Model Optimization

http://shorelinechurch.org/wp-content/uploads/2014/10/Level-Up-DS.jpg

Bias and Variance

$$\mathrm{E}\left[\left(y-\hat{f}\left(x\right)\right)^2\right]=\mathrm{Bias}\left[\hat{f}\left(x\right)\right]^2+\mathrm{Var}\left[\hat{f}\left(x\right)\right]+\sigma^2$$

$$\mathrm{Bias}\left[\hat{f}\left(x\right)\right]=\mathrm{E}\left[\hat{f}\left(x\right)-f(x)\right]$$

$$\mathrm{Var}\left[\hat{f}\left(x\right)\right]=\mathrm{E}[\hat{f}\left(x\right)^2]-\mathrm{E}[\hat{f}\left(x\right)]^2$$

In other words:

Error = (Expected Loss of Accuracy)^2 + Flexibility of model + Irreducible error

https://en.wikipedia.org/wiki/Bias%E2%80%93variance_tradeoff

Question:

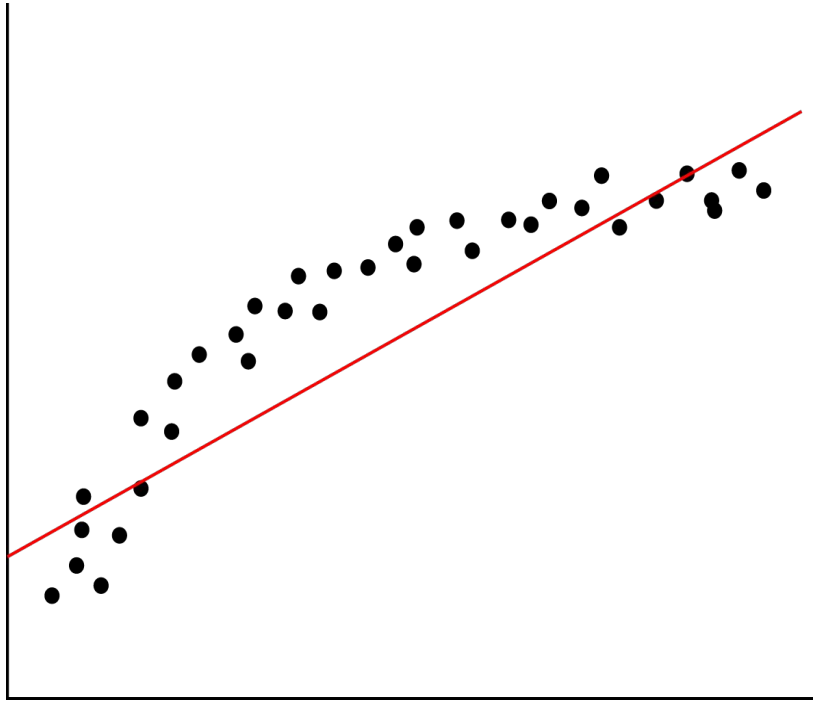
Why would there be a trade-off between bias and variance?

Underfitting

Causes:

1) Lack of relevant variables/factor
2) Imposing severely limiting assumptions
    a) Linearity
    b) Assumptions on distribution
    c) Wrong values for parameters

High Bias and **Inflexible**

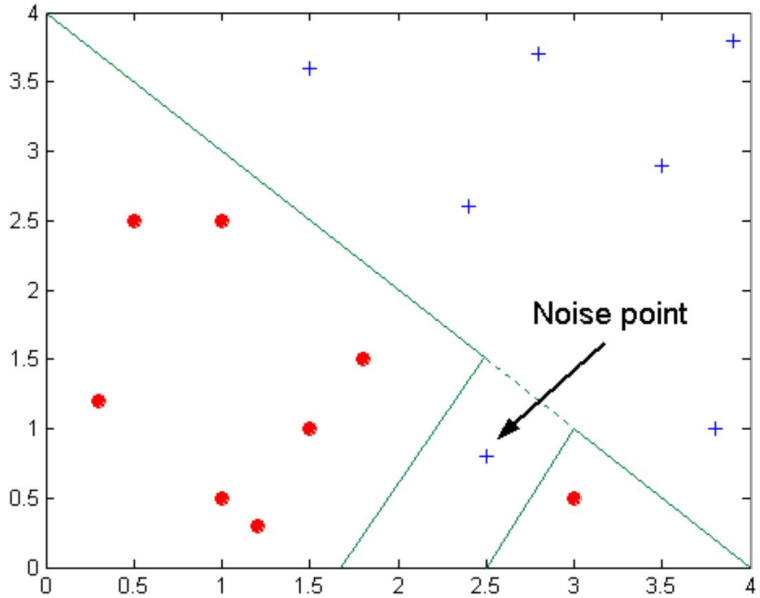


https://xyclade.github.io/MachineLearning/Images/Under-fitting.png

Overfitting

Causes:

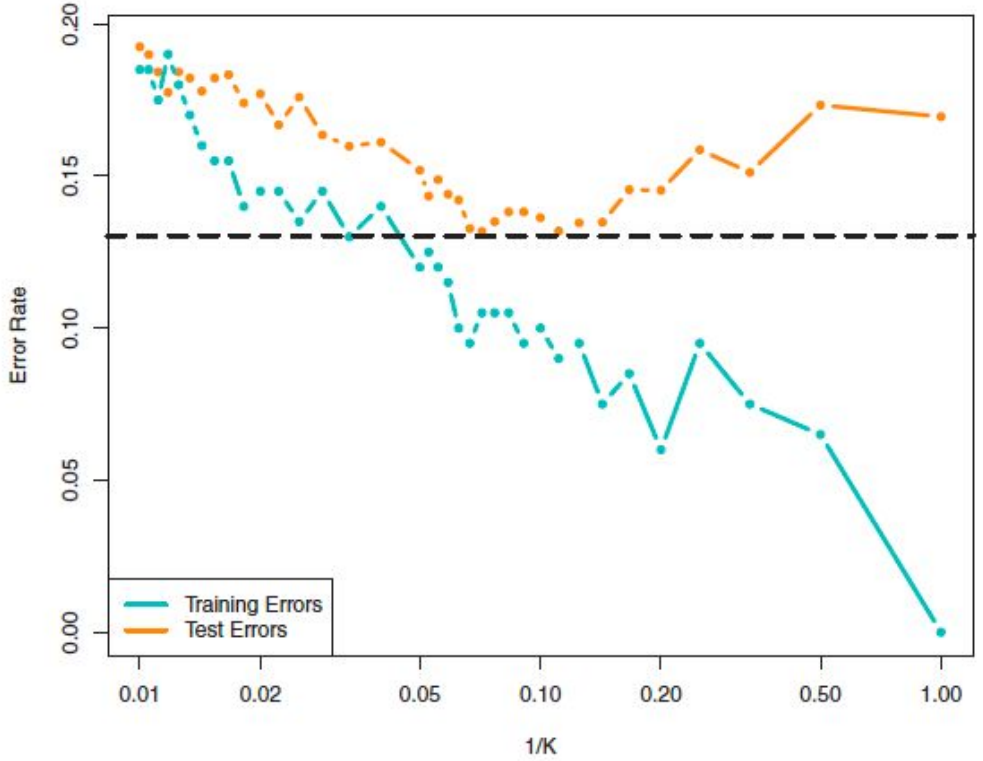
1) Model fits too well to specific cases and doesn't generalize well
2) Model is over-sensitive to noise specific to the sample provided
3) Model introduces too many variables/complexities than needed



Low Bias and **High Flexibility**

http://michael.hahsler.net/SMU/EMIS7332/slides/chap4_basic_classification.pdf

A Tale of Two Datasets



Parsimonious (adj.) - unwilling to spend money or use resources; stingy, frugal.

In data science, *it pays to be parsimonious*. (**Occam's Razor**)

https://i.cbc.ca/1.1674748.1379081034!/httpImage/image.jpg_gen/derivatives/16x9_620/li-620-scrooge-cp-7608083.jpg

Model Goals

When training a model we want our models to:

1) Capture the trends and particularities of the training data
2) Generalize well to other samples of the population
3) Be moderately interpretable

The first two are especially difficult to do simultaneously!

The more sensitive the model, the less generalizable and vice versa

Question:

Why is overfitting more difficult to control than underfitting?

Variance Reduction

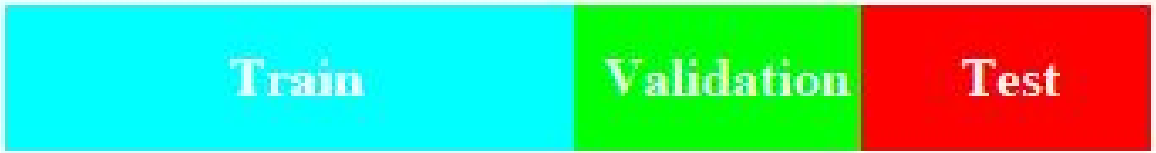
Avoiding overfitting is a **variance reduction** problem

Variance of the model is a function of the variances of each variable

1) Reduce the number of variables to use - **Subset Selection**
2) Reduce the complexity of the model - **Pruning**
3) Reduce the coefficients assigned to the variables - **Regularization**

Cross-validation is used to test the relative predictive power of each set of parameters and subset of features.

Validation - Traditional



About 30% of the training set was reserved as a validation set

Error on validation set served as a good estimate of the test error.

- Advantage: useful especially if a test-set is not available
- Disadvantage: reduces size of available training data

Hastie et al. “Elements of Statistical Learning.”

Cross Validation

Set of validation techniques that uses the training dataset itself to validate model

- Advantage: allows maximum allocation of training data from original dataset
- Advances in processing power makes CV efficient

Cross validation is used to test the effectiveness of any model or its modified forms

Leave-p-Out Validation

For each data point:

- Leave out p data points and train learner on the rest of the data.
- Compute the test error for the p data points.

Define average of these ${}_nC_p$ error values as validation error

http://toryshulman.com/wp-content/uploads/leftout.bmp

K-fold Validation

Often used in practice with *k*=5 or *k*=10.

Create equally sized *k* partitions, or **folds**, of training data

For each fold:

- Treat the *k-1* other folds as training data.
- Test on the chosen fold.

The average of these errors is the validation error

Question:

How are *k*-fold and leave-p-out different?

Subset Selection

- **Best subset selection:** Test all 2^p subset selections for best one
- **Forward subset selection**
  - Iterate over k = 0 ... (p-1) predictors
  - At each stage, select the best model with (p-k) predictors
  - Find best model out of the p-1 selected candidates with CV
- **Backward selection** - Reverse of forward subset selection
  - Start from p predictors and work down

In practice, best subset selection method is rarely used, why?

Regularization

We defined our error up until now as: $SS_{(residuals)} = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$

Minimizing this equation on training data = minimizing **Training Loss.**

To avoid overfitting, we add a penalty term independent of the data, known as **Regularization**

Error = (Training Loss)^2 + Regularization

- Ridge Regression
- Lasso Regression

http://ww2.tnstate.edu/ganter/BIO-311-Ch12-Eq5a.gif

Ridge Regression

Uses L_2 - regularization penalty:

$$\sum_{i=1}^{n}\left(y_i-\beta_0-\sum_{j=1}^{p}\beta_j x_{ij}\right)^2+\lambda\sum_{j=1}^{p}\beta_j^2=\mathrm{RSS}+\lambda\sum_{j=1}^{p}\beta_j^2,$$

Lambda is the penalty threshold constant, and controls sensitivity

- Useful for non-sparse, correlated predictor variables
- Used when predictor variables have small individual effects
- Limits the magnitudes of the coefficient terms, but not to 0

Lasso Regression

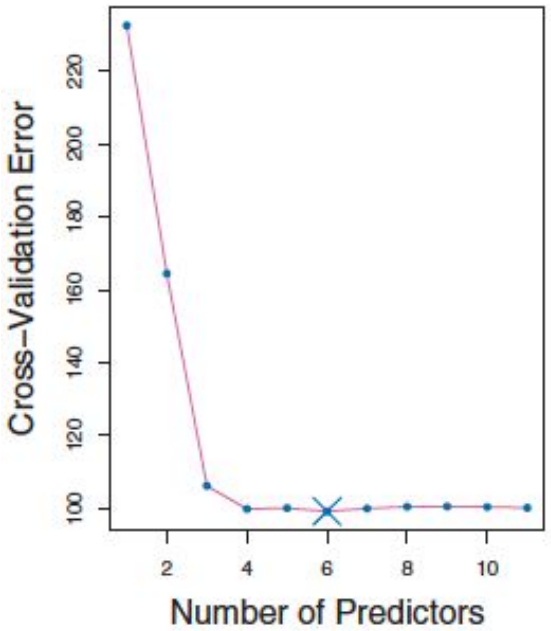
Uses L_1 - regularization penalty:

$$\sum_{i=1}^{n}\left(y_i-\beta_0-\sum_{j=1}^{p}\beta_j x_{ij}\right)^2+\lambda\sum_{j=1}^{p}|\beta_j| = \mathrm{RSS}+\lambda\sum_{j=1}^{p}|\beta_j|.$$

Notice that the penalty term uses absolute, rather than the squares

- Useful for sparse, uncorrelated variables
- Used when there are few variables with medium to high effects
- Performs both shrinkage and feature selection(drives coefficients to 0) when lambda sufficiently large

Training Accuracy vs Test Accuracy



Regularization, cross-validation are all techniques to limit the model's sensitivity

- In practice, if CV error is high:
  - Compare with Training
  - If significantly lower
    - Raise penalty constant
    - Try different subset
    - Try different parameters

Regularization + CV Demo

We'll compute the training error of a CART model.

We'll then use *k*-fold cross validation to get a good approximation of test error.

Finally, we'll compute the real test error.

Demo time!

Coming Up

Your problem set: None

Next week: Things are going to get meta.

See you then!