Overfitting and Underfitting

"No Free Lunch" Theorems

$$
\begin{aligned}
Acc_G(L) &= \text{Generalization accuracy of learner } L \\
&= \text{Accuracy of } L \text{ on non-training examples}
\end{aligned}
$$

$\mathcal{F}$ = Set of all possible concepts, $y = f(\mathbf{x})$

Theorem: For any learner L, $\frac{1}{|\mathcal{F}|}\sum_{\mathcal{F}} Acc_G(L) = \frac{1}{2}$
(given any distribution $\mathcal{D}$ over $\mathbf{x}$ and training set size n)

Don't expect your favorite learner to always be best

Try different approaches and compare

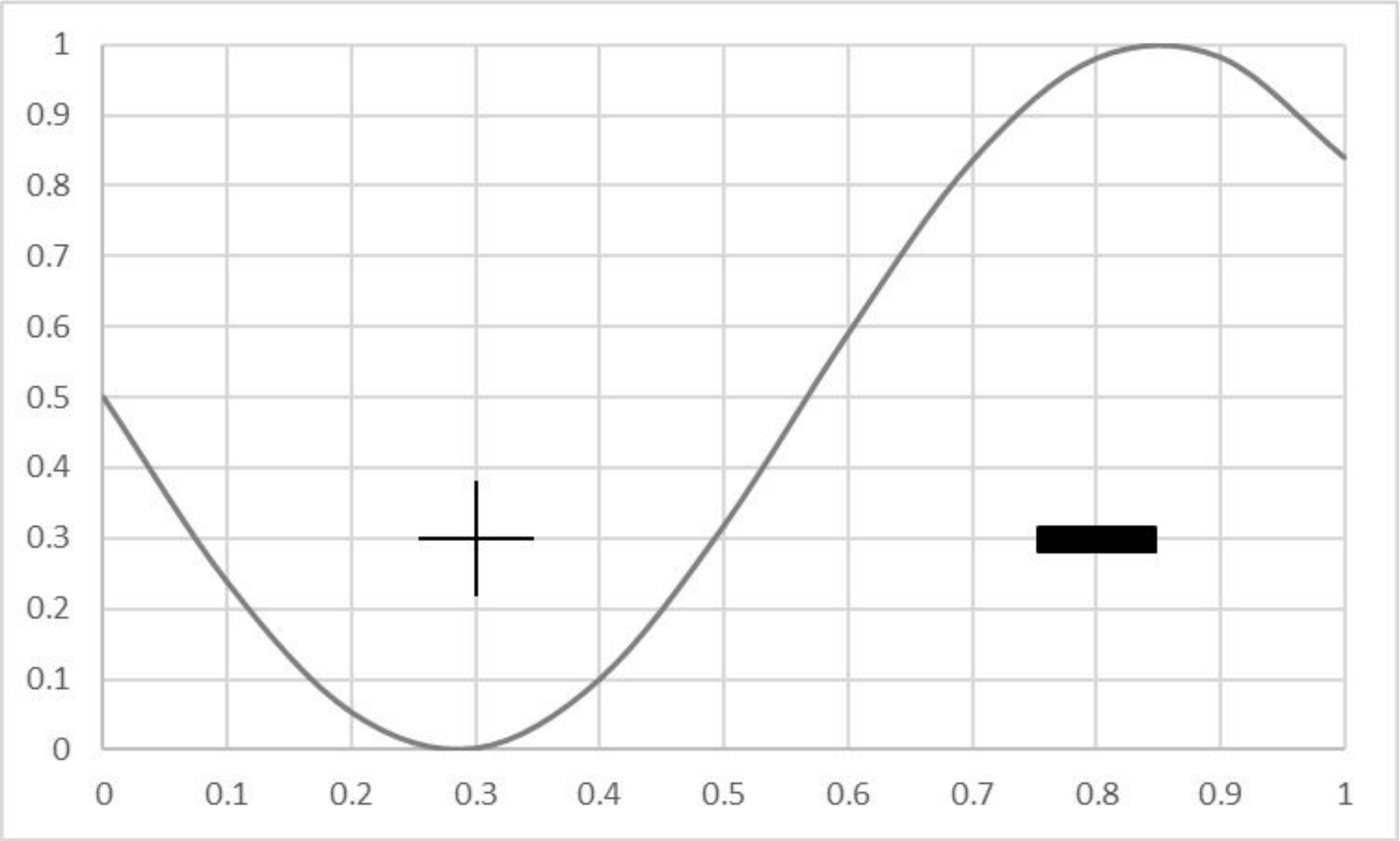
Bias and Variance

- Bias – error caused because the model can not represent the concept
- Variance – error caused because the learning algorithm overreacts to small changes (noise) in the training data

TotalLoss = Bias + Variance (+ noise)

Visualizing Bias

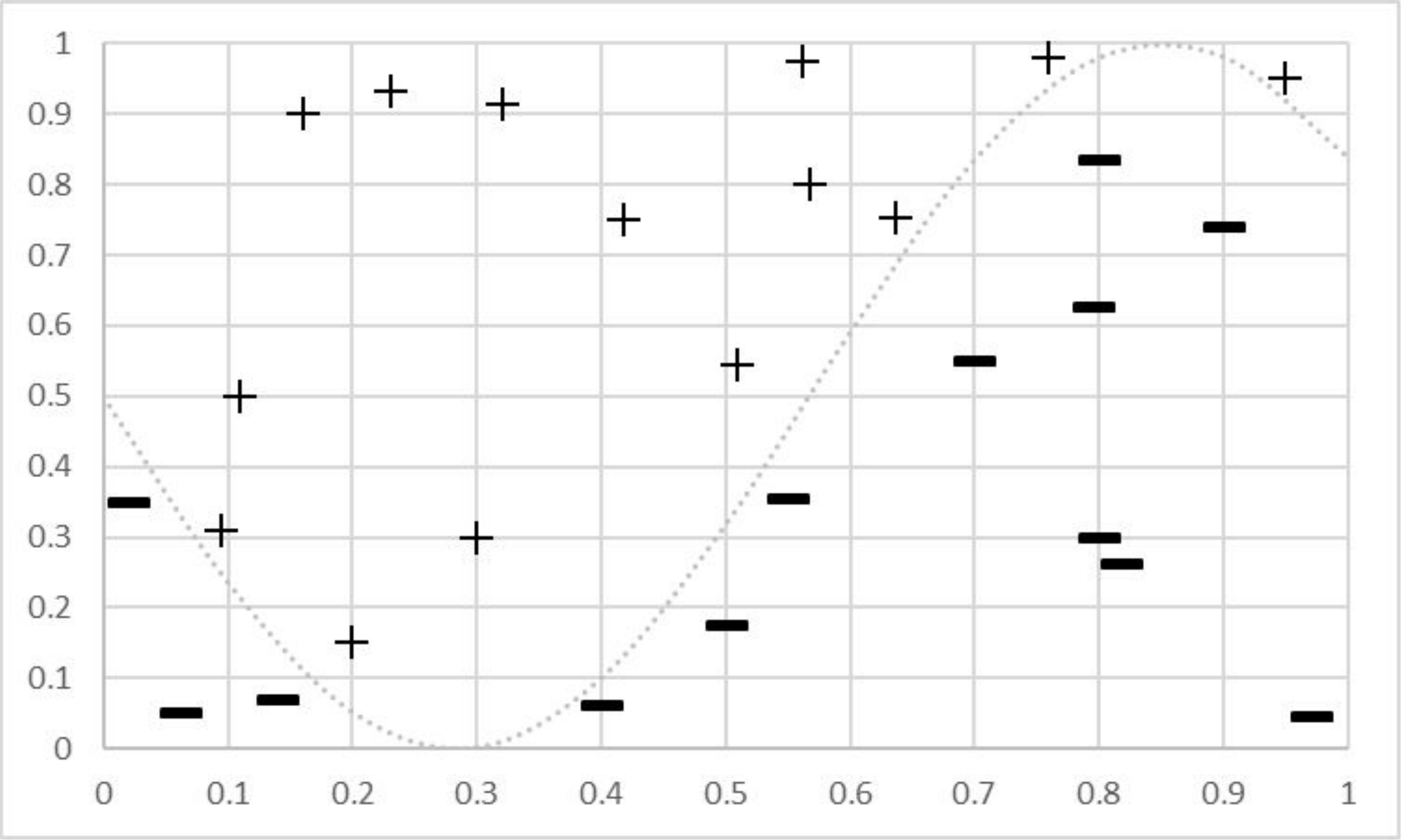
- Goal: produce a model that matches this concept



True Concept

Visualizing Bias

- Goal: produce a model that matches this concept
- Training Data for the concept

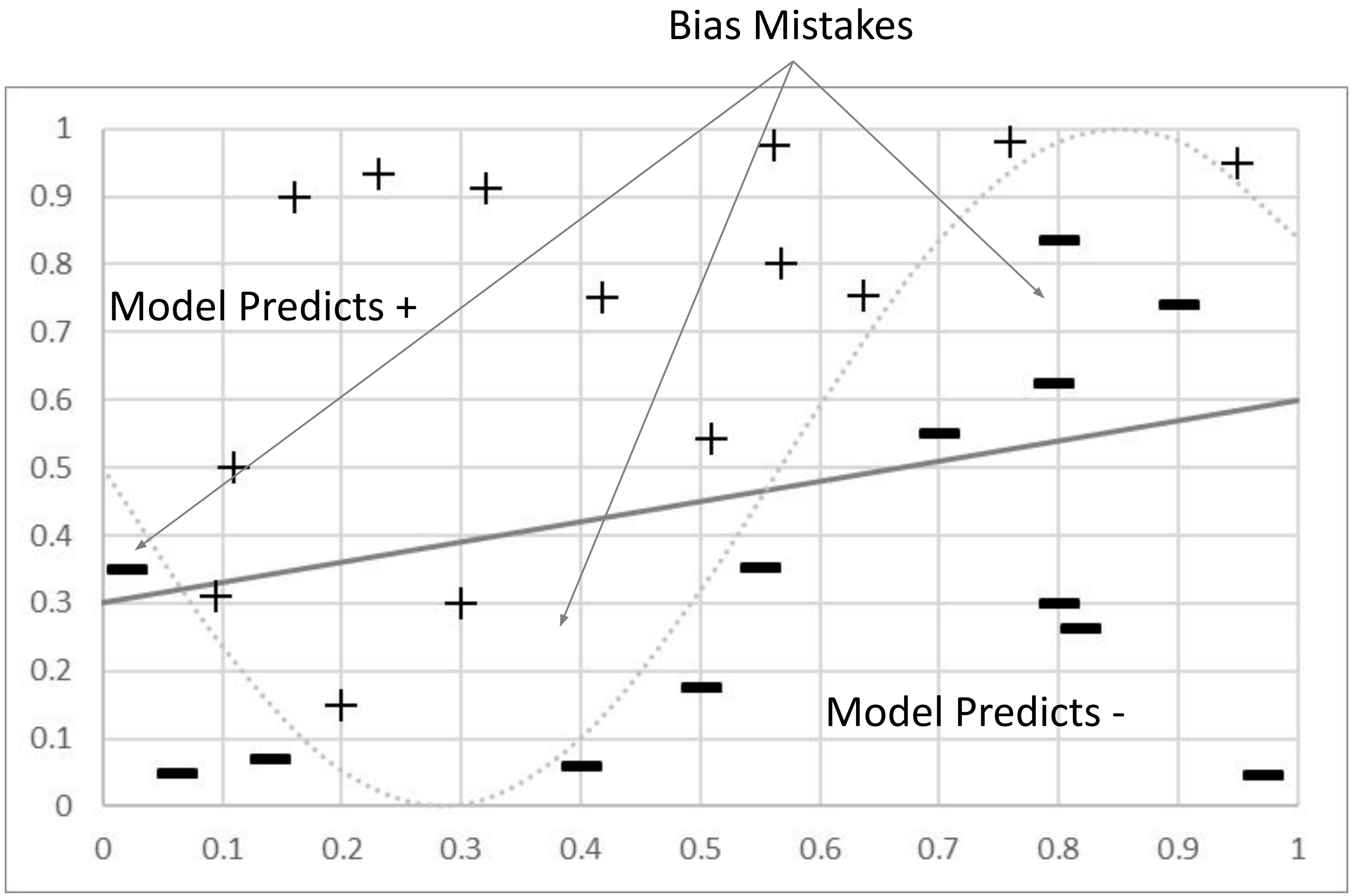


Training Data

Visualizing Bias

- Goal: produce a model that matches this concept
- Training Data for concept

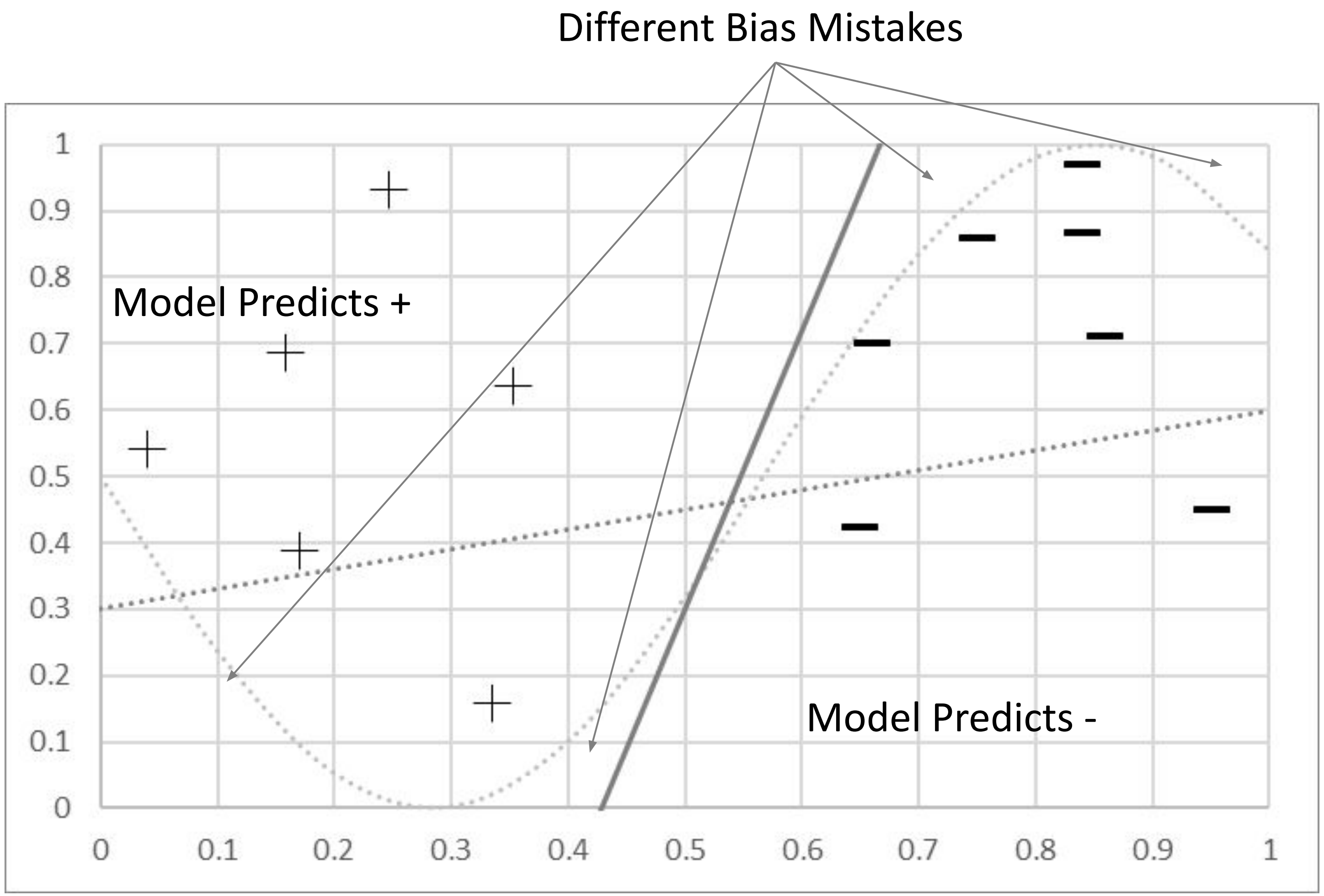
- Bias: Can't represent it…



Fit a Linear Model

Visualizing Bias

- Goal: produce a model that matches this concept
- New data, new model

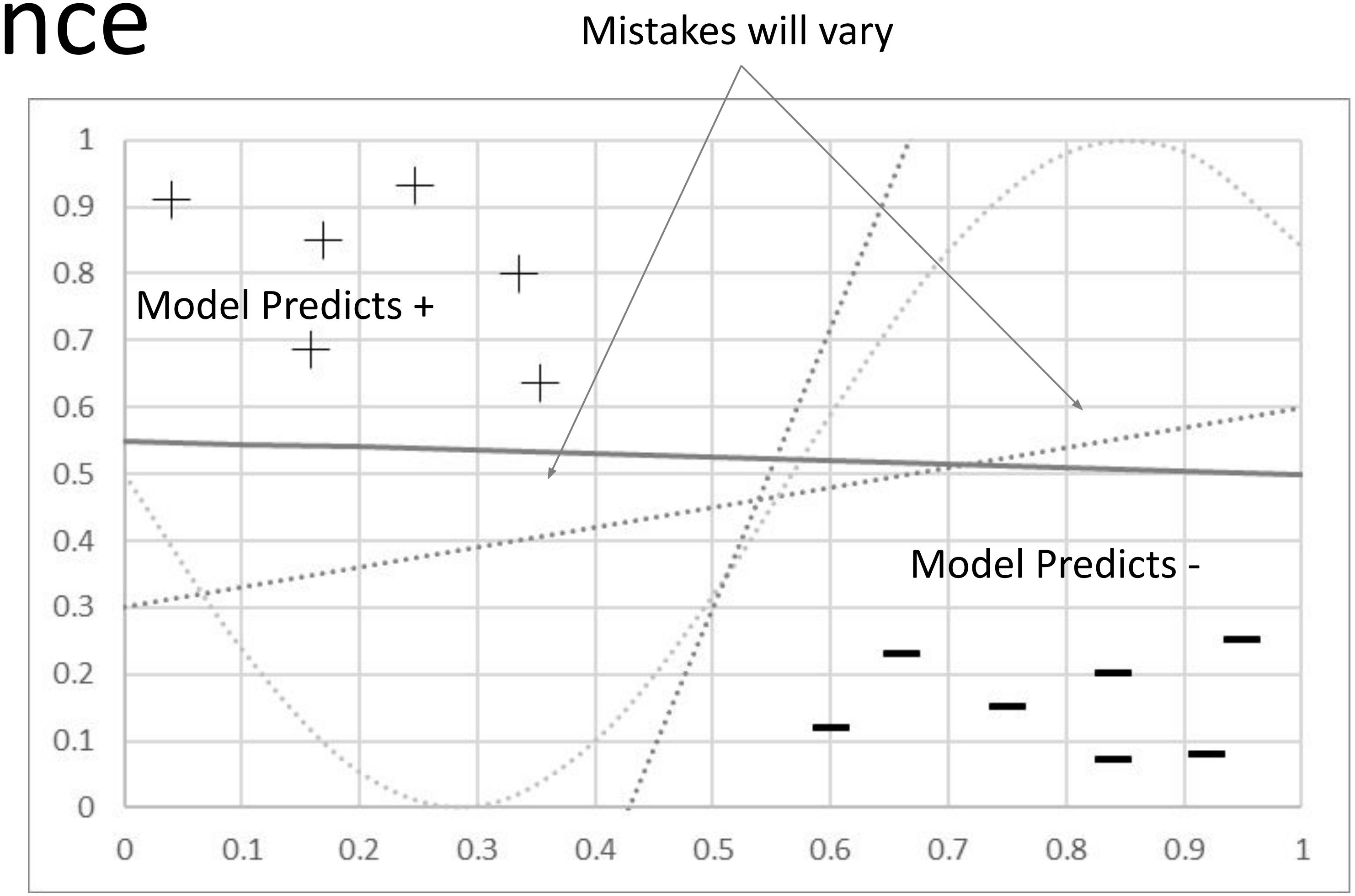


Fit a Linear Model

Visualizing Variance

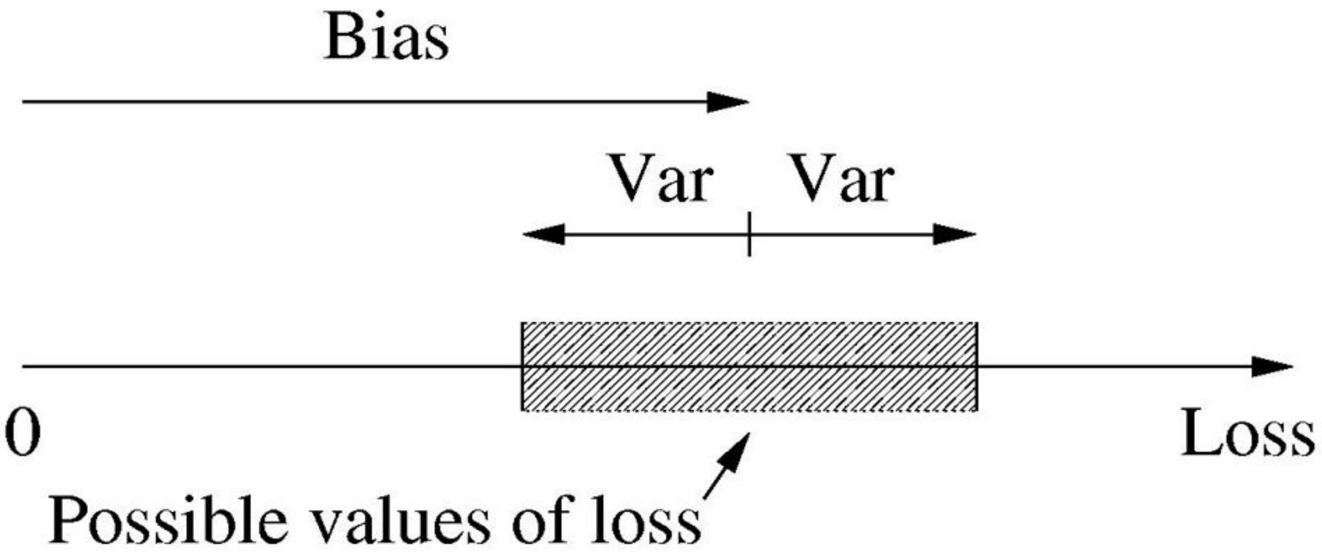
- Goal: produce a model that matches this concept
- New data, new model
- New data, new model…

- Variance: Sensitivity to changes & noise



Fit a Linear Model

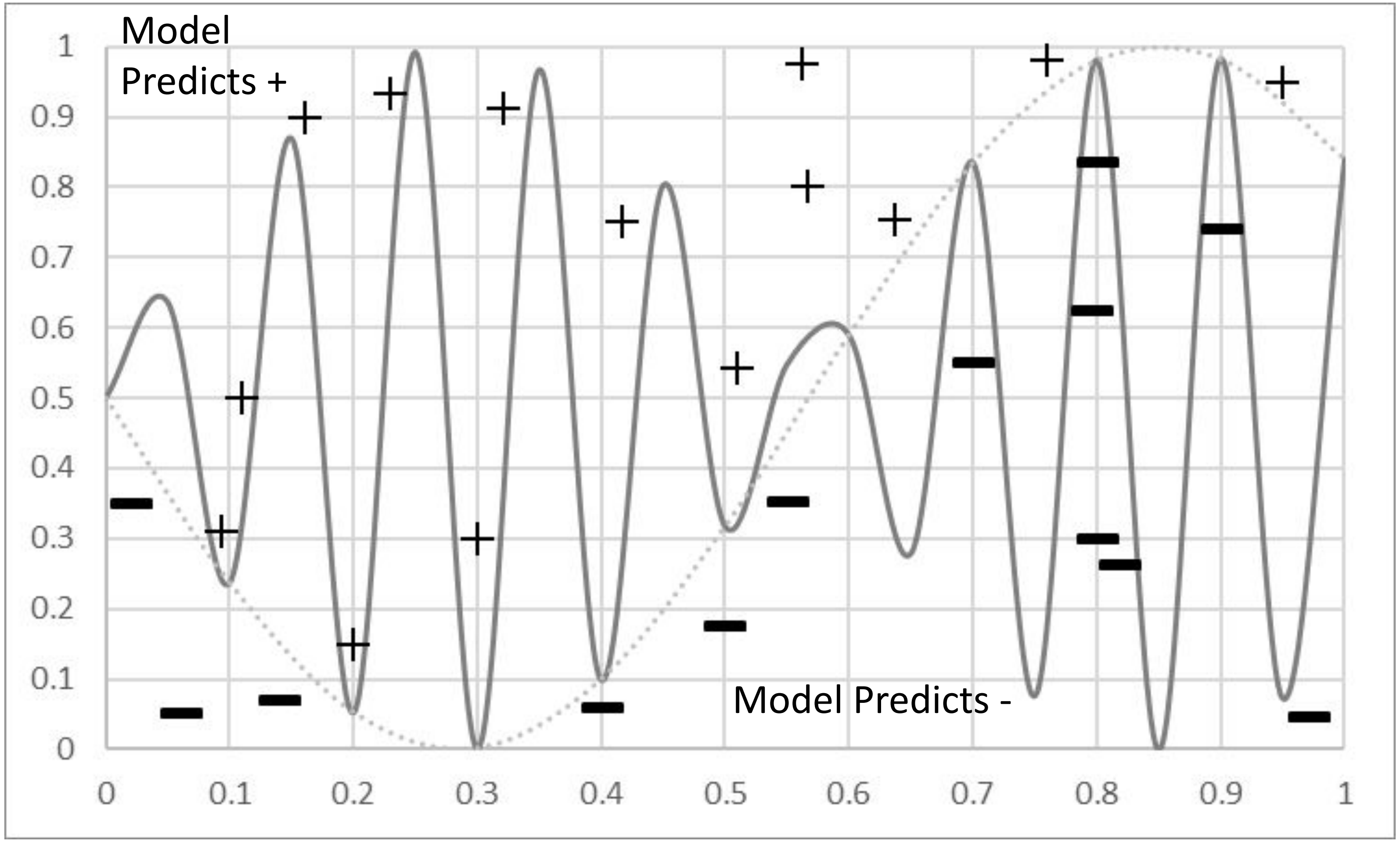
Another way to think about Bias & Variance



Bias and Variance: More Powerful Model

- Powerful Models can represent complex concepts

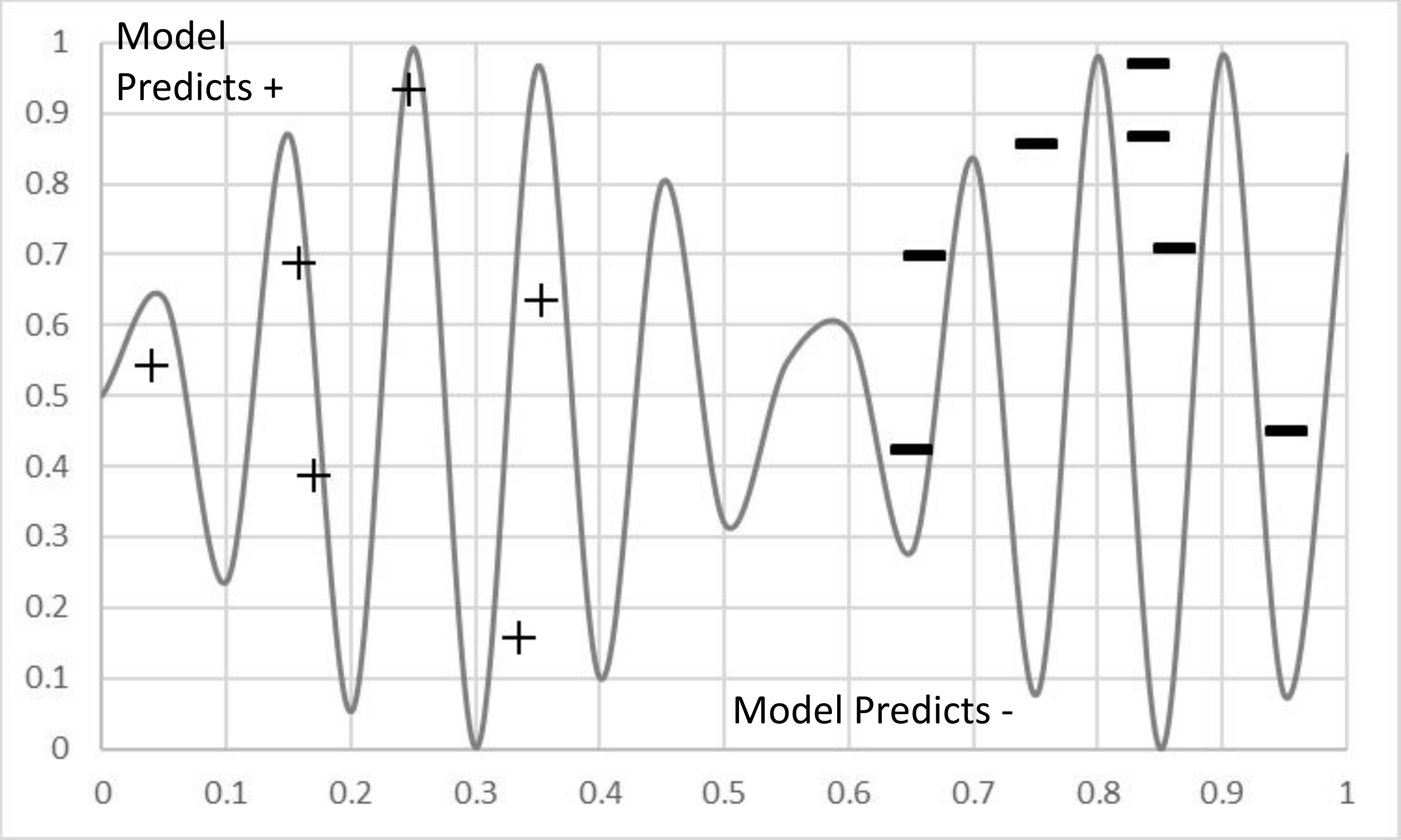
- No Mistakes!



Bias and Variance: More Powerful Model

- But get more data…

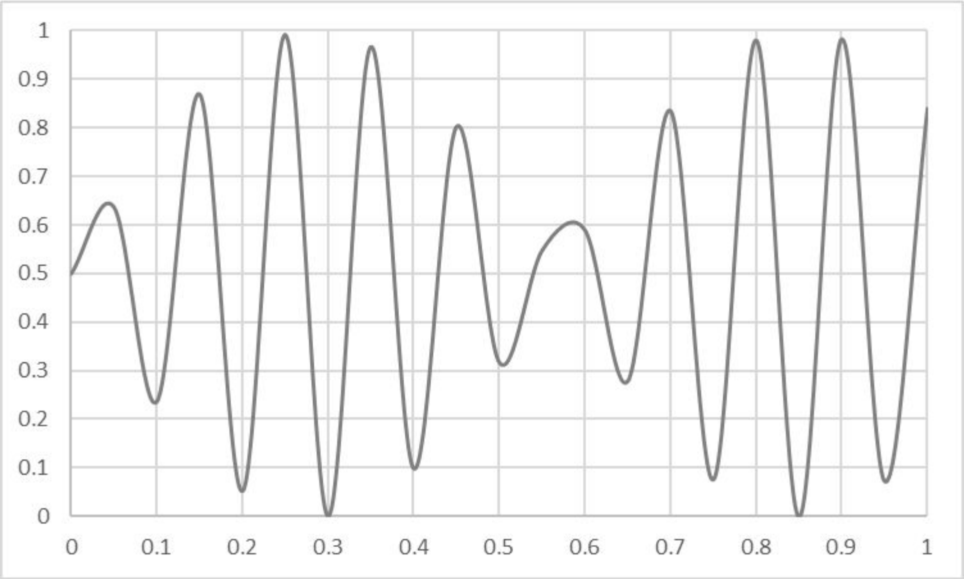
- Not good!



Overfitting vs Underfitting

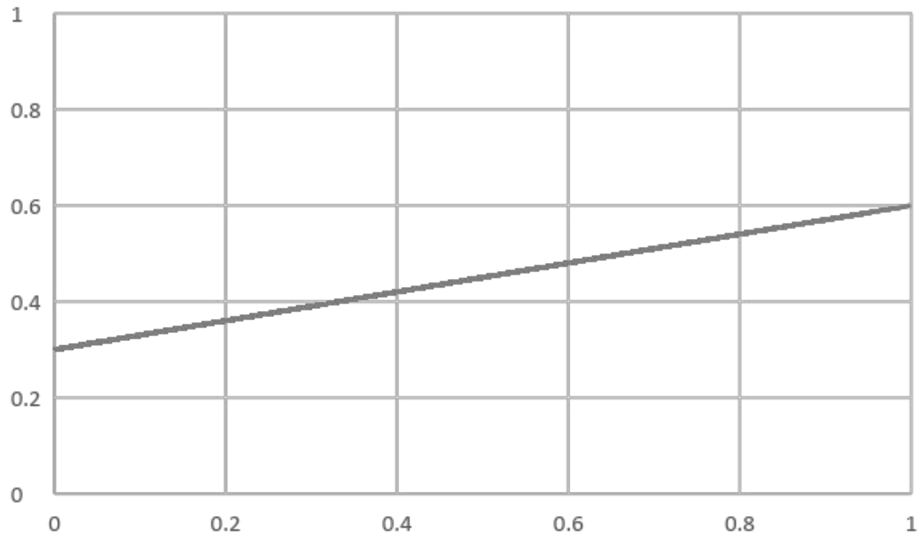
Overfitting

- Fitting the data too well
  - Features are noisy / uncorrelated to concept
  - Modeling process very sensitive (powerful)
  - Too much search

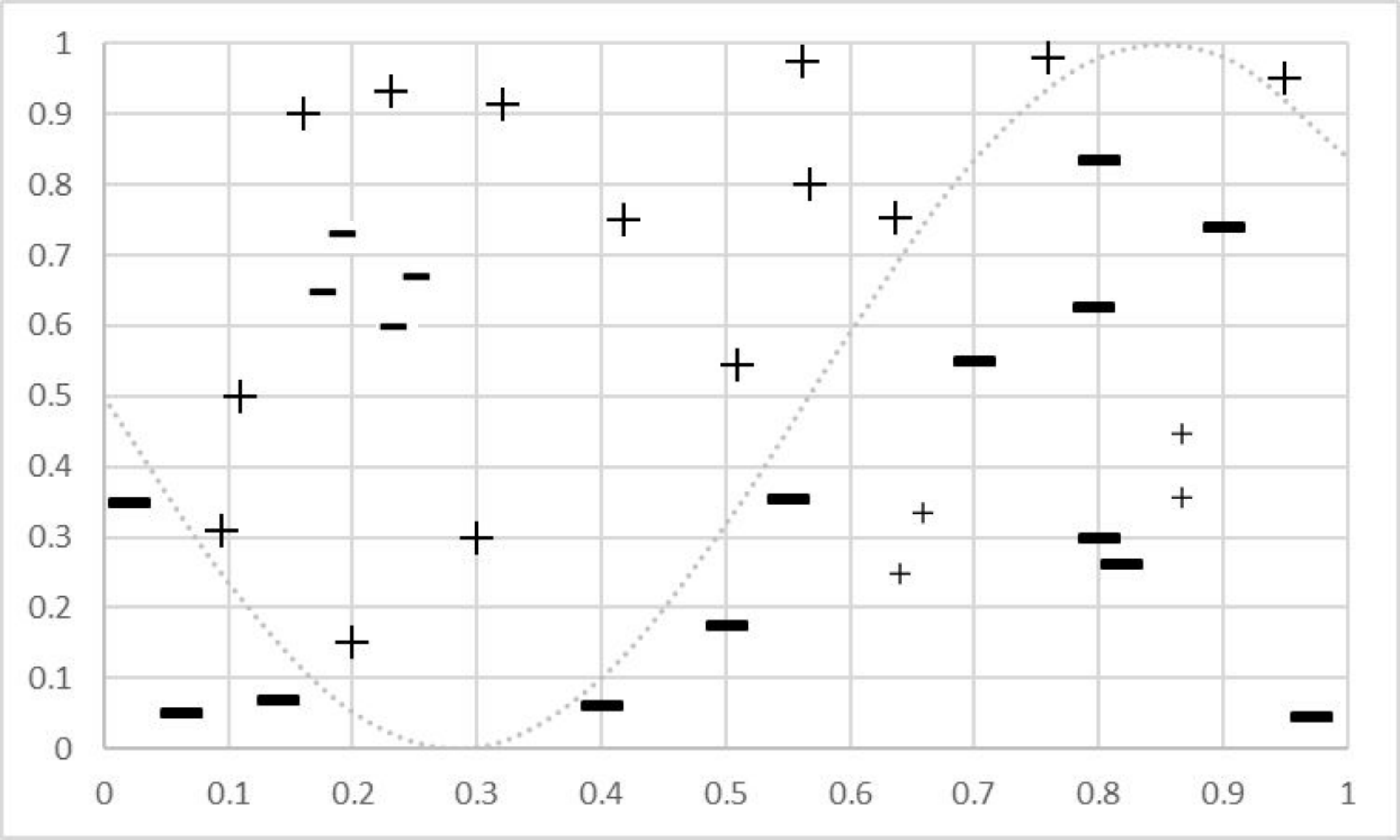


Underfitting

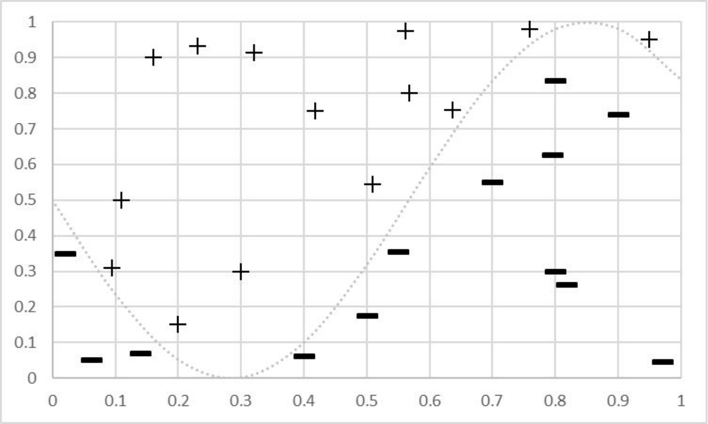
- Learning too little of the true concept
  - Features don't capture concept
  - Too much bias in model
  - Too little search to fit model

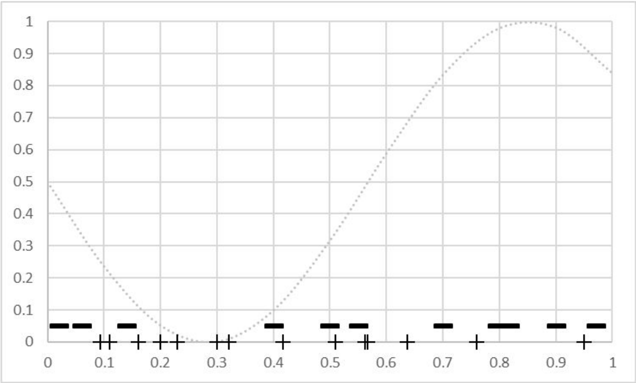


The Effect of Noise



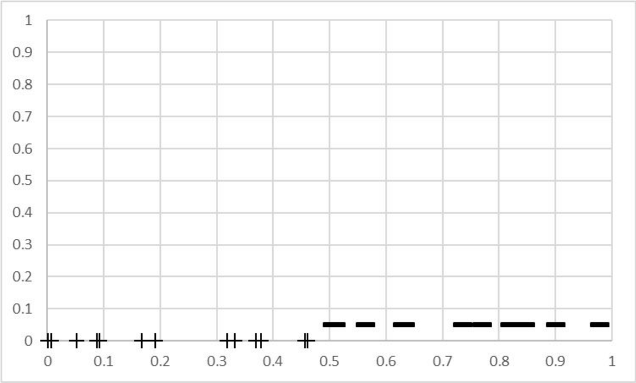
The Effect of Features





Throw out x_2

- Not much info
- Won’t learn well
- Powerful -> high variance



New x_3

- Captures concept
- Simple model -> low bias
- Powerful -> low variance

The Power of a Model Building Process

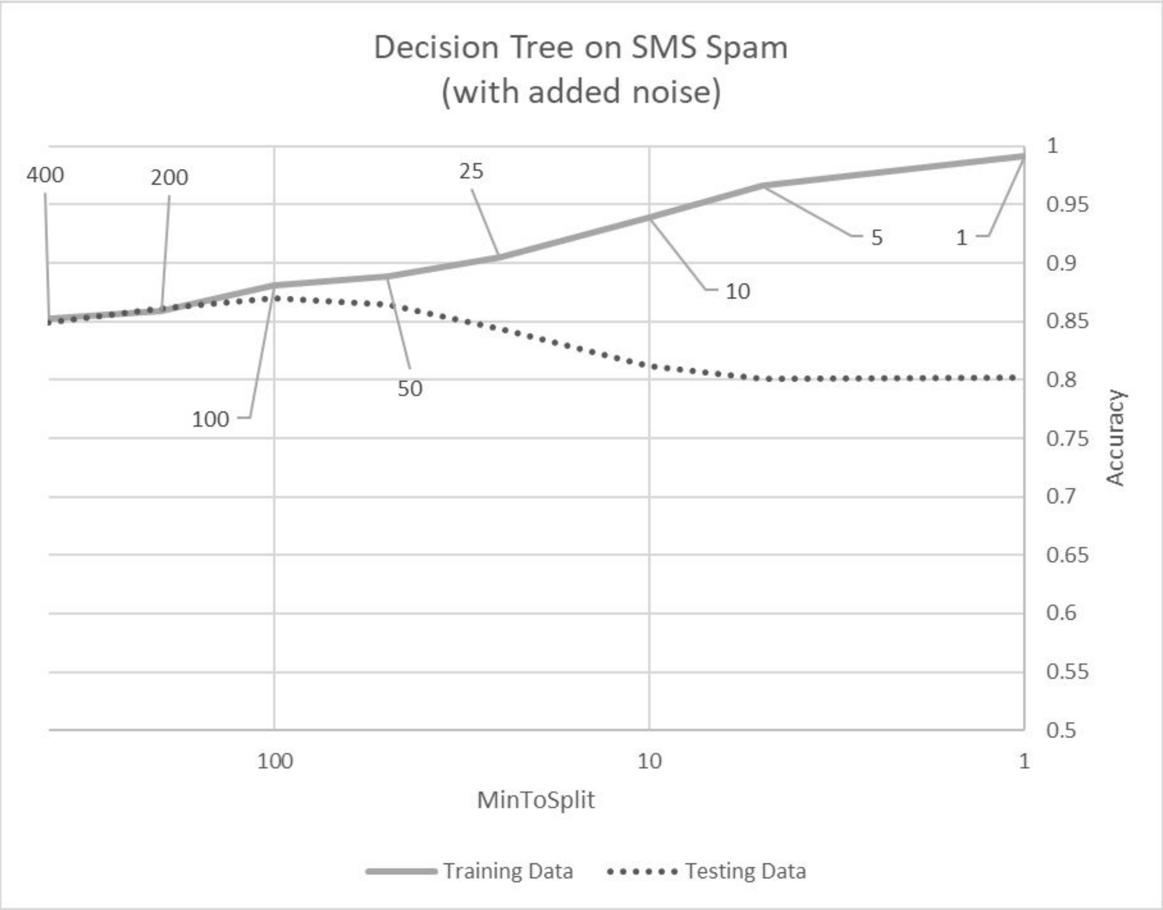
Weaker Modeling Process
(higher bias)

- Simple Model (e.g. linear)
- Fixed sized Model (e.g. fixed # weights)
- Small Feature Set (e.g. top 10 tokens)
- Constrained Search (e.g. few iterations of gradient descent)

More Powerful Modeling Process
(higher variance)

- Complex Model (e.g. high order polynomial)
- Scalable Model (e.g. decision tree)
- Large Feature Set (e.g. every token in data)
- Unconstrained Search (e.g. exhaustive search)

Example of Under/Over-fitting



Ways to Control Decision Tree Learning

- Increase minToSplit
- Increase minGainToSplit
- Limit total number of Nodes
- Penalize complexity

$$Loss(S) = \sum_{i}^{n} Loss(\hat{y_i}, y_i) + \alpha \, Log_2(\# \, Nodes)$$

Ways to Control Logistic Regression

- Adjust Step Size

- Adjust Iterations / stopping criteria of Gradient Descent

- Regularization

$$Loss(S) = \sum_{i}^{n} Loss(\hat{y_i}, y_i) + \alpha \sum_{j}^{\#Weights} |w_j|$$

Modeling to Balance Under & Overfitting

- Data
- Learning Algorithms
- Feature Sets
- Complexity of Concept
- Search and Computation

- Parameter sweeps!

Parameter Sweep

# optimize first parameter
for p in [setting_certain_to_underfit, …, setting_certain_to_overfit]:

    # do cross validation to estimate accuracy

    # find the setting that balances overfitting & underfitting

optimize second parameter
    # etc…

examine the parameters that seem best and adjust whatever you can…

Types of Parameter Sweeps

- Optimize one parameter at a time
  - Optimize one, update, move on
  - Iterate a few times
- Gradient descent on meta-parameters
  - Start somewhere 'reasonable'
  - Computationally calculate gradient wrt change in parameters
- Grid
  - Try every combination of every parameter
- Quick vs Full runs
  - Expensive parameter sweep on 'small' sample of data (e.g. grid)
  - A bit of iteration on full data to refine
- Intuition & Experience
  - Learn your tools
  - Learn your problem

Summary of Overfitting and Underfitting

- Bias / Variance tradeoff a primary challenge in machine learning
- Internalize: More powerful modeling is not always better
- Learn to identify overfitting and underfitting
- Tuning parameters & interpreting output correctly is key