Cornell Data Science

Model Optimization

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

Bias and Variance

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

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

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

Error = (expected loss of accuracy)^2 + flexibility of model + irreducible error

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

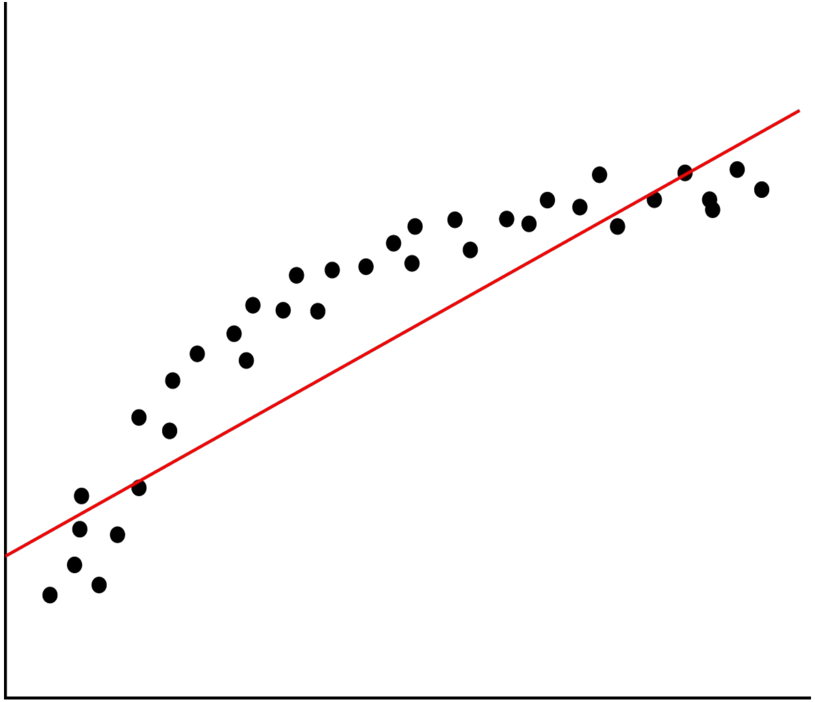
Question:

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

Underfitting

Underfitting means we have high bias and low variance.

- Lack of relevant variables/factor
- Imposing limiting assumptions
  - Linearity
  - Assumptions on distribution
  - Wrong values for parameters



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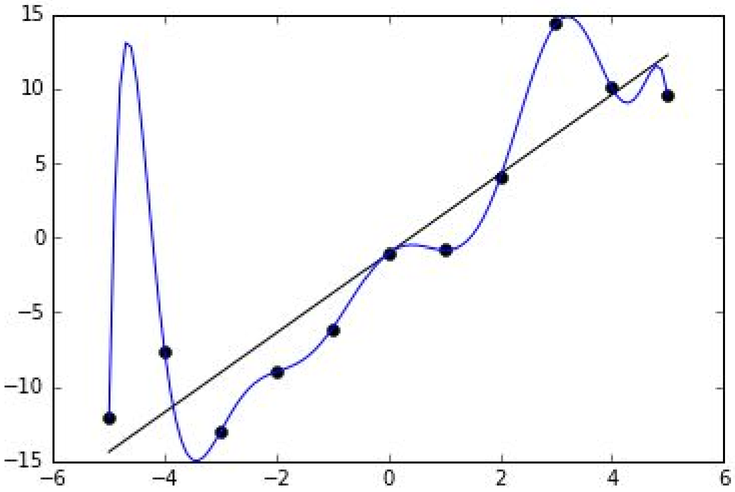
Overfitting

Overfitting means we have low bias and high variance.

- Model fits too well to specific cases
- Model is over-sensitive to sample-specific noise
- Model introduces too many variables/complexities than needed



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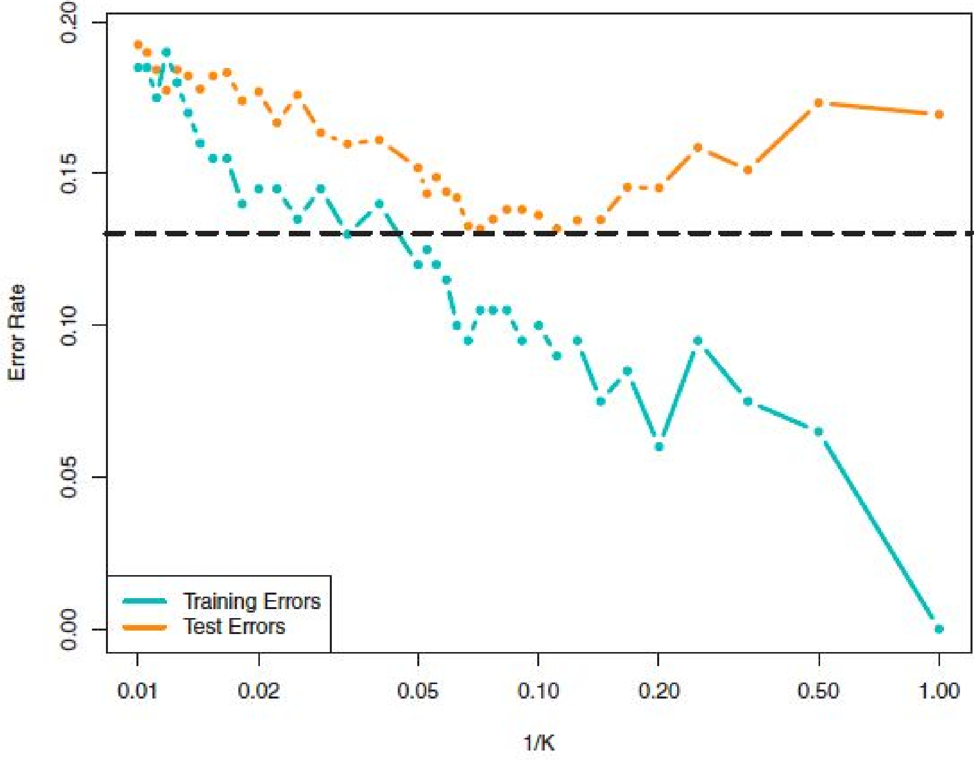
A Tale of Two Datasets



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:

- Capture the trends of the training data
- Generalize well to other samples of the population
- 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

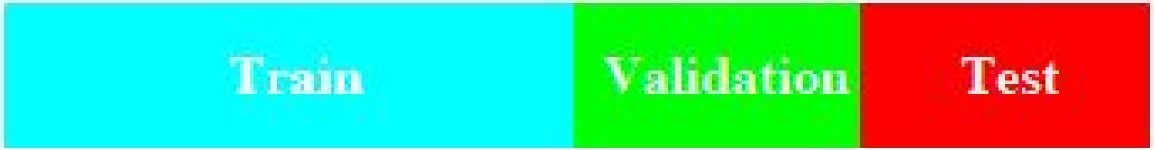
Avoiding overfitting is a **variance reduction** problem

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

- Reduce the number of variables to use [**Subset Selection**]
- Reduce the complexity of the model [**Pruning**]
- 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 is reserved as a validation set.

Error on validation set serves 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.”

More Generally: Cross Validation (CV)

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

- Allows maximum allocation of training data from original dataset
- Efficient due to advances in processing power

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 ${}_{n}C_{p}$ error values as validation error

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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.**

But we can often do better!

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Regularization

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

$$\text{Error} = (\text{Training Loss})^2 + \text{Regularization}$$

Ridge Regression

Lasso Regression

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

Ridge Regression

Uses L_2 - regularization penalty:

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

λ 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

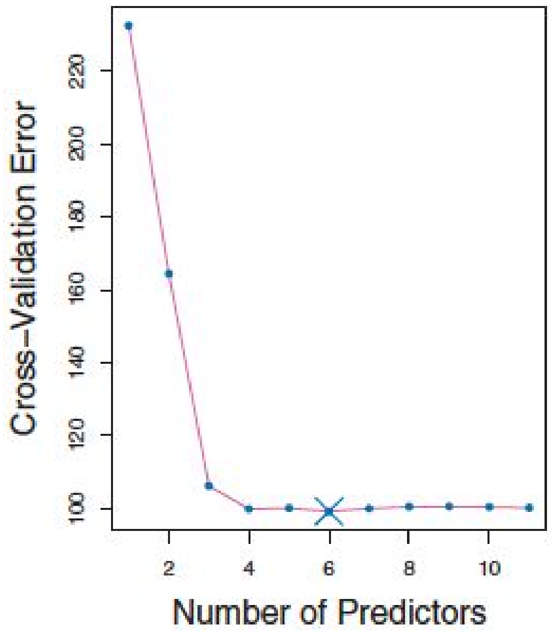
Uses L_1 - regularization penalty:

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

This time the penalty term uses absolute value rather than squaring.

- Useful for sparse, uncorrelated variables
- Used when there are few variables with medium to high effects
- Drives coefficients to 0 when λ sufficiently large (performs feature selection)

Training Accuracy vs Test Accuracy



Key idea: Regularization and cross-validation are 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

Coming Up

Your problem set: None

Next week: Things are going to get meta.

See you then!