Lecture 28: Review

Reading: All chapters in ISLR.

STATS 202: Data mining and analysis

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Announcements

- The Kaggle winners will be emailed today shortly after 4pm!
- Confusion about Kaggle rules:
  - Kaggle allows 2 submissions per day, and each day runs from 4pm to 4pm.
  - Some people who made 2 submissions late yesterday expected to get extra submissions today before the winners are chosen. Unfortunately, this won't be possible.
  - However, you can make submissions until Friday, which will count for the 5% credit (and perhaps bragging rights).
- Remember to submit Homework 8 by Friday.

Unsupervised learning

- In unsupervised learning, all the variables are on equal standing, no such thing as an input and response.
- **Two sets of methods:**
  1. PCA: find the main directions of variation in the data
  2. Clustering: find meaningful groups of samples
     - Hierarchical clustering (single, complete, or average linkage).
     - K-means clustering.

PCA

1. Find the linear combination of variables

$$\theta_{11}X_1 + \theta_{12}X_2 + \cdots + \theta_{1p}X_p$$

   with $\sum_i \theta_{1i}^2 = 1$, which has the largest variance.

2. Find the linear combination of variables

$$\theta_{21}X_1 + \theta_{22}X_2 + \cdots + \theta_{2p}X_p$$

   with $\sum_i \theta_{2i}^2 = 1$ and $\theta_1 \perp \theta_2$, which has the largest variance.

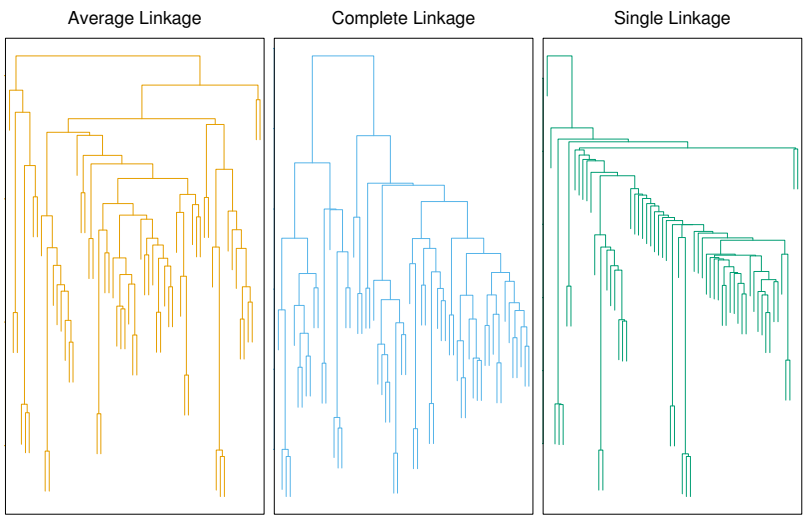
3. ...

- What is a biplot, how is it interpreted?
- What is the proportion of variance explained? A scree plot?
- What is the effect of rescaling variables?

K-means clustering

- The number of clusters is fixed at K.
- Goal is to minimize the average distance of a point to the average of its cluster.
- The algorithm starts from some assignment, and is guaranteed to decrease this average distance.
- This find a local minimum, not necessarily a global minimum, so we typically repeat the algorithm from many different random starting points.

Hierarchical clustering



- Agglomerative algorithm produces a *dendrogram*.
- At each step we join the two clusters that are "closest":
  - **Complete:** distance between clusters is maximal distance between any pair of points.
  - **Single:** distance between clusters is minimal distance.
  - **Average:** distance between clusters is the average distance.
- Height of a branching point = distance between clusters joined.

Supervised learning

Now, we have a response variable y_i associated to each vector of predictors x_i.

Two classes of problem:

- Regression: y_i is numerical

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

- Classification: y_i is categorical

$$0-1 \text{ loss} = \sum_{i=1}^{n}\mathbf{1}(y_i \neq \hat{y}_i).$$

Training vs. test error

Both the MSE for regression, and the 0-1 loss for classification can be computed:

1. On the training data.
2. On an independent test set.

We want to minimize the error on a very large test set which is sampled from the same process as the training data. This is called the *test error*.

Bias-variance decomposition

Consider a regression method, which given some data $(x_1, y_1), \ldots, (x_n, y_n)$ outputs a prediction $\hat{f}(x)$ for the regression function.

If we think of the training data as coming from some distribution, then the function $\hat{f}$ can be considered a random variable as well.

The expected test MSE of $\hat{f}$ has the following decomposition for any fixed x:

$$E([\hat{f}(x) - f(x)]^2) = \underbrace{E([\hat{f}(x) - E\hat{f}(x)]^2]}_{\text{Var}(\hat{f}(x)) > 0} + \underbrace{[E(\hat{f}(x) - f(x))]^2}_{\text{Square bias of } \hat{f}(x). > 0} + \text{Var}(\epsilon)$$

Variance: Increases with the flexibility of the model
Bias: Decreases as the flexibility of the model increases

How do we estimate the test error?

- Our main technique is cross-validation.
- Different approaches:
  1. **Validation set:** Split the data in two parts, train the model on one subset, and compute the test error on the other.
  2. k-**fold:** Split the data into k subsets. Average the test errors computed using each subset as a validation set.
  3. **LOOCV:** k-fold cross validation with $k = n$.
- No approach is superior to all others.
- What are the main differences? How do the bias and variance of the test error estimates compare? Which methods depend on the random seed?

The Bootstrap

- **Main idea:** If we have enough data, the empirical distribution is similar to the actual distribution of the data.
- Resampling with replacement allows us to obtain pseudo-independent datasets.
- They can be used to:
  1. Approximate the standard error of a parameter (say, β in linear regression), which is just the standard deviation of the estimate when we repeat the procedure with many independent training sets.
  2. **Bagging**: By averaging the *predictions* $\hat{y}$ made with many independent data sets, we eliminate the variance of the predictor.

Regression methods

- Nearest neighbors regression
- Multiple linear regression
- Stepwise selection methods
- Ridge regression and the Lasso
- Principal Components Regression
- Partial Least Squares
- Non-linear methods:
  - Polynomial regression
  - Cubic splines
  - Smoothing splines
  - Local regression
  - GAMs: Combining the above methods with multiple predictors
- Decision trees, Bagging, Random Forests, and Boosting

Classification methods

- Nearest neighbors classification
- Logistic regression
- LDA and QDA
- Stepwise selection methods
- Decision trees, Bagging, Random Forests, and Boosting
- Support vector classifier and support vector machines

Self testing questions

For each of the regression and classification methods:

1. What are we trying to optimize?
2. What does the fitting algorithm consist of, roughly?
3. What are the tuning parameters, if any?
4. How is the method related to other methods, mathematically and in terms of bias, variance?
5. How does rescaling or transforming the variables affect the method?
6. In what situations does this method work well?