COMP 543: Tools & Models for Data Science

Over-Fitting and Regularization

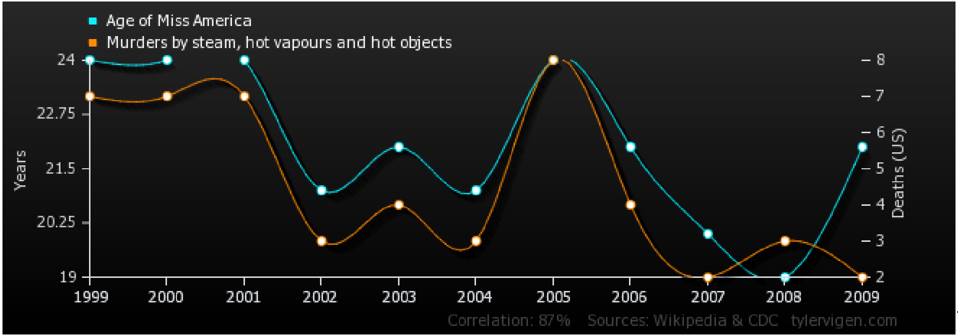
Chris Jermaine & Risa Myers

Rice University

Over-Fitting

- Fundamental problem in data science
  - Given enough hypotheses to check...
  - One of them is bound to be true

Miss America and Murder-By-Steam



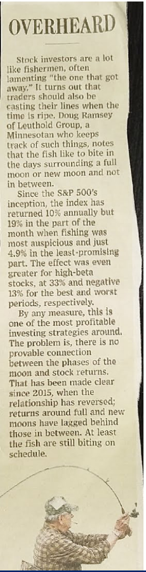
[1]

[1] http://tylervigen.com/view_correlation?id=2948

2

[2] LeinweberDJ.Stupiddataminertricks: overfittingtheS&P500.JournalofInvesting.2007;16(1):15.

Fishing and the S&P 500


OVERHEARD

Stock investors are a lot like fishermen, often lamenting "the one that got away." It turns out that traders should also be casting their lines when the time is ripe. Doug Ramsey of Leuthold Group, a Minnesotan who keeps track of such things, notes that the fish like to bite in the days surrounding a full moon or new moon and not in between.

Since the S&P 500's inception, the index has returned 10% annually but 19% in the part of the month when fishing was most auspicious and just 4.9% in the least-promising part. The effect was even greater for high-beta stocks, at 33% and negative 13% for the best and worst periods, respectively.

By any measure, this is one of the most profitable investing strategies around. The problem is, there is no provable connection between the phases of the moon and stock returns. That has been made clear since 2015, when the relationship has reversed; returns around full and new moons have lagged behind those in between. At least the fish are still biting on schedule.

"Since the S&P 500's inception, the index has returned 10.3% annually but 19% in the part of the month when fishing was most auspicious and just 4.9% in the least-promising part. The effect was even greater for high-beta stocks at 33.4% and negative 13.4% for the best and worst periods, respectively."

"By any measure this is one of the most profitable investing strategies around. The problem is, there is no proveable connection between the phases of the moon and stock returns. That has been made clear since 2015, when the relationship has reversed–returns around full and new moons have lagged those in between. At least the fish are still biting on schedule."[a]

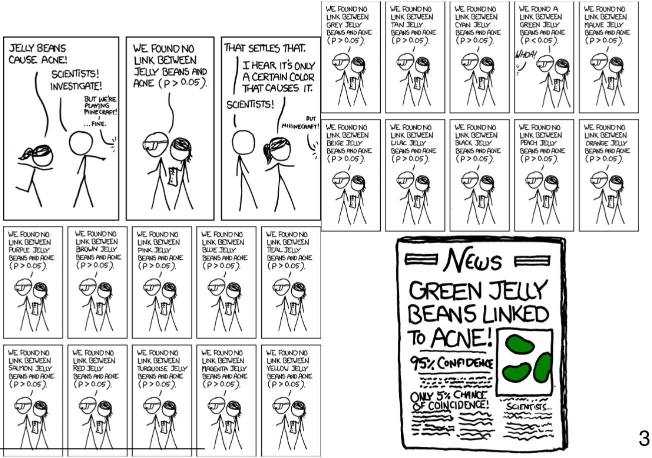
---

[a] https://blogs.wsj.com/moneybeat/2018/06/01/this-trading-strategy-is-the-reel-dea

None of these Models Likely to Generalize

- That means:
  - They’ve learned the input data
  - Not any underlying truth
  - When deployed in the field, likely to fail

- Was originally a derogatory term used by stats
  - Meant that you could always find something if you look hard enough



[3]

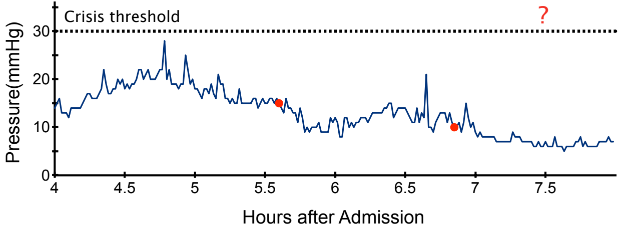
[3] https://xkcd.com/882/

Detecting Over-Fitting

- Detection method number 1: sniff test
  - E.g.: do the regression coefficients make sense?
- Detection method number 2: independent validation and test sets
  - Avoid temptation!
- Detection important...
  - Avoiding altogether is as well!

Sniff Test Example

- 4-hour time series epochs
- 239 patients
- Researchers started with > 1,000 features
- Reduced to 50
  - 68th and 143rd most recent observations



Avoiding Over-Fitting: Occam's Razor

- The Razor stated simply: When you have many hypotheses that match observed facts equally well, the simplest one is preferred.
  - Been around for a long time!
  - Credited to William of Ockham (died 1347)
  - First stated explicitly by John Punch, 1639: "Entities must not be multiplied beyond necessity"
- Example:
  - What's the next number in this sequence?
  - 1, 3, 5, 7, ?

Overly Complex Sequence

- 1, 3, 5, 7, ?
  - 9

    f(x) = x + 2
  - 217341[4]

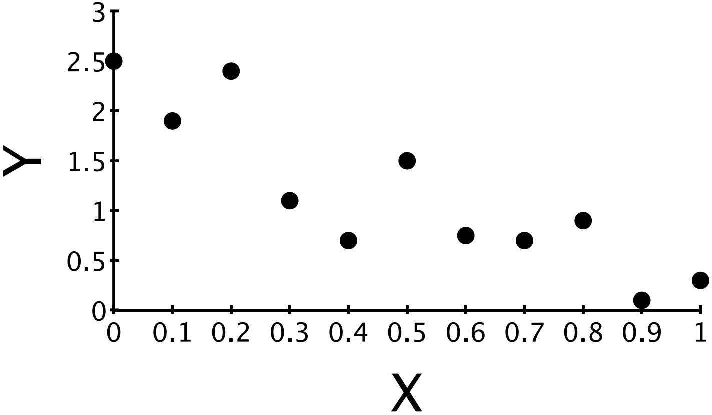
$$f(x) = \frac{18111}{2}x^4 - 90555x^3 + \frac{633885}{2}x^2 - 452773x + 217331$$

[4] https://ml.berkeley.edu/blog/2017/07/13/tutorial-4/

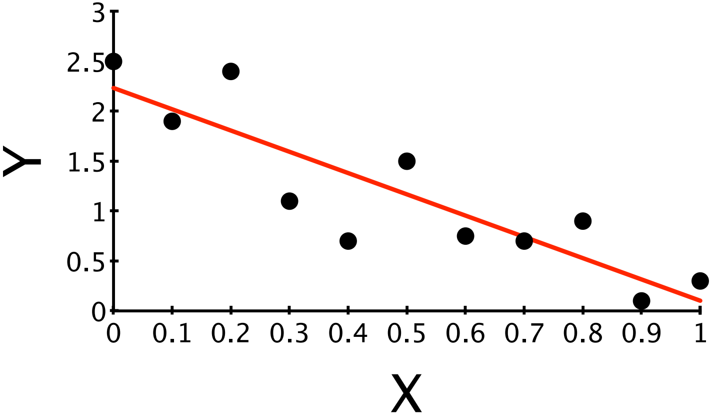
Avoiding Over-Fitting: Occam's Razor

- Of course, not that simple
  - You never have a large number of equally good hypotheses
  - Best you can do: have a bias towards simple models...
  - Under the assumption they will generalize well

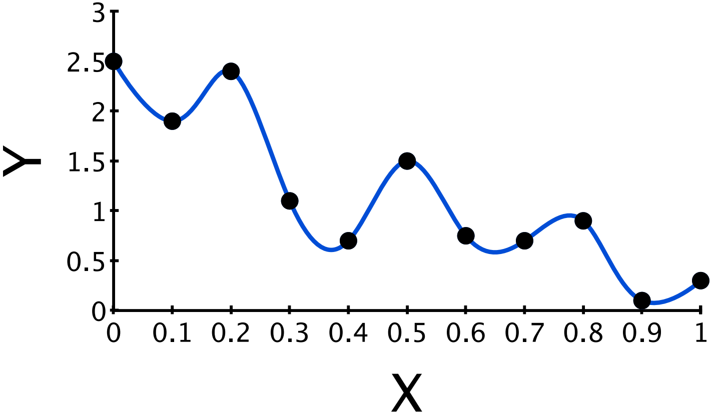
Avoiding Over-Fitting: Example Data



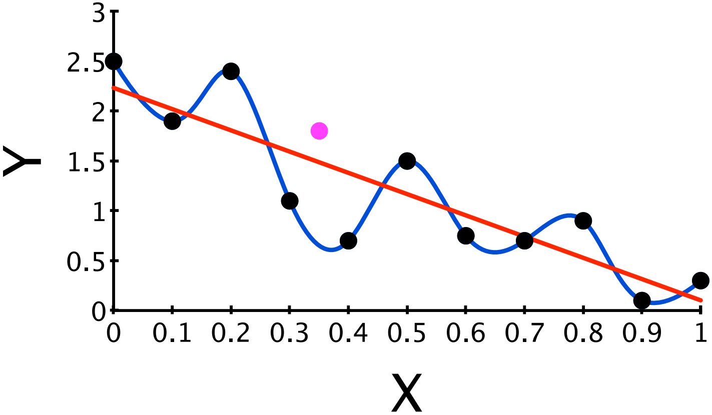
Avoiding Over-Fitting: Example Linear Regression



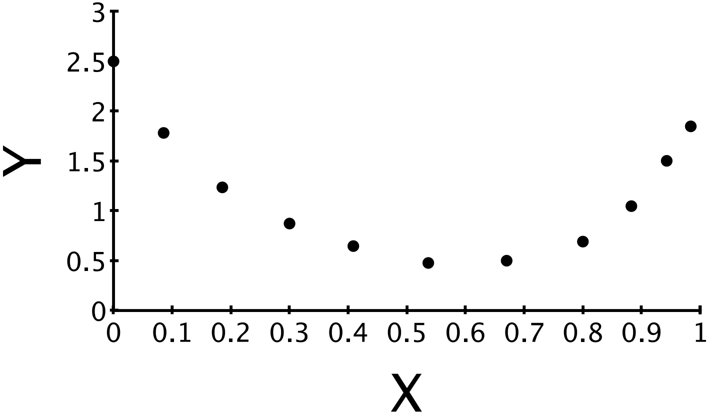
Avoiding Over-Fitting: Example Over-fitting



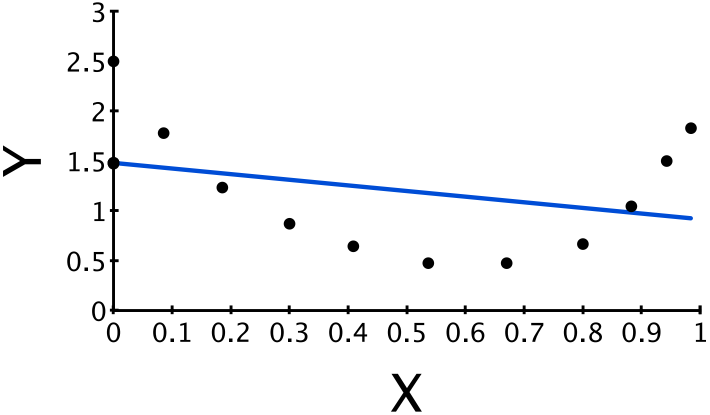
Avoiding Over-Fitting: Example New Point



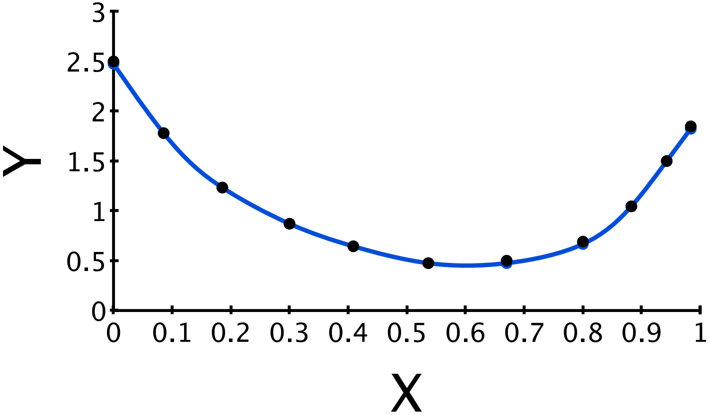
Avoiding Under-Fitting: Example Data



Avoiding Under-Fitting: Example Under-fitting



Avoiding Under-Fitting: Example Fitting



The Bias-Variance Trade-Off

- In a nutshell, we have two main sources of error in machine learning
  - “Bias”: error from incorrect model assumptions
  - “Variance”: sensitivity of model to bad data

`http://scott.fortmann-roe.com/docs/BiasVariance.html`

What is Bias?

- Difference between what our model predicts and the truth
- Imperfect models
  - Simplifying assumptions to make the model easier to learn
  - What are common simplifying assumptions?

`http://scott.fortmann-roe.com/docs/BiasVariance.html`

What is Bias?

- Difference between what our model predicts and the truth
- Imperfect models
  - Simplifying assumptions to make the model easier to learn
  - What are common simplifying assumptions?
    - iid data
    - data distributed normally

http://scott.fortmann-roe.com/docs/BiasVariance.html

What is Variance?

- Variability of a model's prediction for a data point
- If we build multiple models, how consistent are the predictions across these models?
- Sensitivity of the output to small fluctuations in the training set
- The model is highly dependent on our selection of training data
  - A good distribution of training data will enable us to predict new data well
  - If our training data has a lot of outliers or non-standard values, our predictions will be off

`http://scott.fortmann-roe.com/docs/BiasVariance.html`

The Bias-Variance Target

- Suppose we have a number of DIFFERENT training sets for the same problem
- Train the same algorithm on each of the training sets
- Each hit on the target is generated by a single model
- A perfect classifier would hit the bulls-eye

`http://scott.fortmann-roe.com/docs/BiasVariance.html`

Understanding the Trade-Off

- Expected squared error or any prediction is:

$$E[(Y - \hat{f}(X))^2]$$

- Here:
- Y is the output we are trying to predict
- $\hat{f}(.)$ is the model we are learning (is a random variable!)
- X is the observed data (ex: set of regressors)
- Y is the value we are trying to predict from X

Some Definitions

- $Var(X) = E[(X - \mu)^2]$
- $Bias_\theta[\hat{\theta}] = E_{x|\theta}[\hat{\theta}] - \theta = E_{x|\theta}[\hat{\theta} - \theta]$

Understanding the Trade-Off

- Expected squared error of any prediction is $E[(Y-\hat{f}(X))^2]$
  - Expanding:

$$
\begin{aligned}
E[(Y-\hat{f}(X))^2] &= E[Y^2+\hat{f}^2(X)-2Y\hat{f}(X)] \\
&= E[Y^2]+E[\hat{f}^2(X)]-E[2Y\hat{f}(X)] \\
&= Var(Y)+E^2[Y]+E[\hat{f}^2(X)]-E[2Y\hat{f}(X)] \\
&= Var(Y)+E^2[Y]+Var(\hat{f}(X))+E^2[\hat{f}(X)]-E[2Y\hat{f}(X)] \\
&= Var(Y)+Var(\hat{f}(X))+(E^2[Y]-E[2Y\hat{f}(X)]+E^2[\hat{f}(X)]) \\
&= Var(Y)+Var(\hat{f}(X))+Bias^2(\hat{f}(X))
\end{aligned}
$$

  - Means error is a sum of:
  - "Looseness" of relationship between X and Y
  - Sensitivity of the learner to variability of the training data (variance)
  - Inability of the learner $\hat{f}$ to learn the relationship between X and Y (bias)
- It is the second one (variance) that leads to over-fitting

Irreducible Error

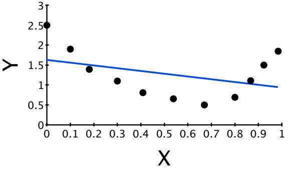
$$E[(Y-\hat{f}(X))^2] = Var(Y) + Var(\hat{f}(X)) + Bias^2(\hat{f}(X))$$

- Var(Y) is irreducible error
  - Inherent variability in the outcomes
  - Noise

Ideally, Reduce Both Bias and Variance!

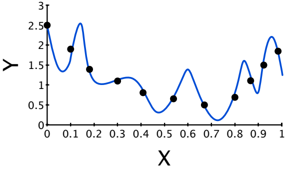
- Unfortunately, not possible
- “In real life”
  - We don’t know the real model–bias is guaranteed
  - Since we ARE wrong, choose a general model and lots of features
  - Hence variance (over-fitting) is also guaranteed
  - Best we can do: choose sweet spot where error is minimized

Underfitting vs. Overfitting



Low Complexity
High Bias
Low Variance

Complexity
$\longrightarrow$



High Complexity
Low Bias
High Variance

Model Complexity vs. Error

http://scott.fortmann-roe.com/docs/BiasVariance.html

$$\frac{dBias}{dComplexity} = -\frac{dVariance}{dComplexity}$$

Finding the Sweet Spot

`http://scott.fortmann-roe.com/docs/BiasVariance.html`

- In practice, there's no way to measure this
  - Try models of different complexity
  - Choose the one with the overall lowest error
  - Relies on choice of error measurement

Regularization

- Massively important idea in data science
  - In a nutshell:
  - Give learning algorithm ability to choose complexity of model
  - Automatically choose the correct trade-off between bias and variance
- Done by adding a penalty term to objective function
  - Penalizes model for complexity

Regularization

- Typically, penalty is based on l_p norm
- Recall, l_p norm of a vector $\langle x_1, x_2, \ldots \rangle$ computed as:

$$\left(\sum_{i=1}^{n} |x_i|^p \right)^{1/p}$$

- Common penalties are l_1, l_2

Example: Logistic Regression

- Standard objective function is:

$$\sum_i y_i \theta_i - \log(1 + e^{\theta_i})$$

  where θ_i is $\sum_j x_{i,j} r_j$

- Change objective function to:

$$\sum_i \left(y_i \theta_i - \log(1 + e^{\theta_i})\right) - \lambda (||r||_p)^p$$

  $(||r||_p)^p$ is the l_p norm of the regression coefficients raised to power p

Example: Logistic Regression

- If $p = 1$ have "the lasso"
- If $p = 2$ have "ridge regression"
- λ controls the magnitude of the penalty
  - Typically, try different values of λ during validation
  - Usually scale λ with n
  - Keeps loss balanced between prediction and regularization parts as data size changes

Ridge Regression

- As known as [Andrey] Tikhonov regularization
- Used when we want an solution to a problem that does not have a unique solution
- “Ridge" local optimums
- Reduces coefficient values
- Has higher bias, but lower variance than least squares estimator
- l_2 norm

Lasso Regression

- Least Absolute Shrinkage and Selection Operator
- Includes
  - Feature selection
  - Regularization
- Credited to Robert Tibshirani 1996
- Designed for least squares models
- Primary goal to improve accuracy by:
  - Reducing the number of features used in the final model
  - Forces the sum of the regression coefficients to be less than a fixed value
- l_1 norm

Closing Remarks

- When regularizing, important to normalize data
  - That is, transform so mean = 0 and variance = 1
  - ? Why?

Closing Remarks

- When regularizing, important to normalize data
  - That is, transform so mean = 0 and variance = 1
  - Why?
    - So the model doesn't have to work so hard to overcome the differences in feature magnitudes

Questions?