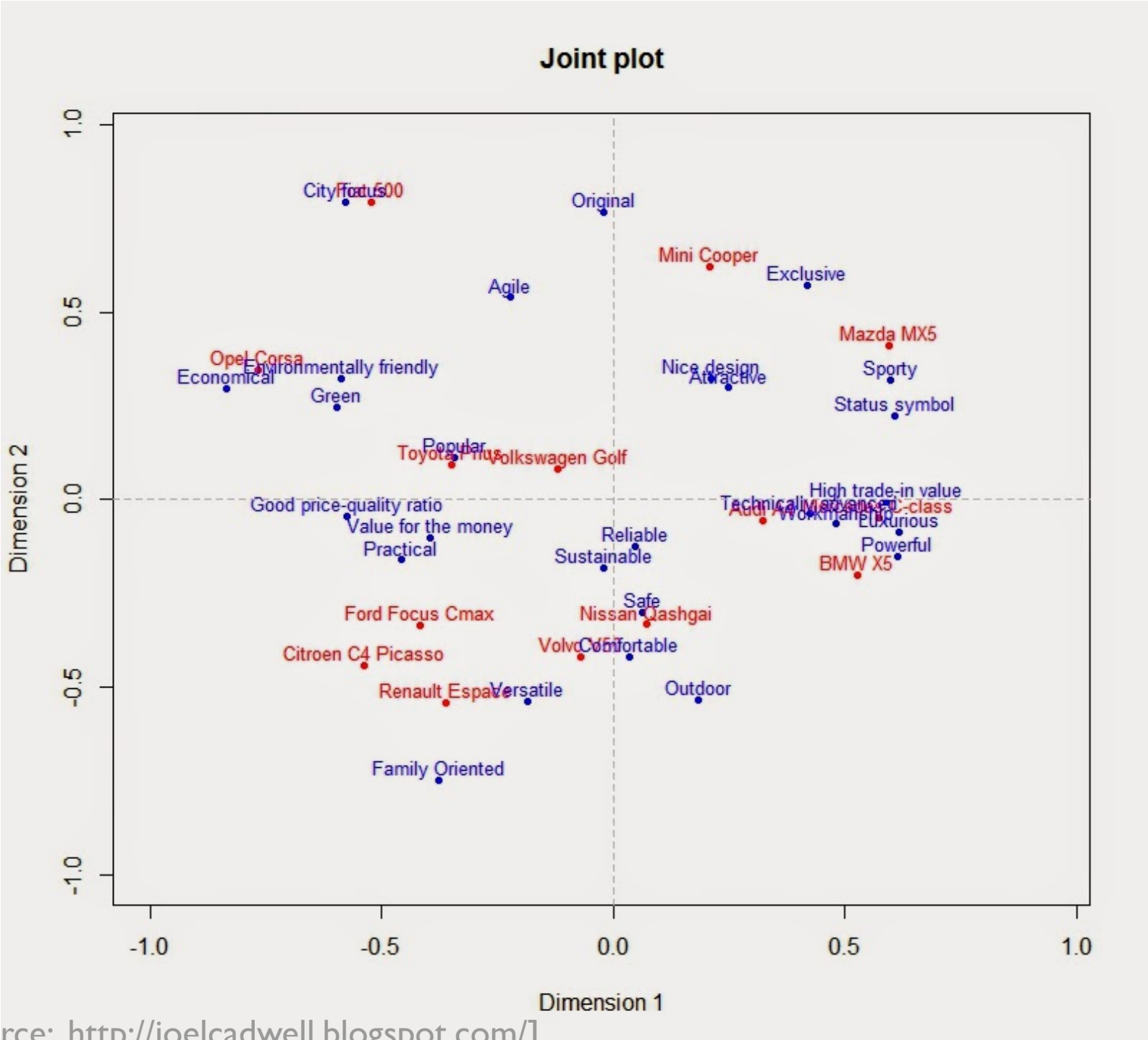


Principal curve

[img source: http://what-when-how.com/]

Correspondence Analysis

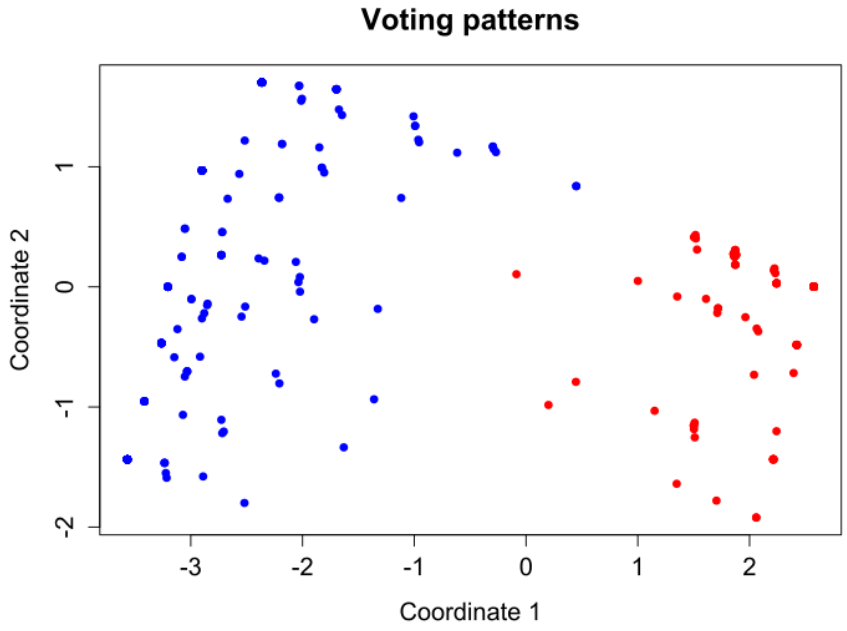
- PCA is great and widely used
- But it's limited to numeric or *ordinal* data
- We may want to perform dimensionality reduction with categorical features
- Correspondence analysis is an extension of PCA that gracefully handles categorical features
- The figure on the next page shows a biplot obtained by running Correspondence analysis on a dataset where consumers were asked to check whether or not they associated particular attributes (blue points) with various car models (red points)



[source: http://joelcadwell.blogspot.com/]

Multidimensional scaling

- Multidimensional scaling (MDS) is a dimensionality reduction methods for visualizing the level of similarity among individuals in a dataset
- Instead of feeding in the data set $\mathbf{X}$, we feed in a distance matrix specifying the pairwise distances between all observations
  - Recall: For hierarchical clustering, we also don't need $\mathbf{X}$. We just operate on the distance matrix
- Here's MDS output from an analysis of voting similarity between Republicans and Democrats (blue) in the house of representatives



Multidimensional scaling: US cities

- Here's an example of what MDS would do if applied to a matrix giving pairwise distances between all of the "major" cities in the US

- Awesome! It doesn't get the right rotation, but we can't expect it to. The reconstruction is otherwise excellent.

Wrapping up

- To wrap up, we'll look at a couple of challenges that commonly arise in real world data

- Topics:
  - Cross-validation: The right way and the wrong way.
  - Classification with imbalanced data

Cross-validation: Right and Wrong

- Suppose we're in a classification setting with $Y \in \{0, 1\}$
- Getting data points is really *expensive*, so we wind up with only $n = 120$ observations
- However, we have *a lot* of features collected on each observation: $p = 5000$
- Fitting a model with $n = 120$ and $p = 5000$ is hopeless, so we take the following approach:
  1. For each of the $p = 5000$ features, calculate the feature's correlation with y. Identify the $q = 100$ predictors that have the highest correlation with the outcome y.
  2. Apply a classifier using just these 100 predictors
- Question: How do we estimate the test error of our classifier?
- Can we apply Cross-validation to just Step 2?

Cross-validation: The wrong way

1. For each of the $p = 5000$ features, calculate the feature's correlation with y. Identify the $q = 100$ predictors that have the highest correlation with the outcome y.

2. Apply a classifier using just these 100 predictors

- It is very wrong to estimate test error by applying Cross-validation just on Step 2
- Doing so would ignore the fact that we *used the y values of the training data in Step 1*
- To get valid error estimates, each step of Cross-validation must go through every part of the model-fitting process that in any way makes use of the outcome variable y
- If we just Cross-validate Step 2, we can easily wind up with a CV error estimate of 0% when the true test error is 50%.

WRONG approach

Step 1

Identify the 100 predictors with the highest value of

$corr(X_j, y)$

Cross-validation

Split data into K folds

For k = 1, 2, ..., K:

-Fit classifier using all the 100 selected predictors on all observations except those in fold k

-Use classifier to predict labels for data in fold k

-Calculate test error on fold k

Return: average test error across all of the folds

RIGHT approach

Cross-validation

Split data into K folds

For k = 1, 2, …, K:

-**Using observations <u>not</u> in fold k, identify the 100 predictors with the highest value of corr(X_j, y)**

-Fit classifier using these 100 selected predictors on all observations except those in fold k

-Use classifier to predict labels for data in fold k

-Calculate test error on fold k

<u>Return</u>: average test error across all of the folds

Classification with imbalanced data

- Suppose that we're trying to identify *fraudulent transactions*
- We build a random forest classifier, and find that it gets 97% accuracy
- Looking back at the data, we see that just 3% of our observations were from fraudulent transactions
- Our random forest got 97% accuracy just by classifying $\hat{y}_i = \texttt{not fraudulent}$ for every observation
- This is an example of imbalanced data
- *Most* classification problems you'll encounter in the real world are imbalanced in this way

Strategies for dealing with imbalanced data

- Stop using *classification accuracy* as your performance metric
  - Instead, assess how well your classifier is doing using more task-relevant metrics: Precision, Recall (Sensitivity), Specificity, PPV, profit

- Artificially improve balance by:
  - Randomly remove instances of your over-represented class (under-sample)
  - Randomly add copies of your under-represented class (over-sample, sampling *with* replacement)
  - Cluster your over-represented observations into a large number of clusters, and select just one representative observation from each class.
  - Create synthetic samples from your under-represented class using a method like SMOTE (Synthetic Minority Over-sampling Technique)

- If using trees or forests: Try growing very deep trees and applying a cost-sensitive pruning technique

Where to go from here?

- We have covered a lot of Data mining methods and concepts in this class
- There is also a lot out there that we didn't get to talk about
- Here's a brief list of things you might be interested in learning more about in the future:
  - Anomaly detection (Outlier detection)
    - If we just get to observe *normally behaved* data, how can we figure out if future observations are anomolous?
    - Approaches: One-class classification, PCA-based and Clustering-based approaches
  - Reinforcement learning:
    - You need to make sequential decisions and learn a good model (a good policy) as you go along.
    - This forces a trade-off between exploration (seeing what happens if you try a *new idea*), and exploitation (going with the best decision according to your current model)
    - E.g., For each customer that browses your site, you need to decide which promos and products to advertise on the landing page. Promos and products change daily, so you need to learn and update your model *on the fly*

More topics

- Text mining
  - Suppose your data set consists of Yelp reviews, and you're trying to use reviews to identify restaurants that are starting to get much better or much worse
  - Key challenge: How can we turn *text* into features?
  - Approaches: Bag-of-words models, TF-IDF representations (term frequency-inverse document frequency), Topic models (Latent Dirichlet Allocation)
- Network analyis
- Recommender systems (e.g., Collaborative filtering)
- Other cool methods
  - Support vector machines (maximum-margin classifiers)
  - Neural networks (lately: Deep learning)
  - Graphical models, Bayes networks…

Acknowledgements

All of the lectures notes for this class feature content borrowed with or without modification from the following sources:

- 36-462/36-662 Lecture notes (Prof. Tibshirani, Prof. G'Sell, Prof. Shalizi)
- 95-791 Lecture notes (Prof. Dubrawski)
- *An Introduction to Statistical Learning, with applications in R* (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani
- *Applied Predictive Modeling*, (Springer, 2013), Max Kuhn and Kjell Johnson