STA 141A Lecture 18a | ISLR 2.1, 2.2 | 2018年11月29日

Efficiency TARP 14

- Statistical Models & Machine Learning
  - So far mostly visualization and point statistics.
  - Modeling is another important part of EDA.
  - Other classes cover theory of models, so here the focus is implementation.
  - We saw performance was an issue for HW 5 with text; it can also be an issue with fitting models.
  - The basic idea of modeling is that we have some inputs $X_1, X_2, \dots$ and we want to predict or understand an output Y.

Tradeoff!

$$Y = f(X_1, X_2, \dots) + \varepsilon$$

ε ← error term

$$\hat{Y} = \hat{f}(X_1, X_2, \dots)$$

- Training Set

Test Set

X_{11}	Y_1
X_{21}	Y_2
$\vdots$	$\vdots$

$n =$ number of observations

Y: response, dependent

X: feature, predictor, independent

- Parametric vs non-parametric
  - Parametric models assume a shape form for f, then estimate parameters
  - Non-parametric models do not assume a shape for f, but do assume other properties, like smoothness. More obs needed
- Supervised (response) vs unsupervised (no response)
- Regression vs classification

- We use mean squared error to measure error in regression models:

$$\frac{1}{n}\sum_{i=1}^{n}\left(y_i-\hat{f}(x_i)\right)^2$$

Other measurements are possible and can change how the model fits.

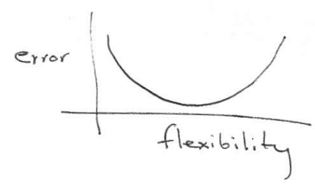
- We care about test error, not training error! This is where $\boxed{\text{overfitting}}$ can be a problem. } Revisit in CV example

- Bias-variance tradeoff:

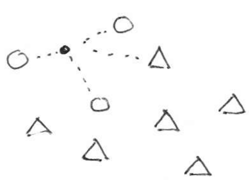
$$\mathbb{E}\left(y_0-\hat{f}(x_0)\right)^2 = \underbrace{Var\left(\hat{f}(x_0)\right)}_{\text{model variance}} + \underbrace{\left[Bias\left(\hat{f}(x_0)\right)\right]^2}_{\text{model bias}} + \underbrace{Var(\varepsilon)}_{\text{error variance}}$$

Variance — how $\hat{f}$ changes with different train set
Bias — error due to approximation

bias, inference $\longleftrightarrow$ variance, flexibility



- k-nearest neighbors



Use k-nearest training points to predict class

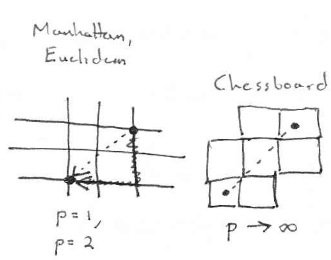
Ties!

$$\mathbb{P}\left(Y_\bullet=\Delta \mid X_{1\bullet}=x_{10}, X_2=x_{30}\right)=\frac{\#\,\Delta}{k}$$

Bayes classifier approximation

The choice of k makes a difference!
Similarly, how we measure distance makes a difference!

- Minkowski distances:
  - Euclidean $p=2$
  - Manhattan $p=1$



$$\left(\sum_{i=1}^{n}|a_i-b_i|^p\right)^{1/p} \qquad p\geq 1$$

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- How to actually implement kNN?
  - What are the inputs? The outputs?

    Input: $x_1, x_2, \ldots$ predictors
    k number of neighbors
    $\{(x,y)_i\}$ training set

    Output: $\hat{y}_0$ predicted label

  - So what are the steps?

    1. Find k nearest neighbors to x_0
       - How do we tell which points are "near"?
       - Compute distances, find smallest distances
         dist() sort() order()
    2. Use neighbor labels to "vote"
       table()
       - Break ties
         sample()
    3. Return "winning" label

- Is kNN "fast"?
- Is kNN flexible? Where is bias-variance tradeoff?

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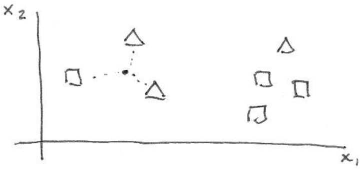
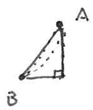
- References: ISLR 2, 5.1 / TARP 8, 14
- 5-min reminder of kNN



- Minkowski distance

$$\left(\sum_{i=1}^{d} |a_i - b_i|^p \right)^{1/p} \quad p \geq 1$$



Effect of k on model flexibility

- How to implement kNN?

predict_knn()

Inputs: new point, train points, k, metric

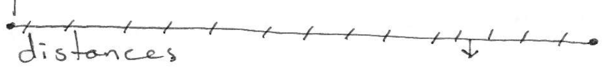
Outputs: class label

Steps:

Find:

1. Compute distances from new point(s) to all train points — dist(), as.matrix()

For each new point



2. Sort/order distances — order()
3. Take top k train points — [ ]

Vote:

4. Count classes for top k points — table()
5. Return winning class, possibly breaking ties. — which.max() / max()

Break the voting step (including ordering) into a separate function.

apply(new_points, 1, vote) ...

- Error rates: how can we tell how well the model works?

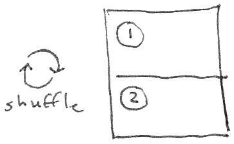
$$\sum \frac{\text{actual == pred}}{\text{total}}$$

Fit on train → predict on train → underestimate

Fit on train → predict on test → Why not use test to train?

* Cross-validation (m-fold) *

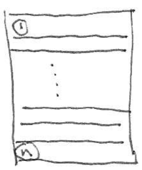
Idea: fit multiple times and average



Iteration	1	2
Train	1	2
Test	2	1
Error	e_1	e_2

$$\hat{e} = \frac{e_1 + \dots + e_m}{m}$$

Two folds doesn't give us much to average.
Error rate will vary depending on how we choose folds, and model doesn't get to see all the data } High bias



n error estimates Leave-one-out CV

Train all others
Test 1 2 ... n

Now we have to fit the model n times — not feasible for large n or slow model.
Estimates are highly dependent! → high variance

Usually we compromise and use $m = 5$ or $m = 10$

* Error rates

Bias - variance tradeoff

* How to implement CV?

cv_error_knn()

Inputs: m, train set, k, metric

Outputs: CV error estimate

Steps:

1. Shuffle the rows or sample row ids. sample()
2. Split rows into folds. rep() split()
3. Loop over test folds; remaining are train folds
   a. Fit model on train folds
   b. Predict for test fold
   c. Compute error rate
4. Return average of error rates. mean()

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- Cross-validation (Lecture 19)
- Implementing CV (Lecture 19)
- Performance considerations for CV
  - Compute distances within training set once, <u>before</u> looping over the folds
  - Split row indexes instead of actual observations, and look up appropriate rows (distances) for each fold
- Recap designing functions / ideas to code:
  - List inputs, outputs, and steps — This requires careful thought
  - Draw pictures or make simple examples of the problem. Work these out by hand
  - Divide-and-conquer: complicated steps can be written as separate functions
  - Test on simple/small examples first
- Function examples?

  dist() order() table() split()
  sample() rep() indexing
- Where to go from here?
  - STA 141B focuses on collecting data, interactive visualizations, and uses Python
  - STA 141C focuses on programming for statistics and uses R (possibly with some C)
  - STA 135/108
  - ECS 171 machine learning