

Lecture 28: Review

Reading: Relevant chapters in ISLR.

STATS 202: Data mining and analysis

Jelena Markovic

slide credits: Sergio Bacallado

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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

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

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- ▶ What is the effect of rescaling variables?

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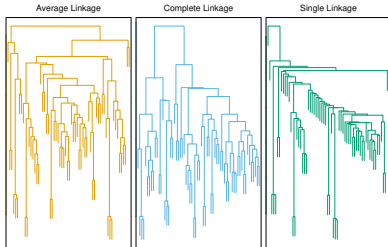
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- ▶ Goal is to minimize the average distance of a point to the average of its cluster.
- ▶ The algorithm starts from some assignment, and is guaranteed to decrease this average distance.
- ▶ This find a local minimum, not necessarily a global minimum, 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.

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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

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

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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

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

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

Variance: Increases with the flexibility of the model

Bias: Decreases as the flexibility of the model increases

Regression methods

- ▶ Nearest neighbors regression
- ▶ Multiple linear regression

Classification methods

- ▶ Nearest neighbors classification
- ▶ Logistic regression
- ▶ LDA and QDA

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5. How does rescaling or transforming the variables affect the method?
6. In what situations does this method work well? What are its limitations?

Evaluating a classification method

We have talked about the 0-1 loss:

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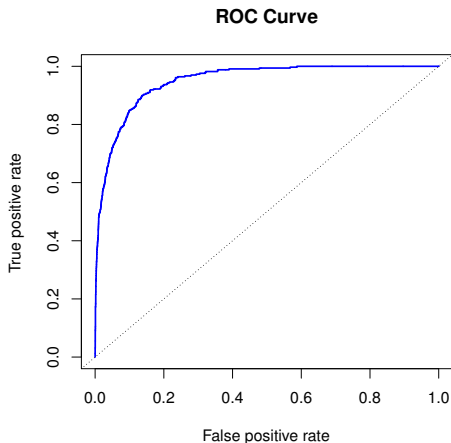
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A much more informative summary of the error is a **confusion matrix**:

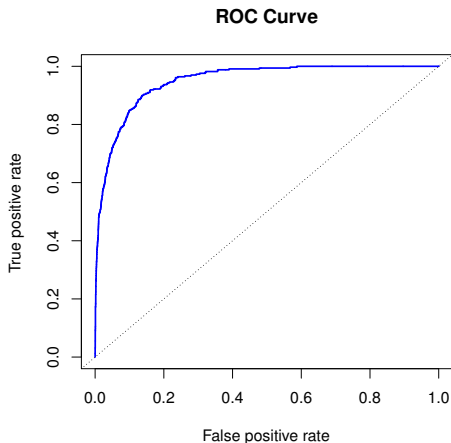
		<i>Predicted class</i>		
		– or Null	+ or Non-null	Total
<i>True class</i>	– or Null	True Neg. (TN)	False Pos. (FP)	N
	+ or Non-null	False Neg. (FN)	True Pos. (TP)	P
	Total	N*	P*	

The ROC curve



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The ROC curve



- ▶ Displays the performance of the method for any choice of threshold.
- ▶ The area under the curve (AUC) measures the quality of the classifier:
 - ▶ 0.5 is the AUC for a random classifier
 - ▶ The closer AUC is to 1, the better.

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- ▶ 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 datasets mimicing how original data was selected.