Data Mining & Machine Learning

CS37300
Purdue University

Oct 2, 2023

Today's topics

- Finish Linear regression
- What is "error"?
- Overfitting
- Model Selection / hyper-parameter tuning

Setup

- Data $\{x_i, y_i\}$ Total *n* data points, $x_i \in R^d, y \in R$.
- $y \sim w^\top x$
- Cost function:

$$\min_w \sum_i |y_i - w^\top x_i|^2$$

- Interpretation: Minimize the "residuals" $(y_i - w^\top x_i)$ i.e. leftover after fitting the model

Last time

- Closed form solution
- Calculating inverses to get the closed form solution
- Extension to GLMs
- Interpretability
- Evaluation

A taste of evaluation

- How do we check whether the learnt model is reasonable?
- MSE
- Coefficient of determination or R^2 statistic = $\frac{\sum_i (y_i - w^T x_i)\text{^}2.}{\sum_i (y_i - \bar{y})\text{^}2}$
  - Intuitively, ratio of variance explained and total variance

Ridge regression

- Alternate cost function using regularization:
  - $\min_w \sum_i |y_i - w^\top x_i|^2 + \lambda ||w||^2$
- "Want to fit the data but don't want w to be too big"
- Also has closed form solution: $w^\star = (X^T X + \lambda I)^{-1} X^T y$
  - The inner matrix is always invertible
- Bias-variance tradeoff (more on this later!)

Sparse modeling

- Instead of using all the features, start with using a few
- Iteratively add or remove features that improve “performance” (e.g. MSE or R^2)
- Alternatively, use LASSO

$$\min_w \sum_i |y_i - w^\top x_i|^2 + \lambda \left|\left|w\right|\right|_1 \quad ,$$

where $\left|\left|w\right|\right|_1 = \sum_i |w|$ is the L1 norm of w.

- Commonly used: Elastic net

$$\min_w \sum_i |y_i - w^\top x_i|^2 + \lambda_1 \left|\left|w\right|\right|^2 + \lambda_2 \left|\left|w\right|\right|_1$$

Error

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- Would you use this classifier?
- Confusion Matrix:

	Classified Good	Classified Defective
Actually good	990 (True Positive)	9 (False Negative)
Actually defective	1 (False Positive)	0 (True Negative)

  - Good: TP, TN
  - Bad: FP, FN

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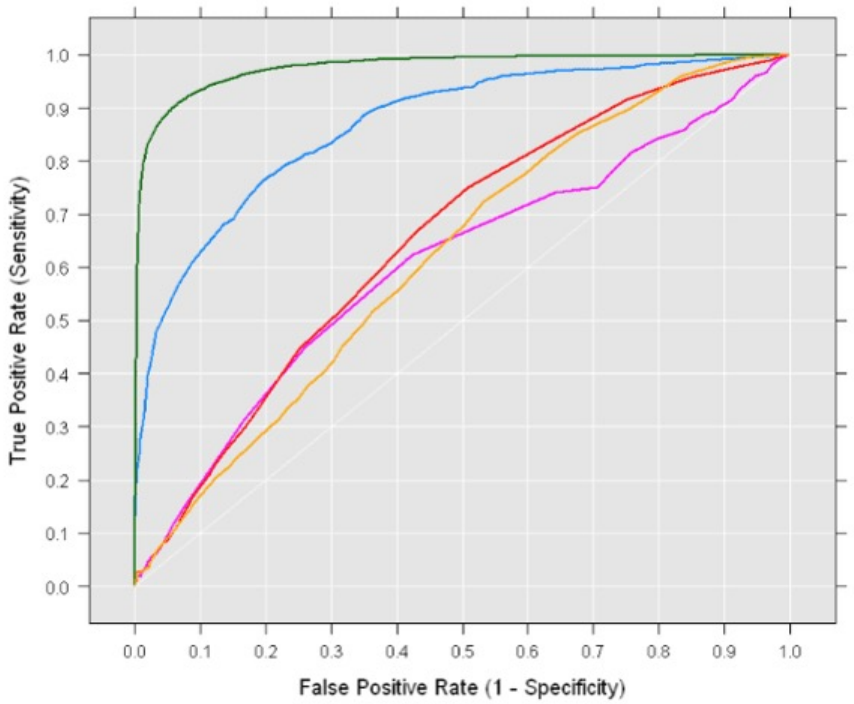
- Regression Error Measures:
  - Mean Absolute Error: $\frac{1}{N}\sum_{i=1}^{N}|\hat{y}_i - y_i|$
  - Mean Squared Error: $\frac{1}{N}\sum_{i=1}^{N}(\hat{y}_i - y_i)^2$

Some typical measures

- Area Under the Curve (AUC): Used to measure a tradeoff between true positives and false positives
  - True Positive Rate / Recall / Sensitivity: TP / (TP+FN)
  - False Positive Rate (1- specificity): FP / (FP + TN)
  - Receiver Operating Curve (ROC): Tradeoff between TPR and FPR
- Better classifiers have a higher "area under the curve"



Bias/Variance trade-off

Bias/Variance

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  - Move to a higher dimension
  - Pick small K in KNN
  - Large decision trees
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How can we tell?

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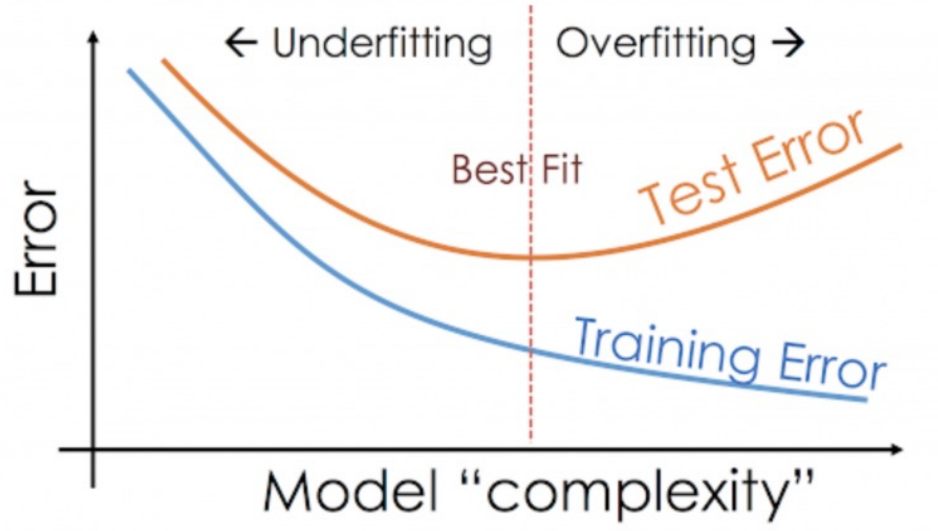
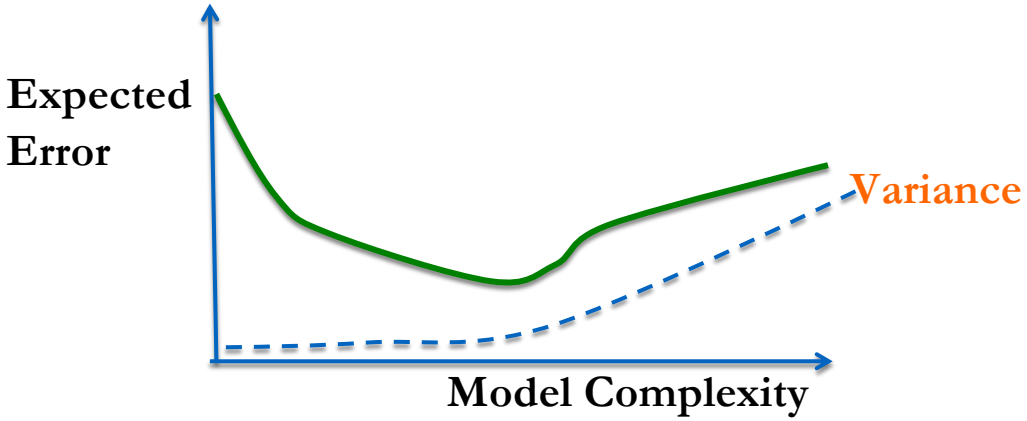


- For a given data set size, there is a trade-off between
  - Model expressiveness (more expressive → smaller training error rate)
  - Overfitting (more expressive → true error rate > training error rate)

The "Variance" of the Learner



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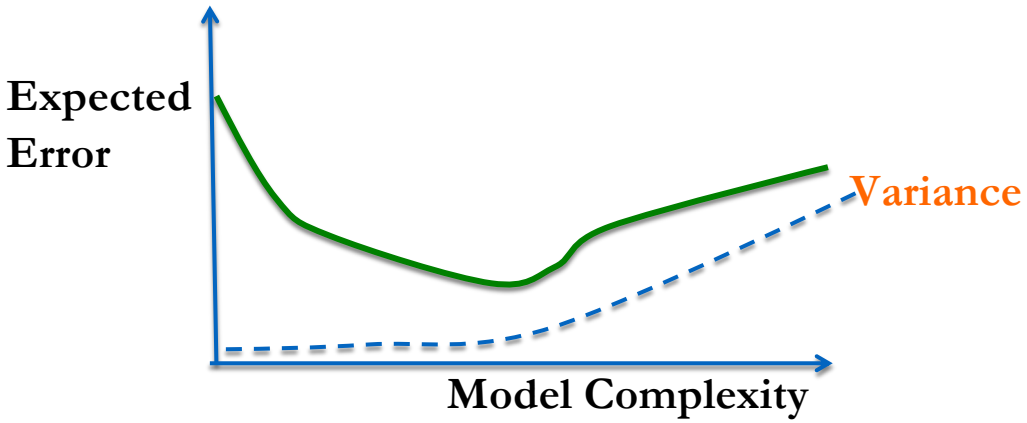

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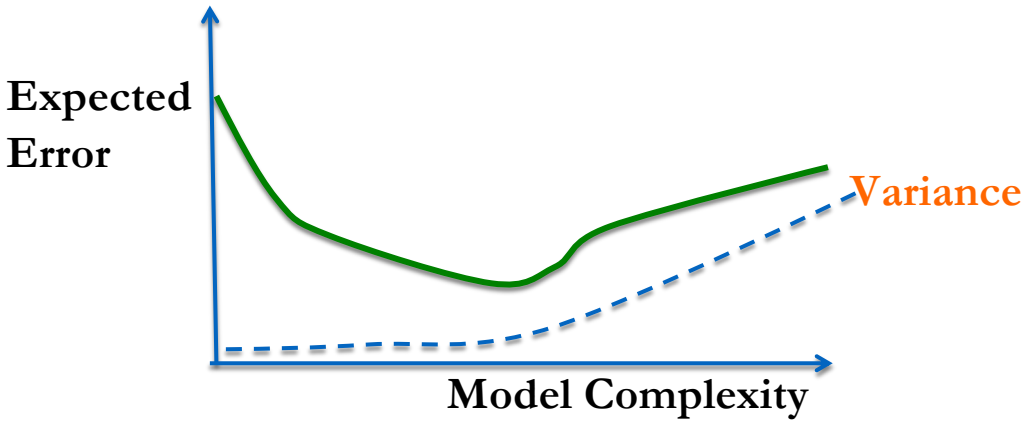

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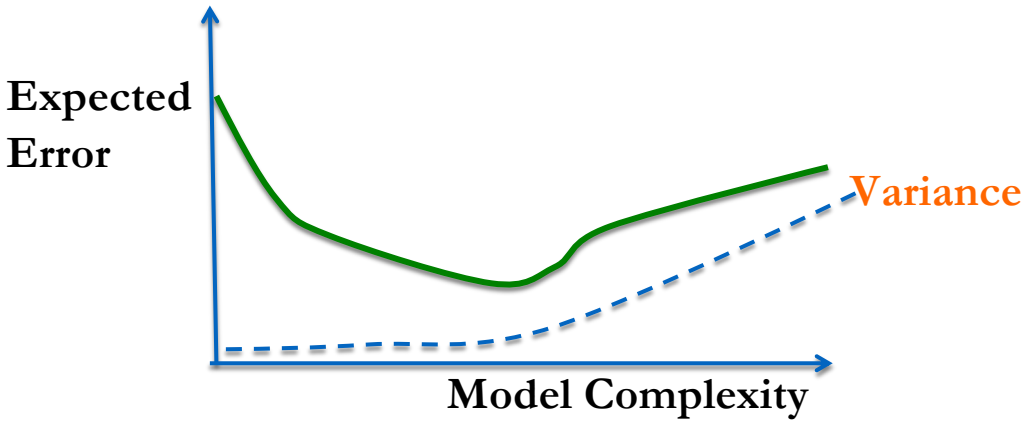

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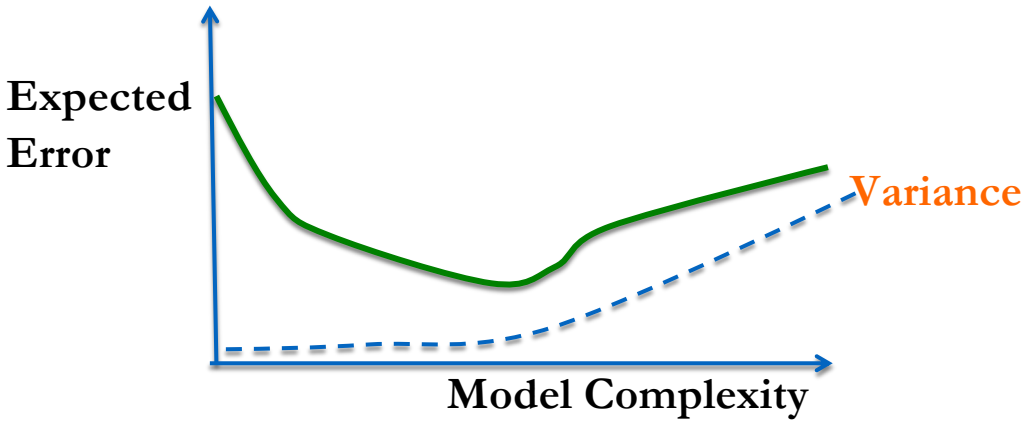

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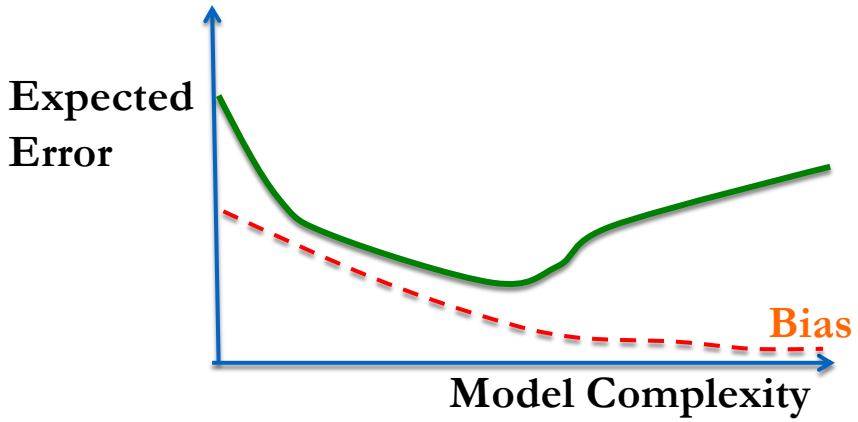
Variance increases with model complexity!

Bias of the Learner



Simpler models have higher "bias": "Trust data less"
meaning they strongly favor specific types of solutions

How likely is the learner to identify the target hypothesis?

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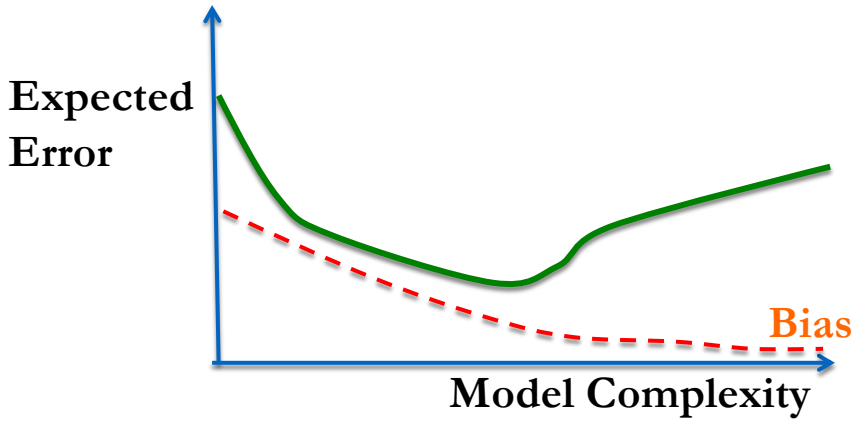

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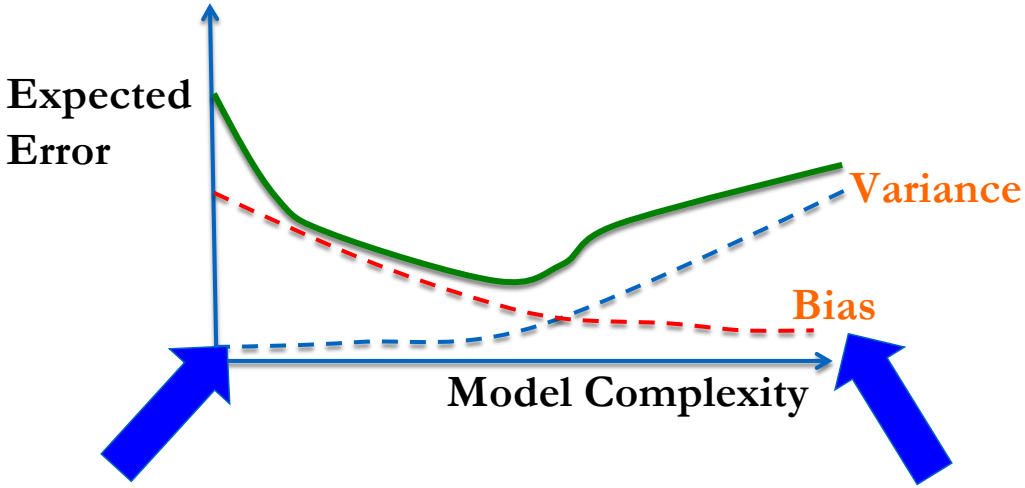
- **What will happen if we train on a different sample?**

Bias is high when the model is too simple

Model Complexity



Simple models:
High bias and low variance

Complex models:
High variance and low bias

Expected Error ≈ Bias + Variance

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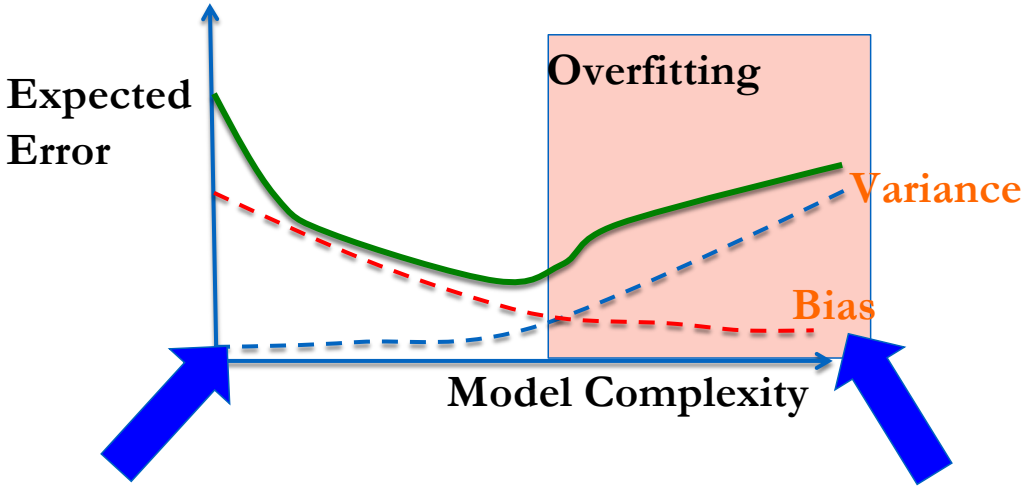

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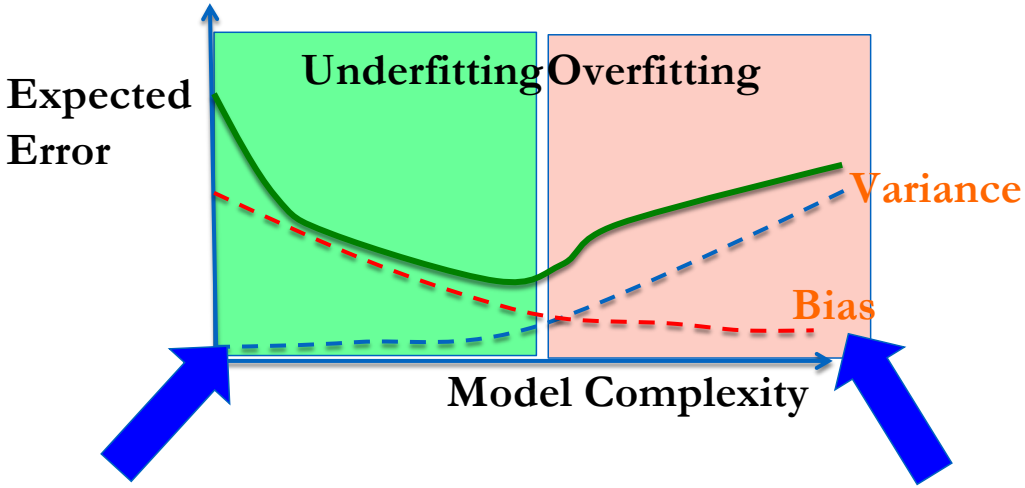

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Bias-Variance Tradeoff in Practice

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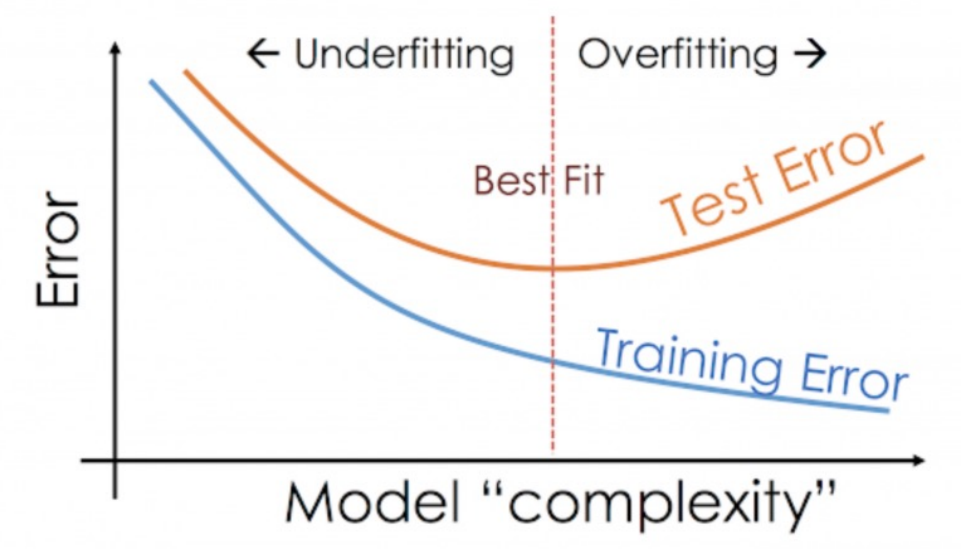
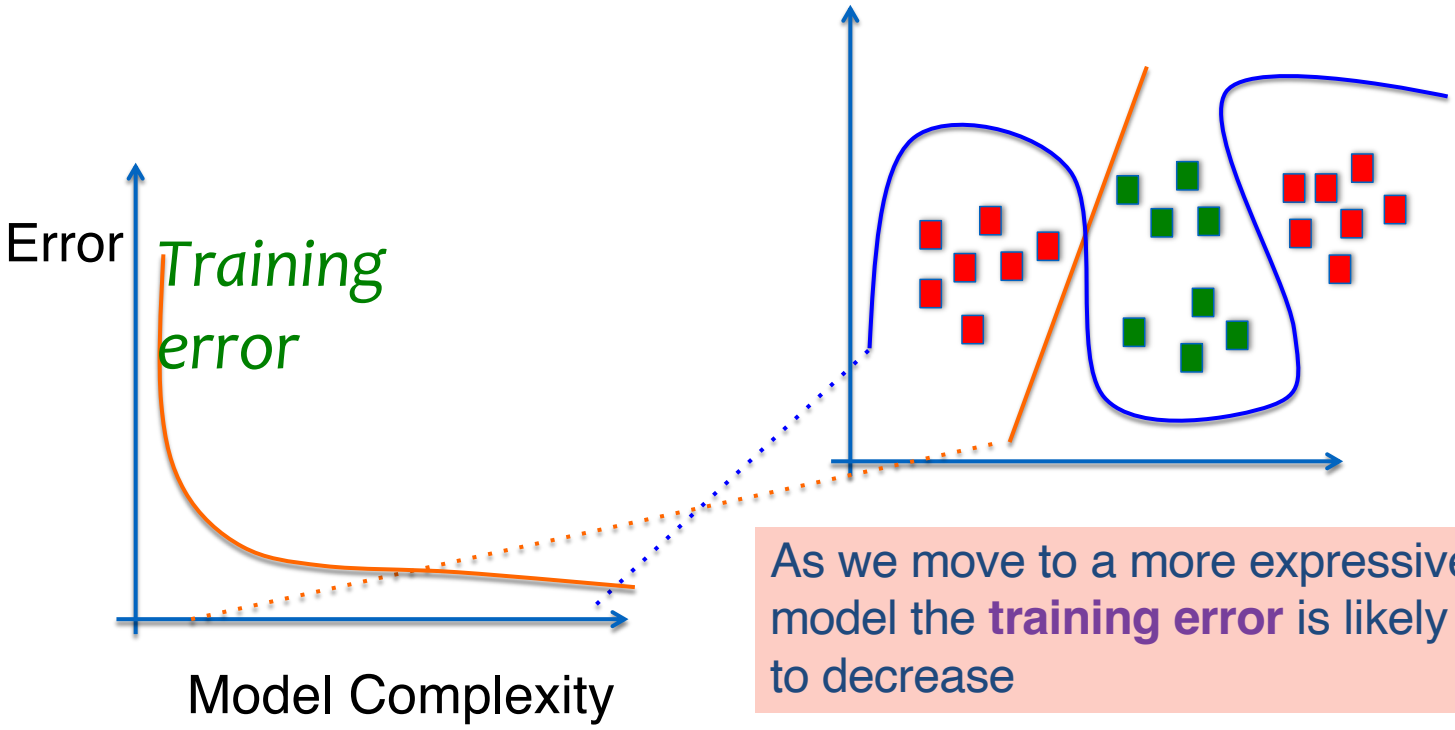
- *How can we diagnose each one of these scenarios?*

Overfitting



- Question 1: How do we detect overfitting?
- Question 2: How do we prevent / correct overfitting?

Bias-Variance Analysis



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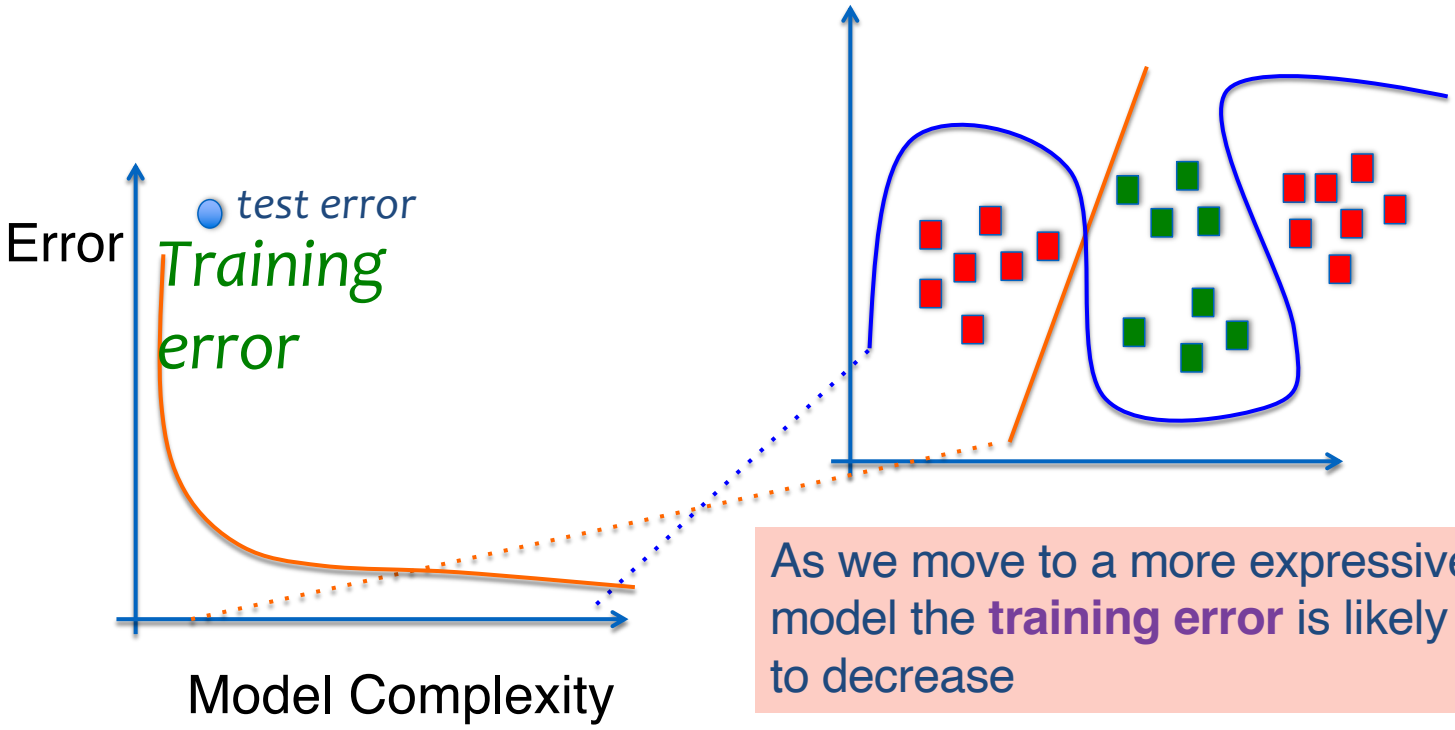
Bias-Variance Analysis

*When we are using a **simple model**, it's very likely we'll underfit resulting in a **high test** error*



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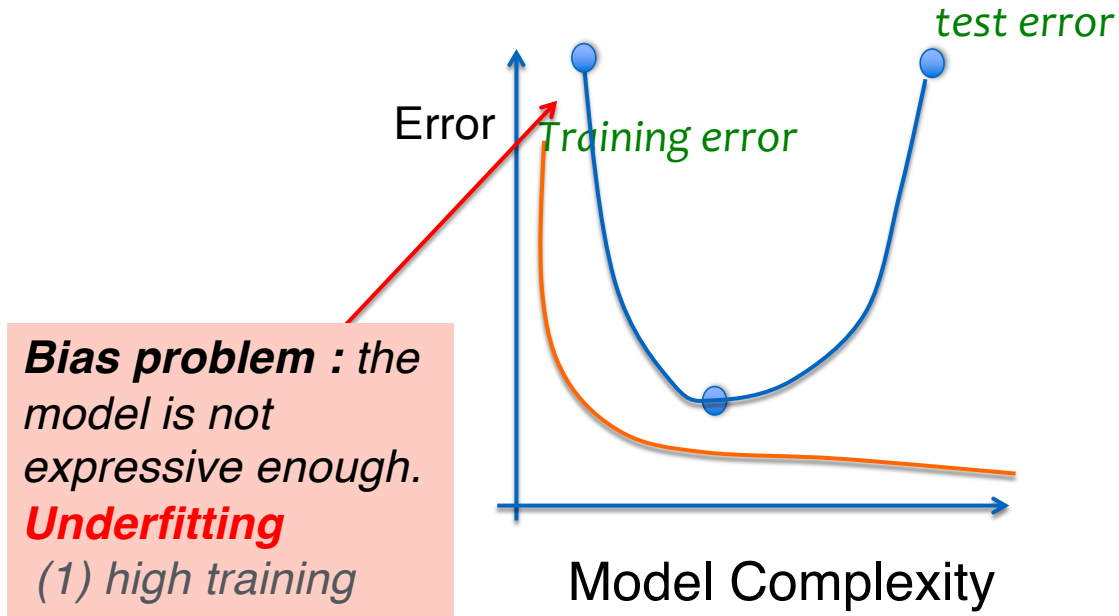
Interpolating over the points: two curves that we can use for ***diagnosis***



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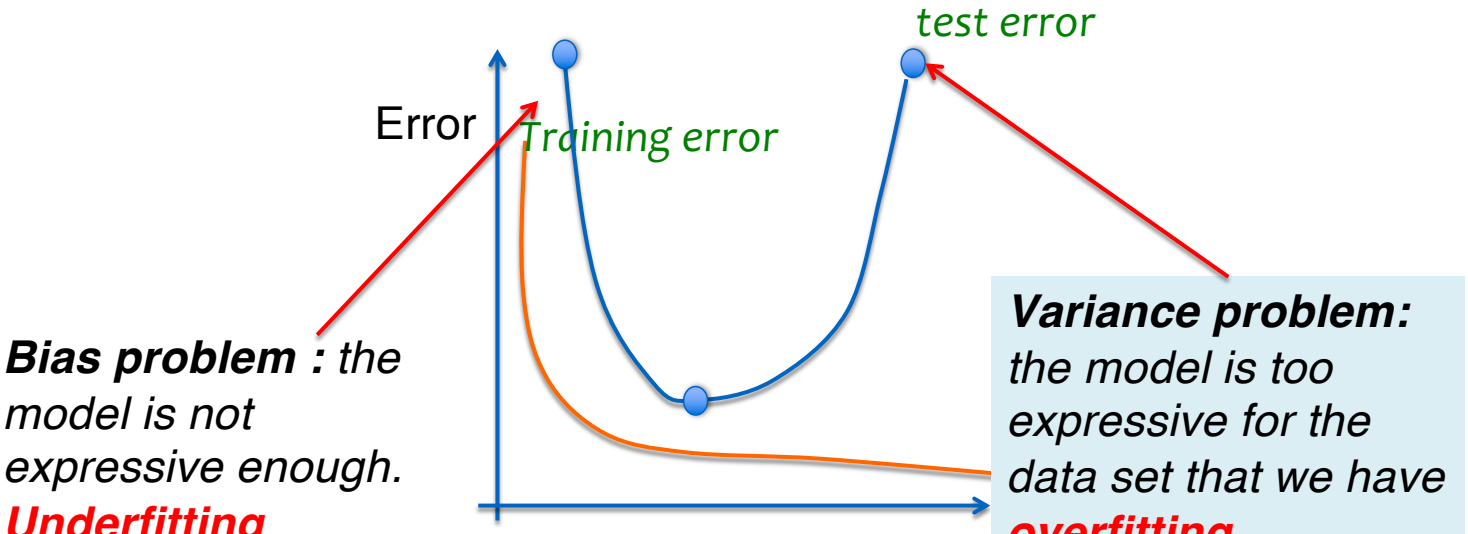

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Variance problem: *the model is too expressive for the data set that we have*
overfitting
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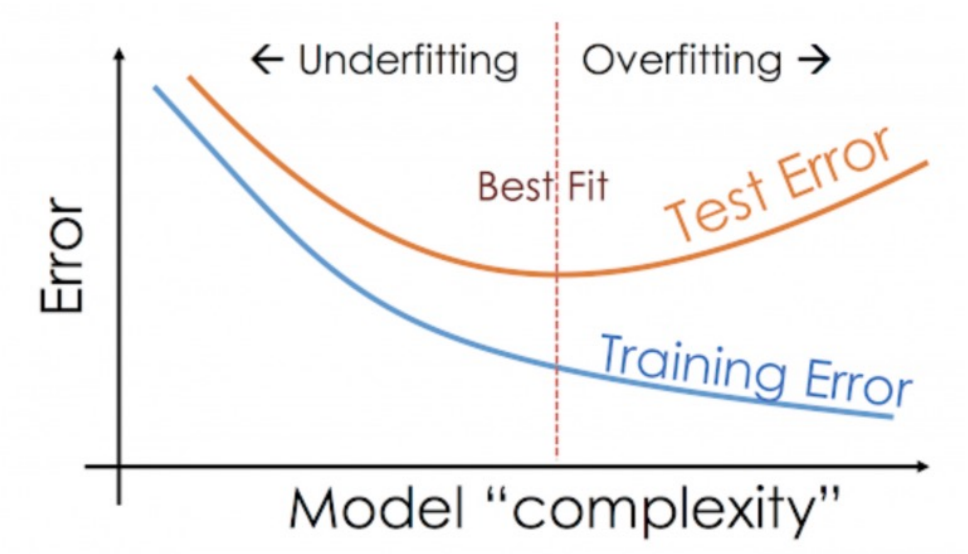
Overfitting



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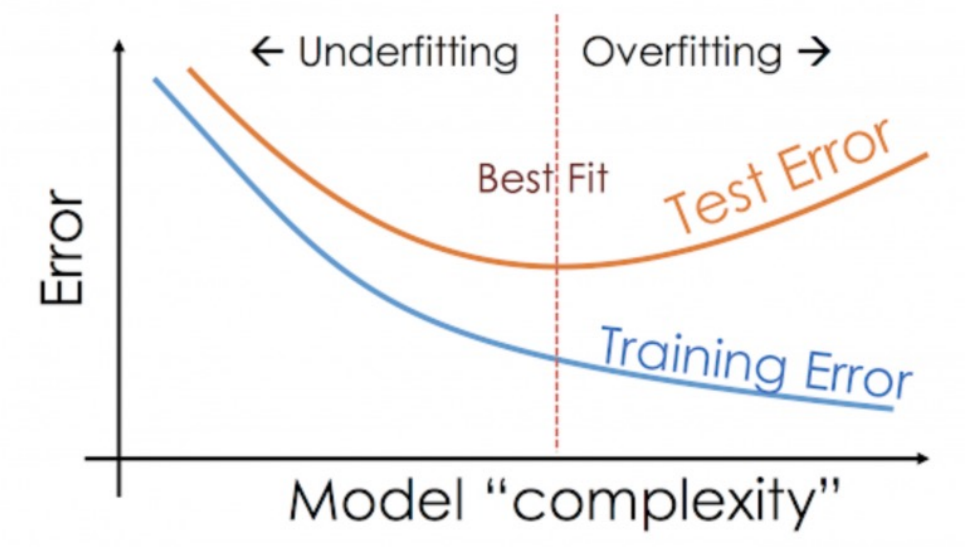

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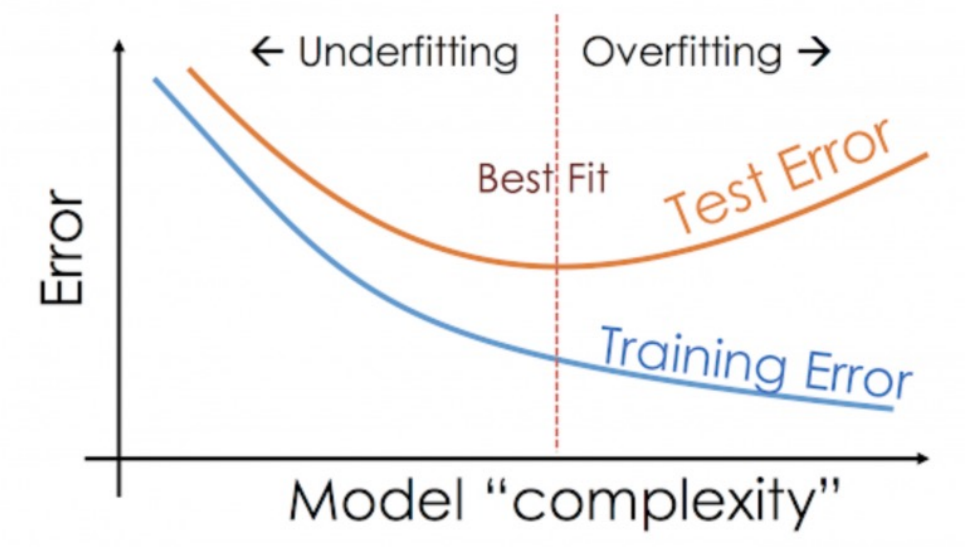
Preventing / Correcting Overfitting



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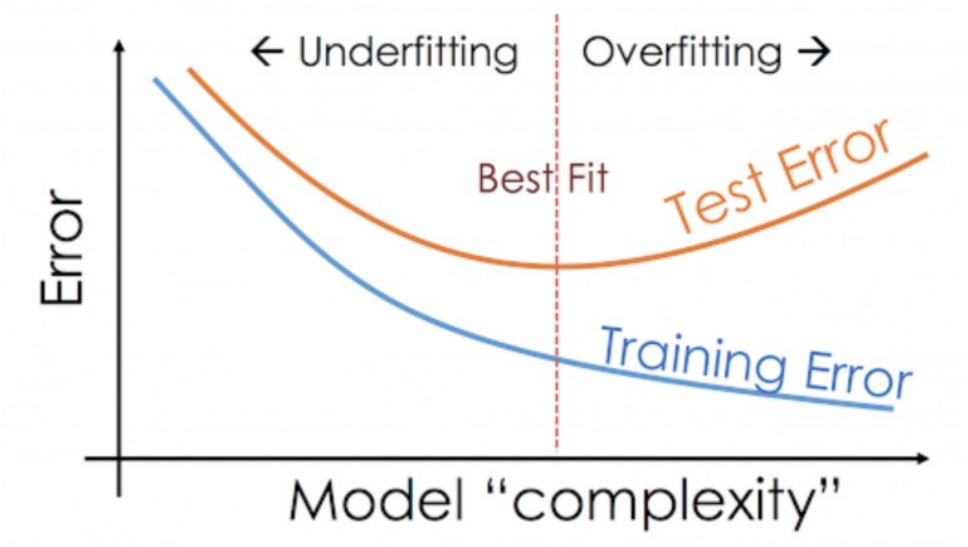

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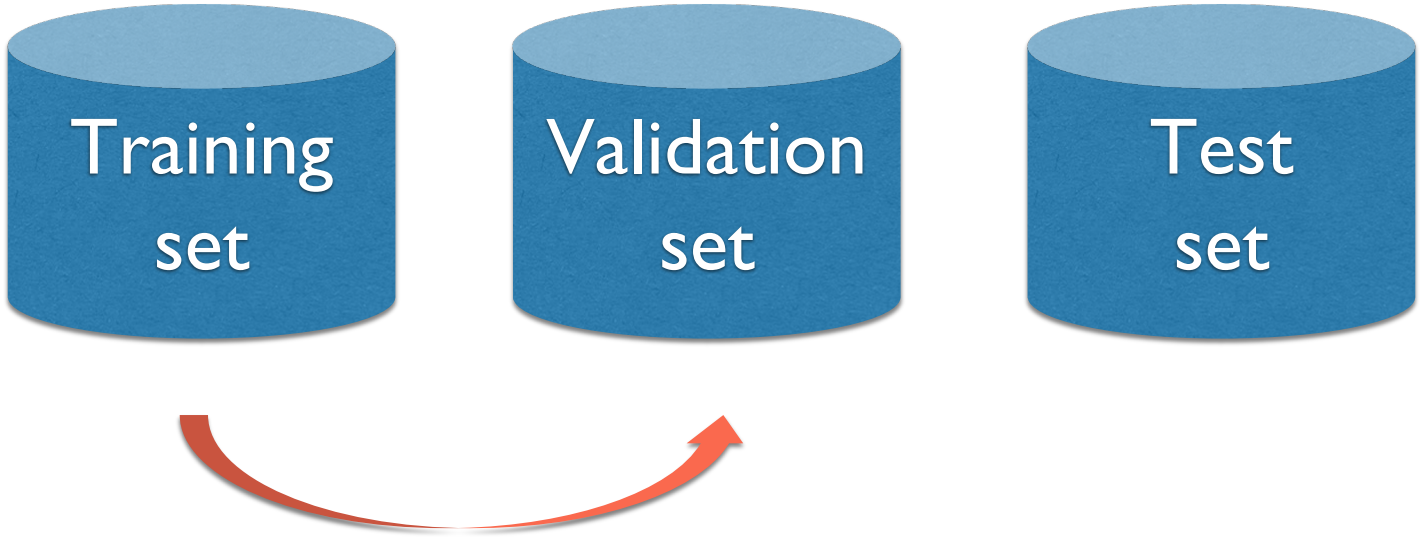
    (e.g., k in kNN, bandwidth in kernel regression, C in Soft-SVM)
  - Sometimes more involved: e.g., post-pruning in decision trees
- A few ways to do this:
  - Validation set (or cross-validation)
  - Theoretical approaches [Structural Risk Minimization]

Training, Validation, Testing

- Split data set into **three** data sets: **training**, **validation**, **test**

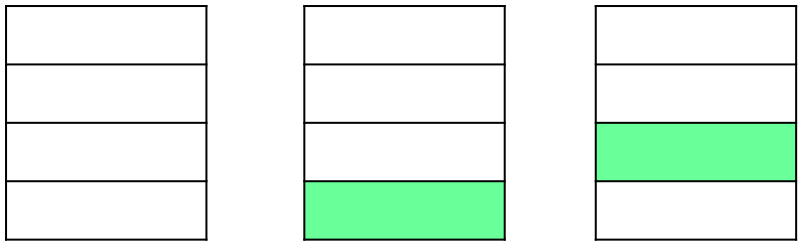


Try different hyper-parameters
(for instance: C=0.1, C=1, C=10 for SVM, or k=1,2,3,…n for kNN)

Report test error rate for the hyper-parameter value
that gave smallest validation error rate

Cross-validation

- Problem: What if the training set is an "unlucky" distribution
  - Error on the test set doesn't match real data
- Solution: Use *all* of the data as test data
  - But then we don't have any data to train on!
- Instead, cross-validation
  - Multiple training/test runs
  - Each uses a different subset as test data



Cross-validation

- **K-fold cross-validation**:
  - Randomly partition the training data into K equal-size subsets $S_1,\ldots,S_K$
  - For each i
    - Train on $S_1 \cup \cdots \cup S_{i-1} \cup S_{i+1} \cup \cdots \cup S_K$ (all the data except S_i)
    - Call this classifier $\hat{h}_i$
    - Evaluate error rate on S_i : $\text{error}_{S_i}(\hat{h}_i)$
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- We can use this to tune hyper-parameters
  - For each setting of the hyper-parameters
  - Run K-fold cross validation
  - Choose the hyper-parameter values with lowest cross-validation error
  - Retrain on the **entire** training set, using the chosen hyper-parameter values

Cross-validation

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Cross-validation

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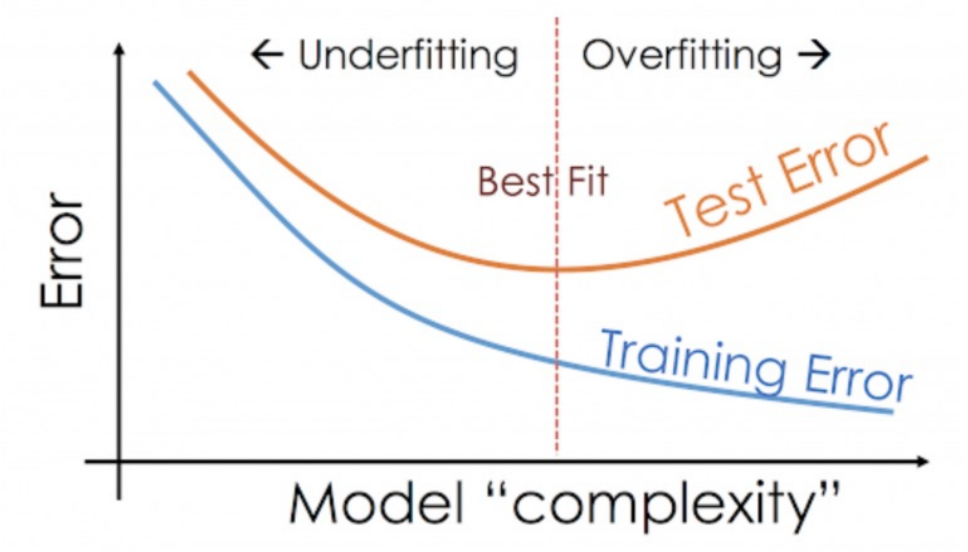
- Most popular in practice: K=10
- If K=n, it's called "leave one out" cross-validation:
  - Every training point (x_i,y_i) gets its own fold $S_i=\{(x_i,y_i)\}$
  - But this is computationally expensive
  - Also can sometimes have higher variance

Cross-validation

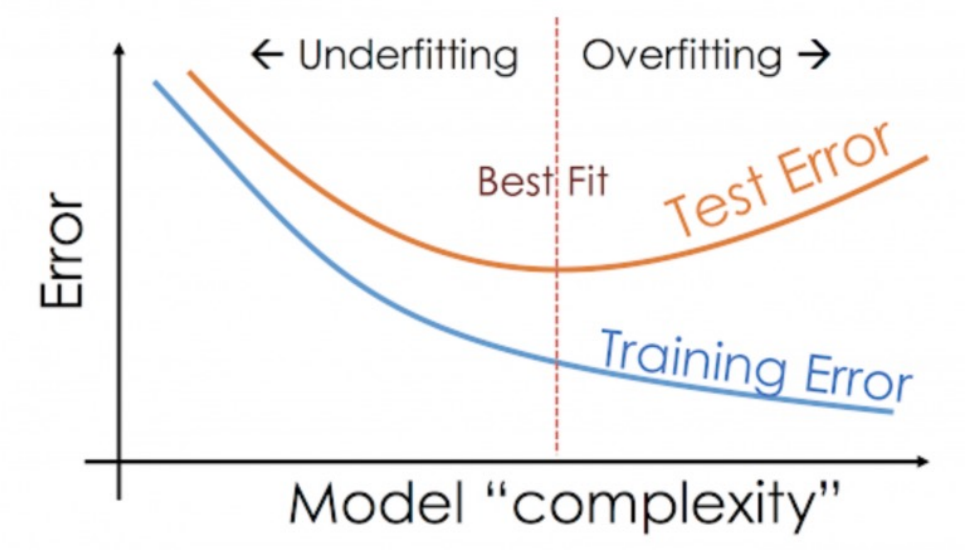
- How do we pick K?
- Most popular in practice: K=10
- If K=n, it's called "leave one out" cross-validation:
  - Every training point (x_i,y_i) gets its own fold $S_i=\{(x_i,y_i)\}$
  - But this is computationally expensive
  - Also can sometimes have higher variance
- To estimate the error rate in the end,
  we would still need a separate held-out test set

Preventing / Correcting Overfitting



- Other approaches:
  - Regularization (e.g., minimizing ||w|| in SVM optimization)
  - Dimensionality reduction / feature selection

Preventing / Correcting Overfitting



- Other approaches:
  - Regularization (e.g., minimizing ||w|| in SVM optimization)
  - Dimensionality reduction / feature selection
- Note: sometimes the appropriate units for x-axis aren't easy to identify.
  - Sometimes large neural networks overfit less than smaller
  - Possibly because the optimization finds good solutions more easily