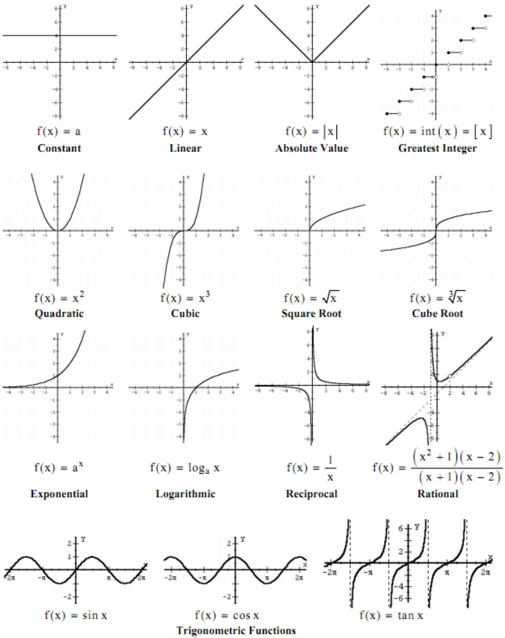
Regularization/Shrinkage

Schwartz

November 8, 2017

Functions



f(x) = a
Constant
f(x) = x
Linear
f(x) = |x|
Absolute Value
f(x) = int(x) = [x]
Greatest Integer
f(x) = x²
Quadratic
f(x) = x³
Cubic
f(x) = √x
Square Root
f(x) = ∛x
Cube Root
f(x) = aˣ
Exponential
f(x) = logₐ x
Logarithmic
f(x) = 1/x
Reciprocal
f(x) = (x² + 1)(x − 2) / (x + 1)(x − 2)
Rational
f(x) = sin x
f(x) = cos x
f(x) = tan x
Trigonometric Functions

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So this works if features are available *before* prediction is needed...

Have X to guess $\hat{Y}$ to help decision making

Model Complexity

1. $\hat{Y} = \hat{\beta}_0 + x\hat{\beta}_1$
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   $\vdots$

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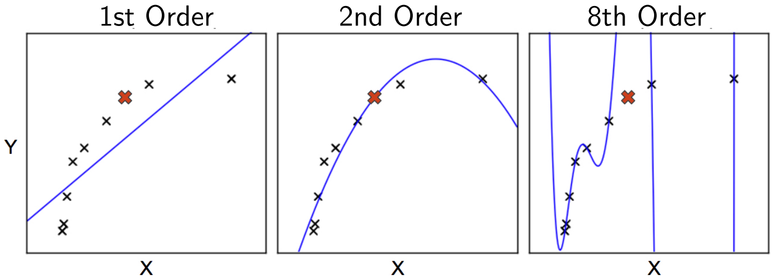

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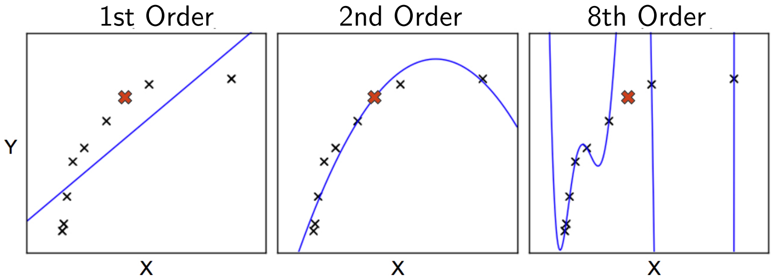

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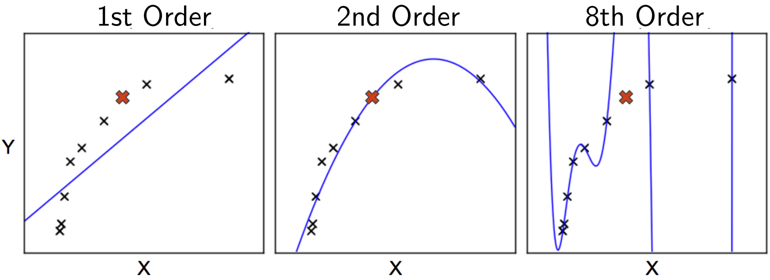


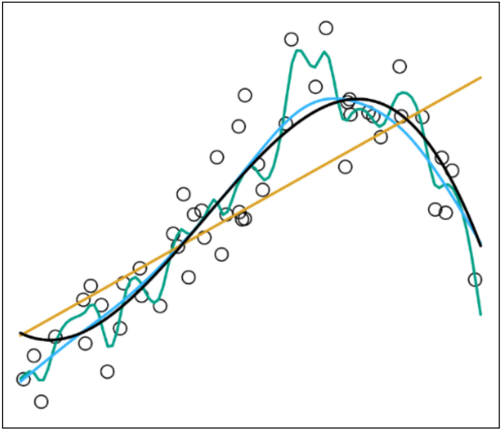
Model fit to the data always improves until *perfect* data fit

R^2 can only get better – never worse – with more features

Variance and Bias

<u>Variance</u>: (1) the volatility of a model prediction from data set to data set; (2) the amount of flexibility/susceptibility the model has to being influenced by idiosyncratic outliers

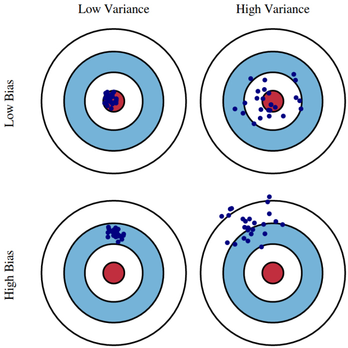
<u>Bias</u>: the rigidity/inability/limitations of the model to flexibly capture complex but true data associations

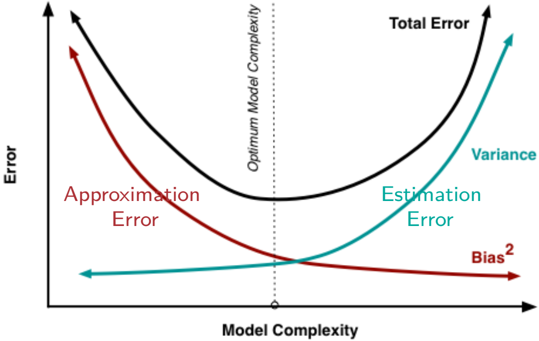


Bias and *Variance* characterize models *robustness* – a neutral word

Variance and Bias and Tradeoff

- In *Machine Learning*, *bias* and *variance* refer to performance accuracy characteristics over hypothetical random data sets





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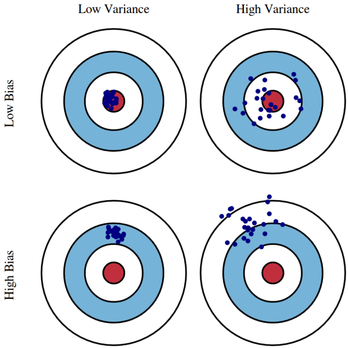

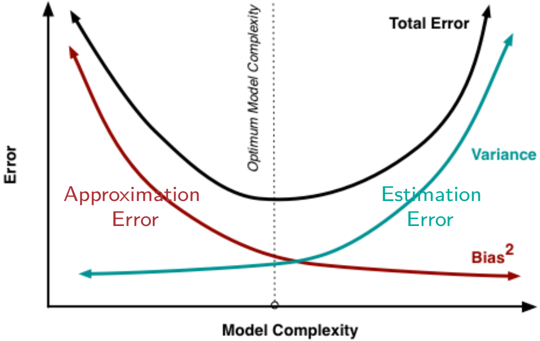

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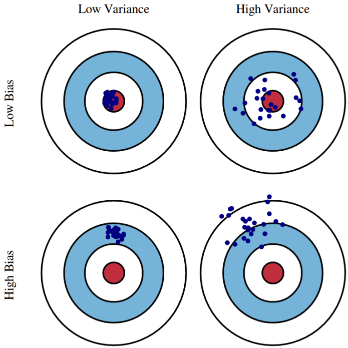
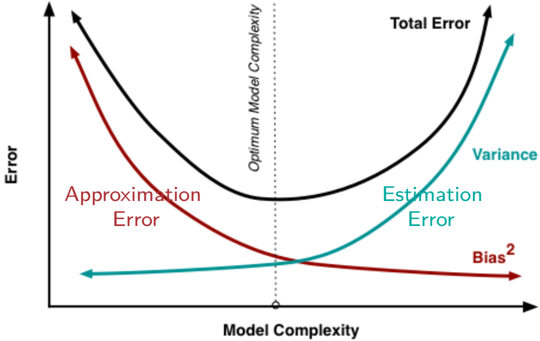
  The Machine Learning objective is finding the right balance





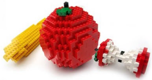
Partition of Variation

Let $y_i = \theta + \epsilon_i$ with $\theta = f(x_0)$ and $\epsilon \sim \mathrm{N}(0, \sigma_\epsilon^2)$
For estimator $\hat{\theta} = \hat{f}(x_0)$,

$$
\begin{aligned}
MSE &= \frac{1}{n}\sum_i \left(y_i - \hat{\theta}\right)^2 \approx \mathrm{E}\left[\left(y_i - \hat{\theta}\right)^2\right] \\
&= \mathrm{E}\left[\left(y_i - \theta + \theta - E[\hat{\theta}] + E[\hat{\theta}] - \hat{\theta}\right)^2\right] \\
&= \mathrm{E}\left[\left((y_i - \theta) + (\theta - E[\hat{\theta}]) + (E[\hat{\theta}] - \hat{\theta})\right)^2\right] \\
&\overset{!}{=} \mathrm{E}\left[(y_i - \theta)^2\right] + \mathrm{E}\left[\left(\theta - E[\hat{\theta}]\right)^2\right] + \mathrm{E}\left[\left(E[\hat{\theta}] - \hat{\theta}\right)^2\right] \\
&= \sigma_\epsilon^2 + \left(\mathrm{E}[\hat{\theta}] - \theta\right)^2 + \sigma_{\hat{\theta}}^2 \\
&= \text{Residual Variance} + \text{Model Bias}^2 + \text{Model Variance}
\end{aligned}
$$

Model Generalizability

- The question isn't how well does the model fit data you have
  - It can fit data you have exactly as closely as you want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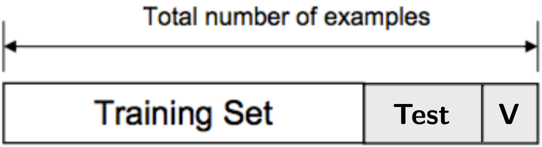
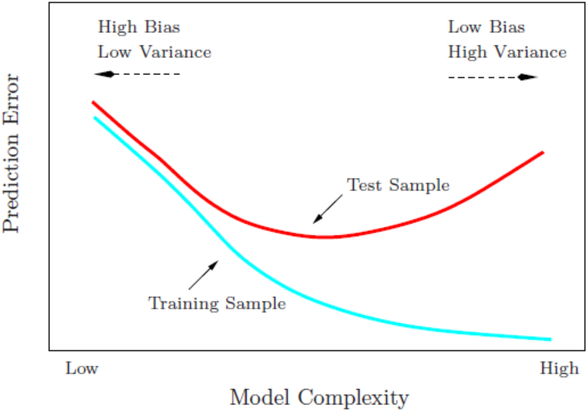
Train/Test split

The Train/Test Split





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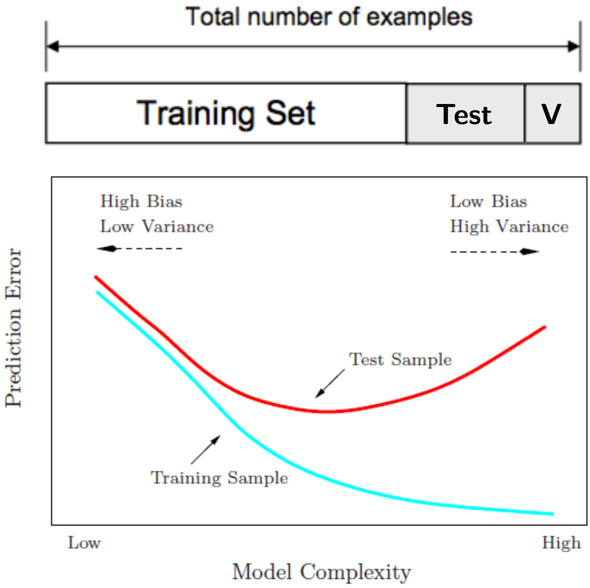

- How do we choose?
- Sampling Variability?
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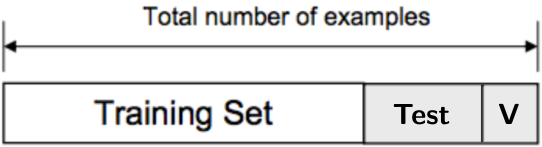

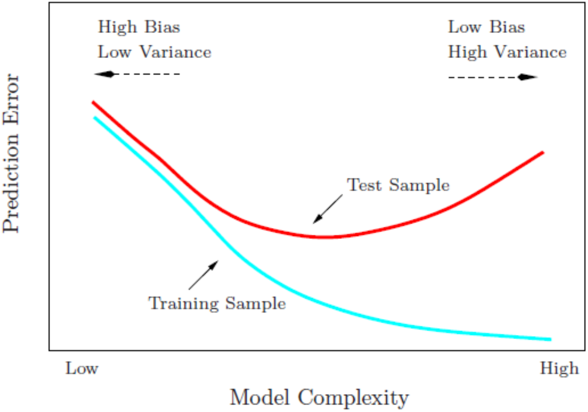

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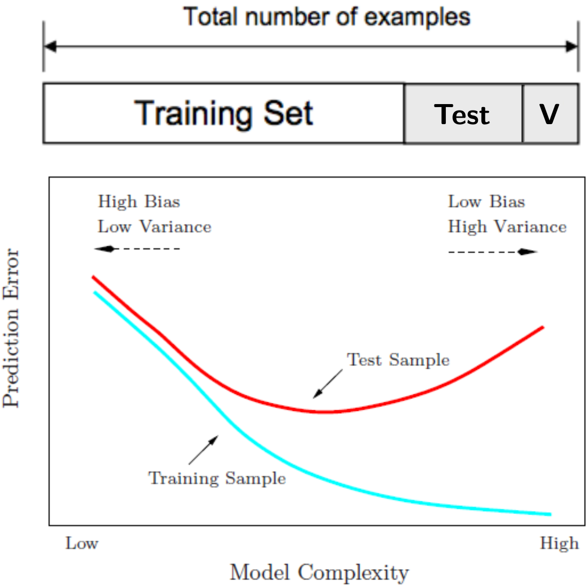

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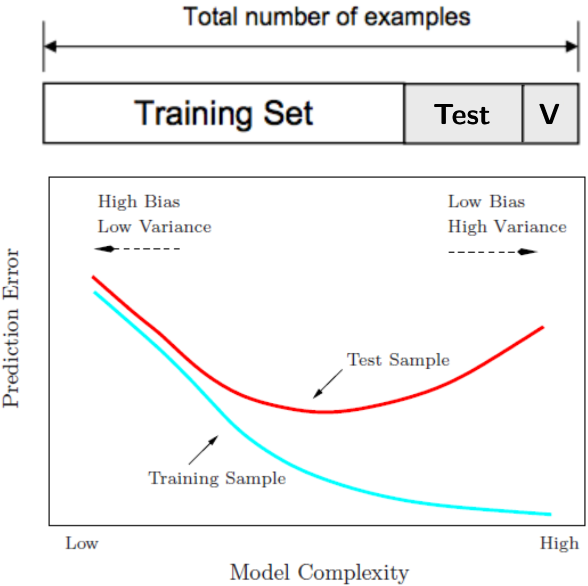

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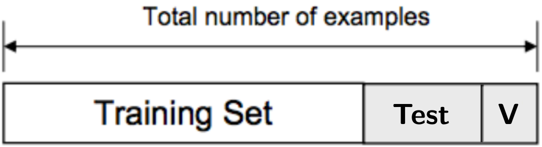

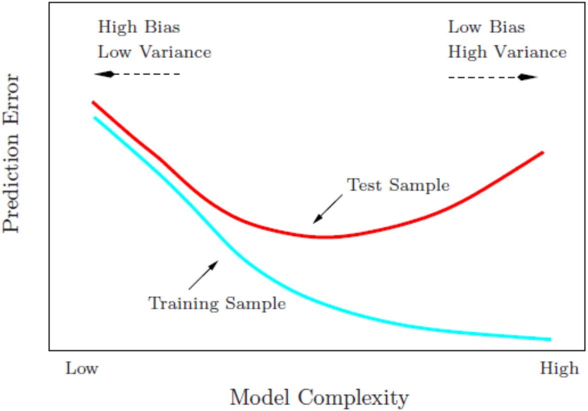

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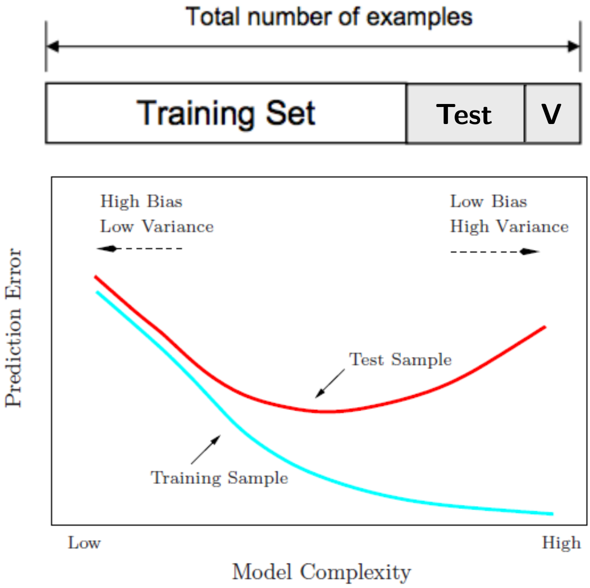

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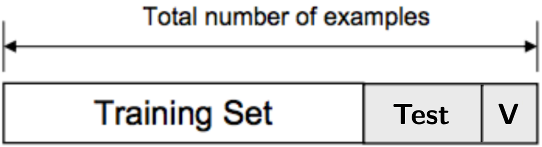

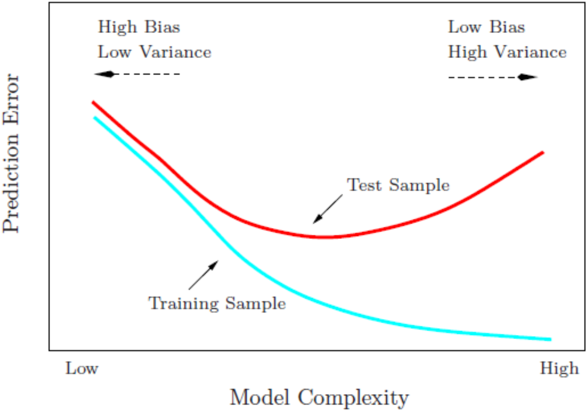

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  <Hold this thought>
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  Complexity choice is "fit" from test data
  The *validation* set V actually "tests wild"

Quiz

What is the “prediction error” on the previous slide?
(let’s have two regression and two classification examples)

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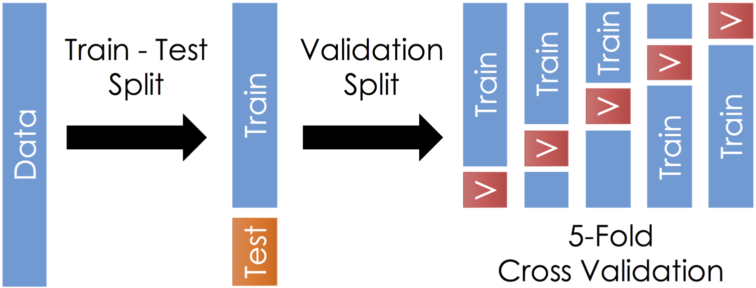
$$RMSE = \sqrt{\sum_{i=1}^{n} \left(Y_i - \hat{Y}_i\right)^2}$$

$$R^2 = \frac{\sum_{i=1}^{n}(Y_i - \bar{Y}_i)(\hat{Y}_i - \bar{\hat{Y}}_i)^2}{\hat{\sigma}_Y \hat{\sigma}_{\hat{Y}}}$$

$$Accuracy = \frac{\sum_{i=1}^{n} 1_{[Y_i = \hat{Y}_i]}}{n}$$

$$Sensitivity = \frac{\sum_{i=1}^{n} 1_{[Y_i = \hat{Y}_i]} 1_{[Y_i = 1]}}{\sum_{i=1}^{n} 1_{[Y_i = 1]}}$$

K-Folds Cross Validation



Benefits?

Challenges?

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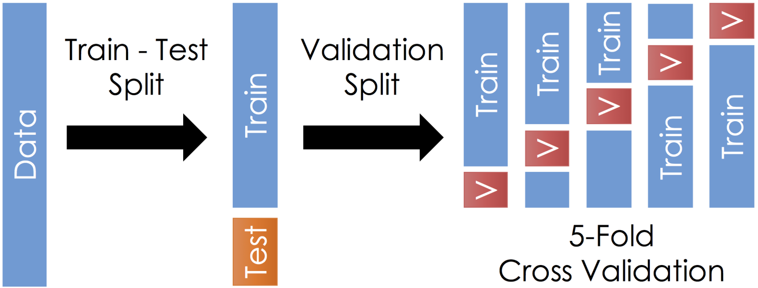

Benefits?

- Uses all the data as "validation" set

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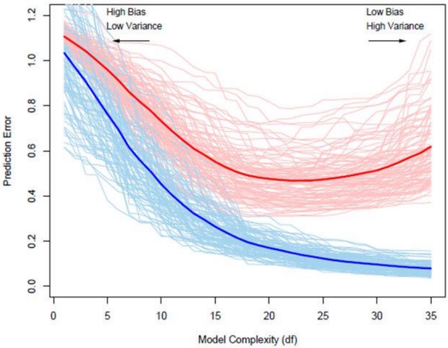

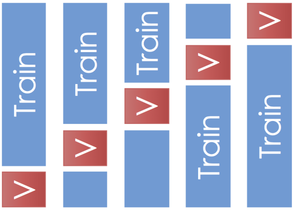

5-Fold
Cross Validation

Benefits?

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- Shows variation in sample accuracy scores

Challenges?

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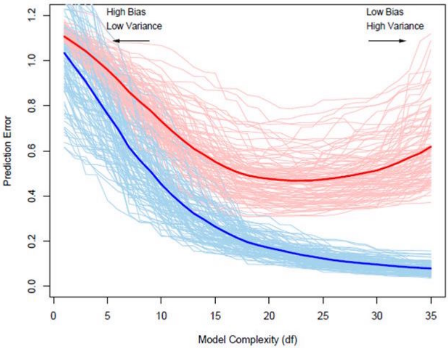

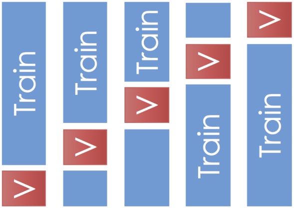

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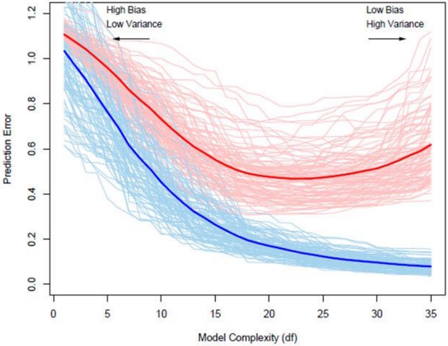

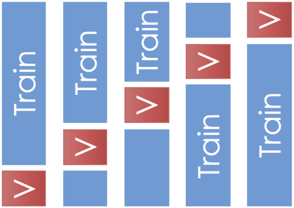

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- Refit with all data at a generalizable complexity level

Overfitting

1. How do you make this simpler/more complex?

$$\beta_0 + x_1\beta_1 + x_2\beta_2 + x_3\beta_3 + x_4\beta_4 + x_5\beta_5 + x_6\beta_6 + x_7\beta_7 + \cdots$$

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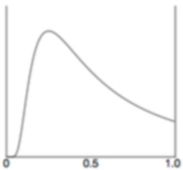
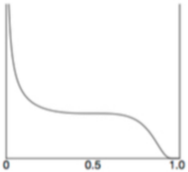
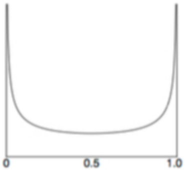
2. What does "dampening"/"suppressing" the β_j towards 0 do?

3. Why might we like this?

4. Suppose every β_j was 1...
   what do you think about the following *shrinkage* profiles?







Bias/Variance Tradeoff