INTRODUCTORY APPLIED MACHINE LEARNING

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Today:

- Overfitting
- Model attribute selection

Outline

- Goal of the lecture
- Overfitting
- Bias-variance tradeoff
- Cross-validation
- Information criteria

Goals

- After this, you should be able to:
  - Understand the risk of overfitting
  - Quantitatively assess the performance of different models
  - Calculate information criteria for regression models
  - Estimate model prediction error using cross-validation

Review – Coefficient of Determination R^2

- R^2 is proportion of the variance in the dependent variable that is predictable from the independent variable, i.e.,

$$R^2 = \frac{SSR}{SST} = \frac{1 - SSE}{SST},$$

where $SSE = \sum_{i=1}^{N} (y_i - \hat{y}_i)^2$

- Usually a larger R^2 implies the model better fits the data
- SSE is also known as <u>residual sum of squares</u> (RSS)
- Note that SSE is calculated with <u>the same set of data</u> (i.e., training data) that are used to generate the model $\hat{y}$

Response Surface Methodology

- The true relationship between the response variable y and the explanatory variables $\boldsymbol{x}$ is usually unknown
- The approximation of the response variable using a set of explanatory variable is called response surface methodology
- In many practical application, high-order polynomial models are employed, i.e.,

$$\hat{y} = f(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \cdots + \beta_M x^M$$

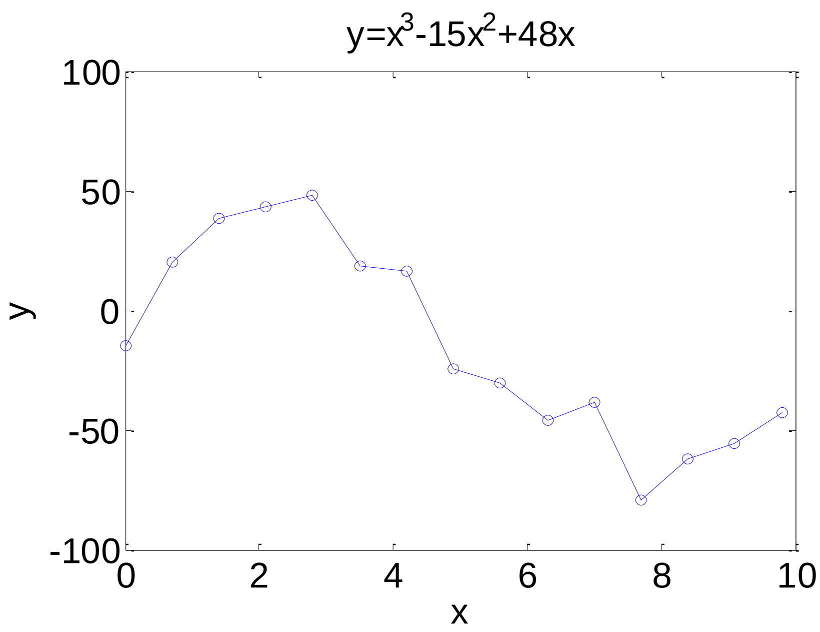
$$\hat{y} = f(x_1, x_2) = \beta_0 + \beta_{11} x_1 + \beta_{12} x_2 + \beta_{21} {x_1}^2 + \beta_{22} {x_2}^2 + \cdots$$

- High-order polynomial models usually gives larger R^2 (why?), but that means high-order models are better???

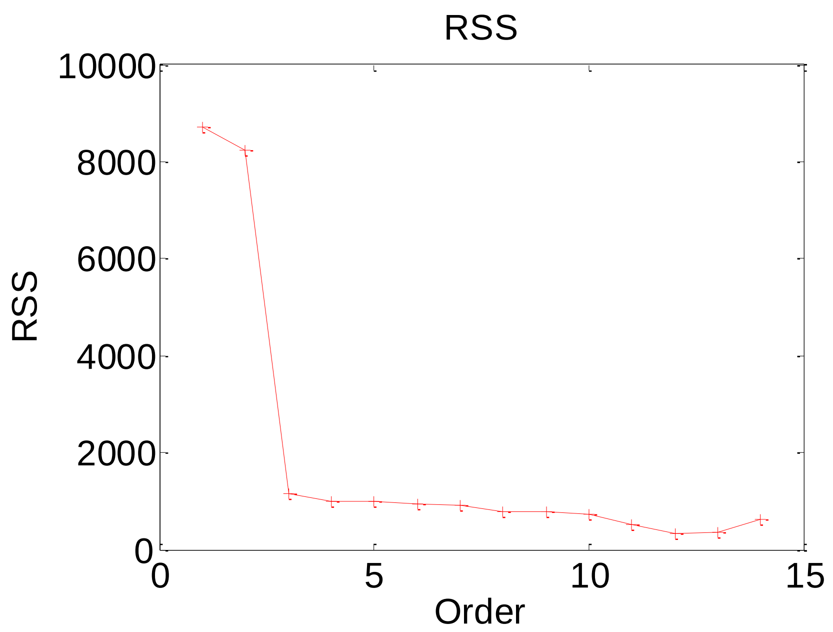
Example – Polynomial Curve Fitting

- Assume the true model is a 3rd-order polynomial with random noise
- RSS decreases when the order of the polynomial increases

3rd-order Polynomial with **Noise**



RSS of Models with Different Orders



Example MATLAB Code

```
clear; close all;
% generate data
x=(0:.7:10)';
y=x.^3-15*x.^2+48*x+10*randn(length(x),1);
plot(x,y, '-ob'); set( gcf, 'Color', 'w');
xlabel('x', 'FontSize', 16); ylabel('y', 'FontSize', 16);
set(gca,'FontSize', 16); title('y=x^3-15x^2+48x');

% regress y with different order of x
for i=1:length(x)-1
    X(:,i)=power(x,i);
    [b,bint,r]=regress(y,[ones(length(x),1) X(:,1:i)]);
    RSS(i)=r'*r;
end
figure; plot((1:14), RSS, '-+r'); set( gcf, 'Color', 'w');
set(gca,'FontSize', 16); xlabel('Order', 'FontSize', 16);
ylabel('RSS', 'FontSize', 16); title('RSS');
```

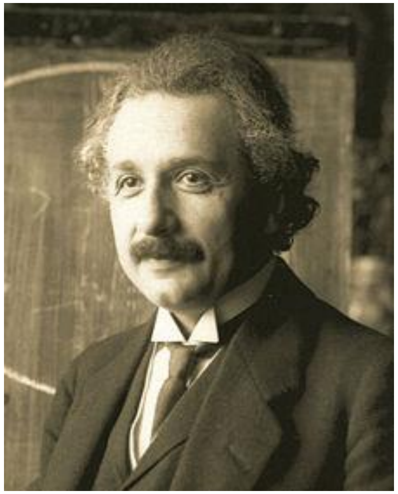
Occam's Razor

William of Occam

Occam's razor:

"*entia non sunt multiplicanda praeter necessitatem*"

Entities should not be multiplied beyond necessity

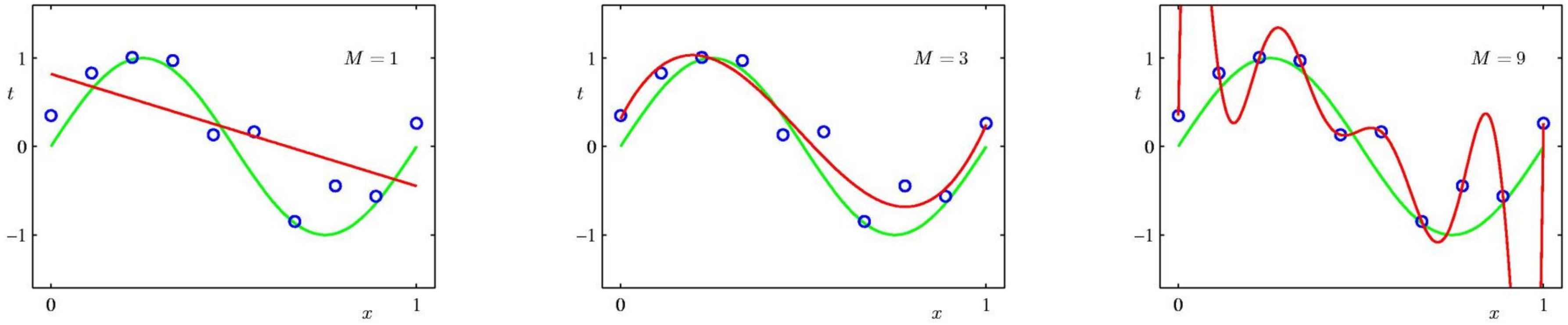


Everything should be made as simple as possible, but not simpler

Albert Einstein

Overfitting – the Problem of Complex Model

- The phenomenon in which a model well predicts the outcome with the data points used to develop the model, but subsequently fails to provide valid predictions in unseen cases
- Data drawn from a sinusoidal model $\sin(x/_{2\pi})$ with noise



Bishop. *Pattern Recognition and Machine Learning*

- Overfitting happens when a model is capturing idiosyncrasies of the data rather than generalities

Understanding Overfitting

- What is the source of overfitting?
- Why do some models overfit more than others?
- How does one tackle overfitting?

Model Performance Estimation

- A loss function is defined as the difference between the true and estimated target values, i.e.,

$$L\big(y, f(\boldsymbol{x})\big) = \begin{cases} \big(y - f(\boldsymbol{x})\big)^2 & \text{squared error} \\ |y - f(\boldsymbol{x})| & \text{absolute error} \end{cases},$$

where f is the model that estimates the target $y \in \Re$ from measurements $\boldsymbol{x} \in \Re^M$, i.e., $\hat{y} = f(\boldsymbol{x})$

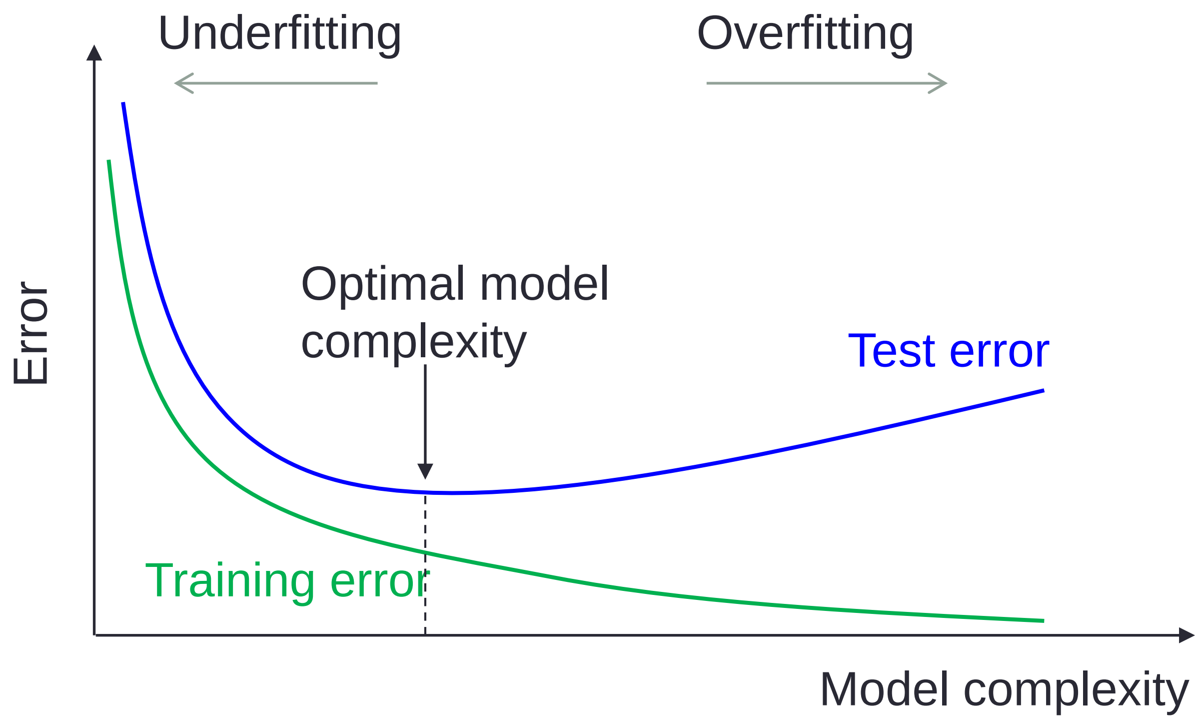
- The training error is $\overline{err} = \frac{1}{N}\sum_{i=1}^{N} L\big(y_i, f_i(\boldsymbol{x})\big)$, where N is the number of samples
- The test (generalization) error is $err = E\big[L\big(y, f(\boldsymbol{x})\big)\big]$

Measuring Model Complexity

- The complexity of the model can be measured by the "degrees of freedom" (number of parameters)
- What is the complexity of this model?

$$\hat{y} = f(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \cdots + \beta_M x^M$$

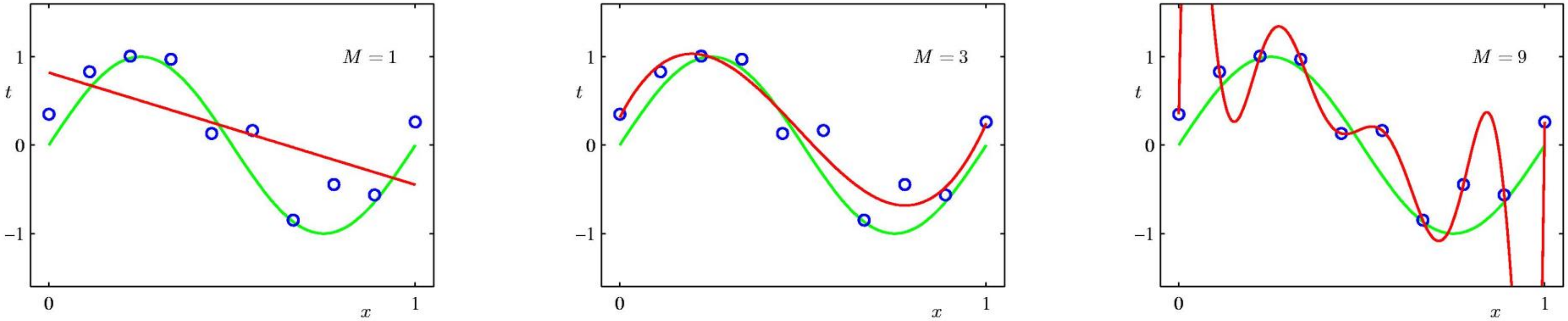
Optimal Model Complexity



- Training error usually monotonically decreasing with increase in model complexity
- Test error bounced back once the complexity increases

Example of Model Complexity vs. Errors

- Errors of the 1st-order, 3rd-order, and 9th-order models
- True model vs. Measured data vs. Regression model
- The distance between the true model and the regression model increases when the complexity of the model increases

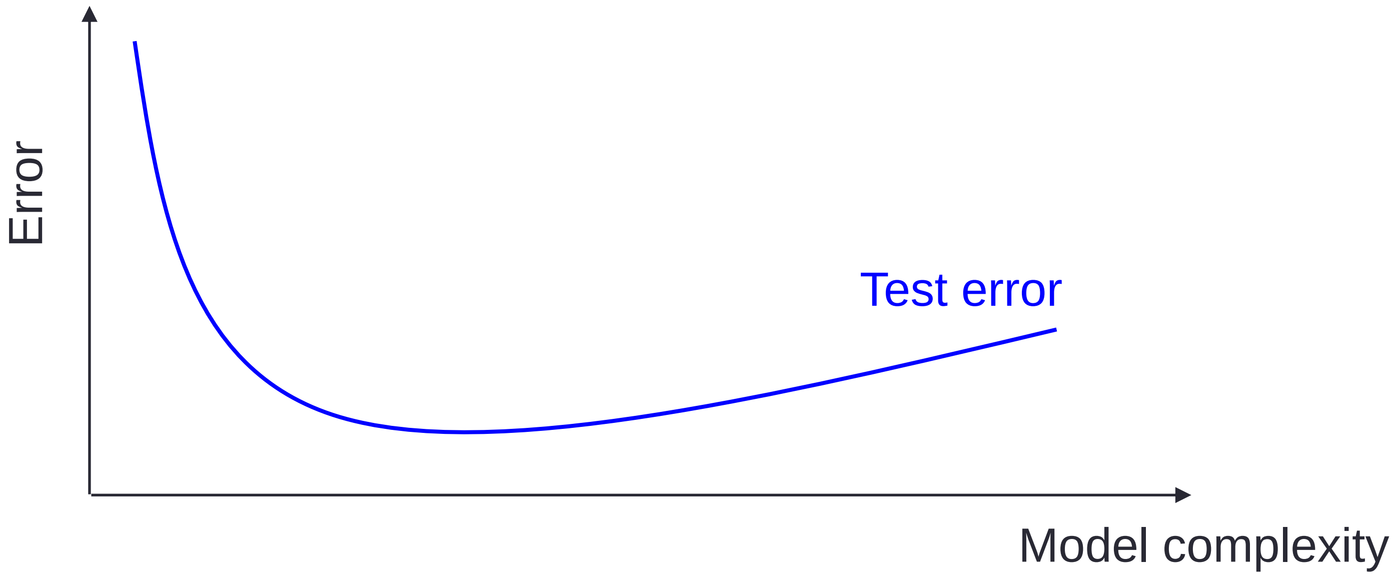


Bishop. *Pattern Recognition and Machine Learning*

Bias and Variance Decomposition

- Why does the test error go up and down as the model complexity changes?
- Test error can be decomposed into

$$(Test\ error)^2 = Bias^2(\hat{y}) + Var(\hat{y})$$



Bias and Variance of An Estimator $\hat{y}$

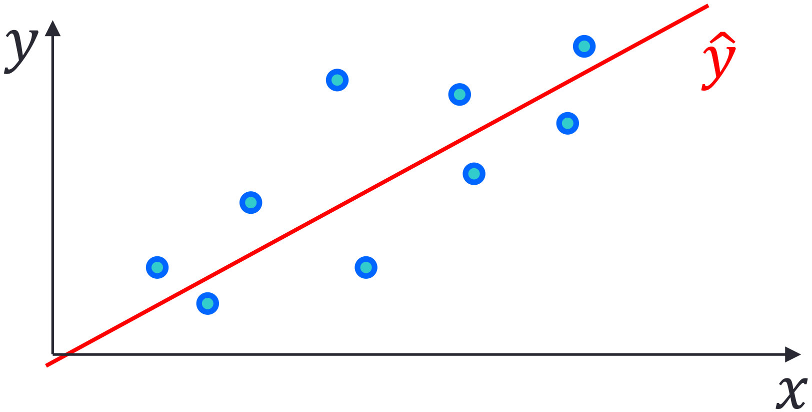
- An estimator $\hat{y}$ is a model for estimating a parameter y
- Bias of $\hat{y}$ is the difference between the estimator's expected value $E[\hat{y}]$ and the true value y, i.e., $Bias(\hat{y}) = E[y - E[\hat{y}]]$

  (NOTE: true value y is usually unknown)

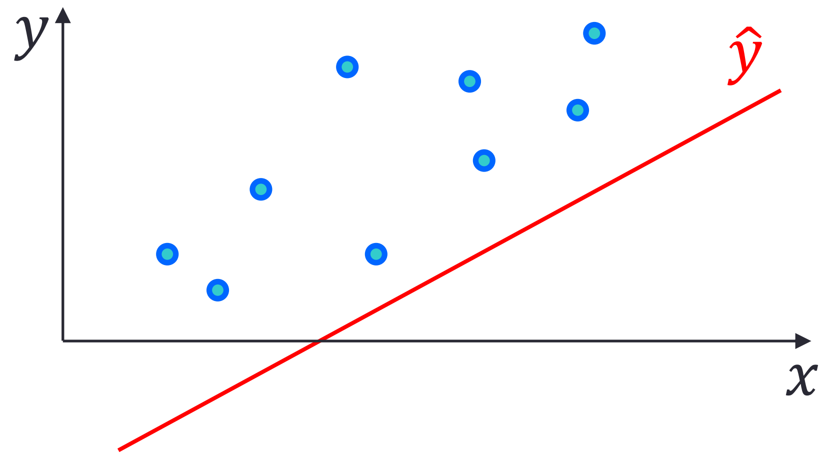
- Variance of $\hat{y}$ is a measure of how far a set of numbers are spread out from each other, i.e., the variance of an estimator $\hat{y}$ is $Var(\hat{y}) = E[(\hat{y} - E[\hat{y}])^2]$

Illustration of Bias and Variance

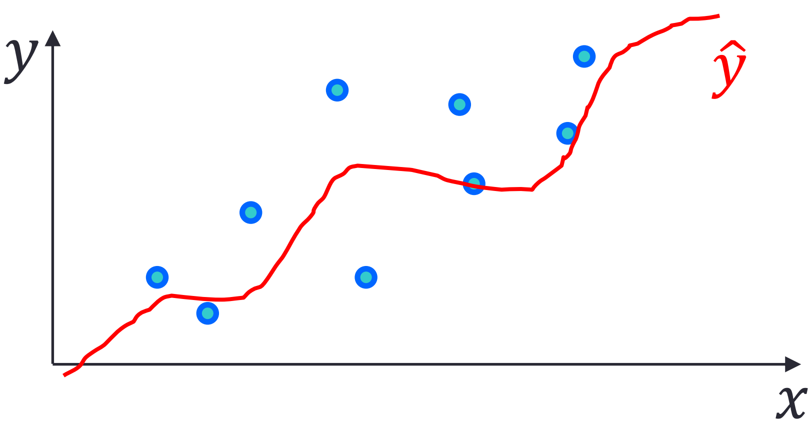
Low bias and low variance



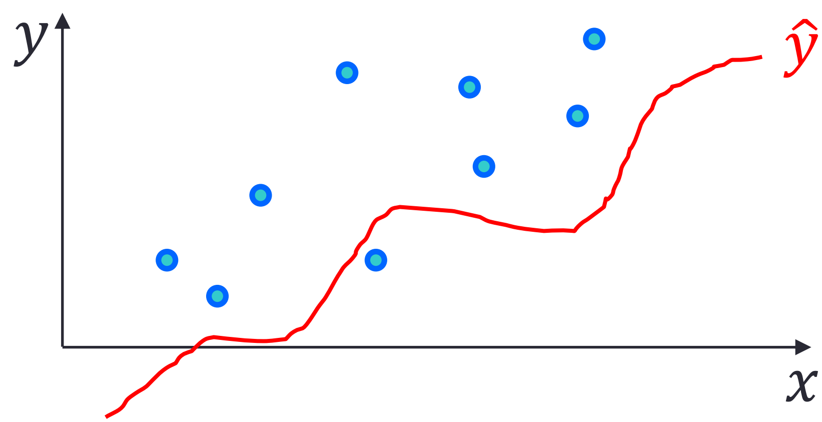
High bias and low variance



Low bias and high variance



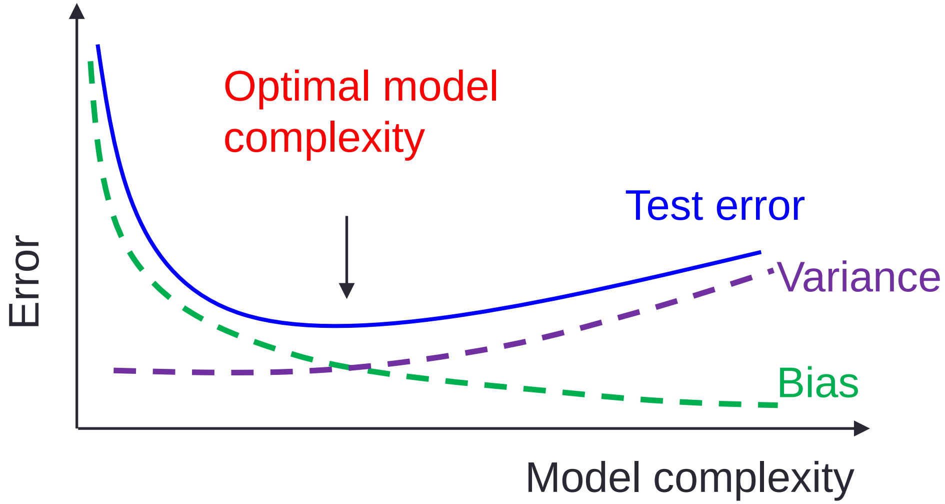
High bias and high variance



Model Complexity and Bias-variance Tradeoff

- Intuition for the bias-variance trade-off:
  - Complex model $\Rightarrow$ sensitive to data $\Rightarrow$ much affected by changes in $\boldsymbol{x}$ $\Rightarrow$ high variance, low bias
  - Simple model $\Rightarrow$ more rigid $\Rightarrow$ does not change as much with changes in $\boldsymbol{x}$ $\Rightarrow$ low variance, high bias

One of the most important goals in machine learning is to find a model with the optimal model complexity



Bias-variance Decomposition of the “Test Error”

- The expectation value of the “squared test error” can be decomposed to:

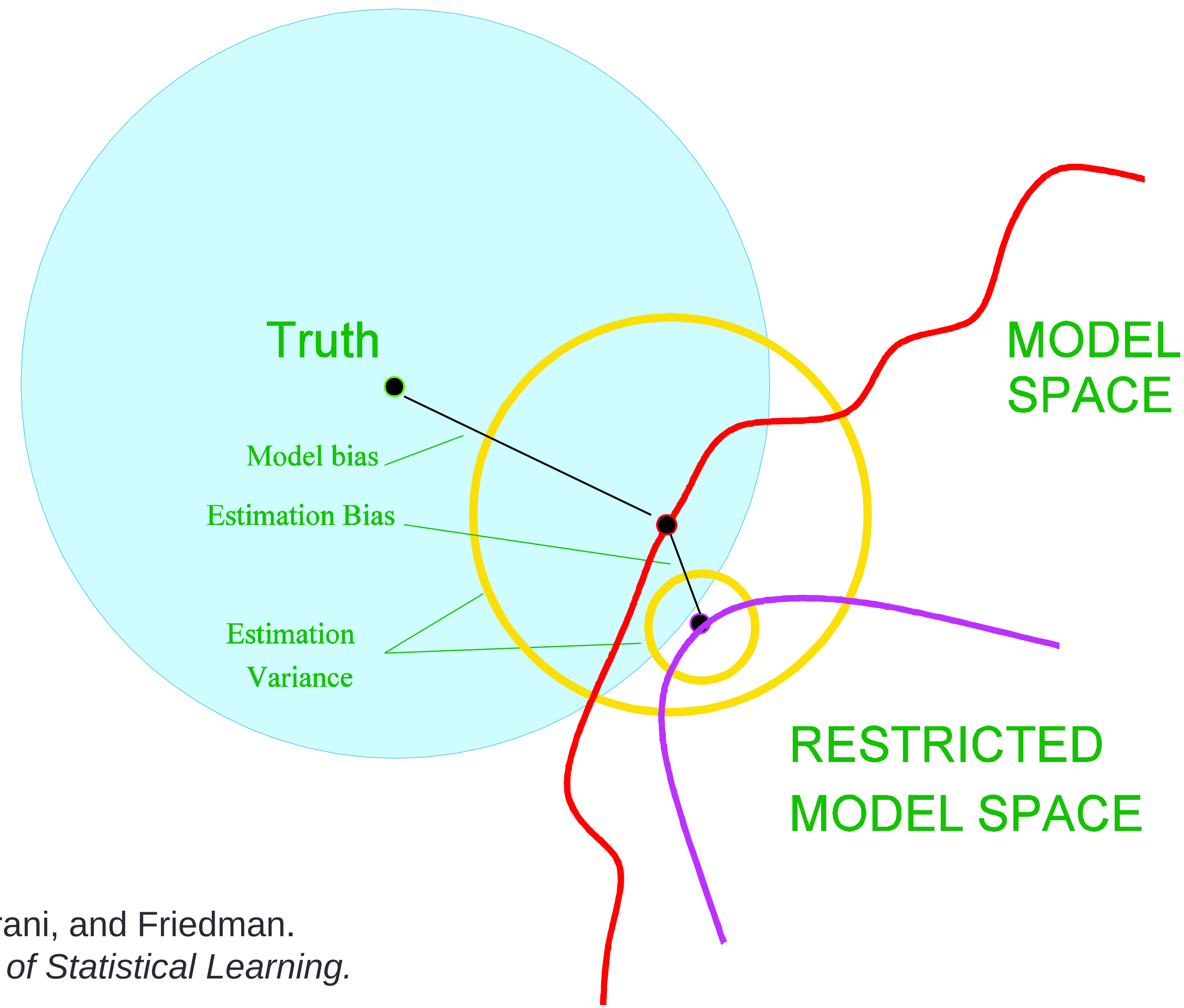
$$(Test\ error)^2 = E[(y-\hat{y})^2] = E[\{(y-E[\hat{y}])+(E[\hat{y}]-\hat{y})\}^2]$$

$$= E[(y-E[\hat{y}])^2] + E[(E[\hat{y}]-\hat{y})^2] + 2E[(y-E[\hat{y}])(E[\hat{y}]-\hat{y})\}]$$

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

$$= Bias^2(\hat{y}) + Var(\hat{y}) + 2(\cancel{E[y]E[\hat{y}]} - \cancel{E[y\hat{y}]} - \cancel{(E[\hat{y}])^2} + \cancel{(E[\hat{y}])^2})$$

Accuracy of Model and Restricted Model



Hastie, Tibshirani, and Friedman.
The Elements of Statistical Learning.

Summary of Overfitting

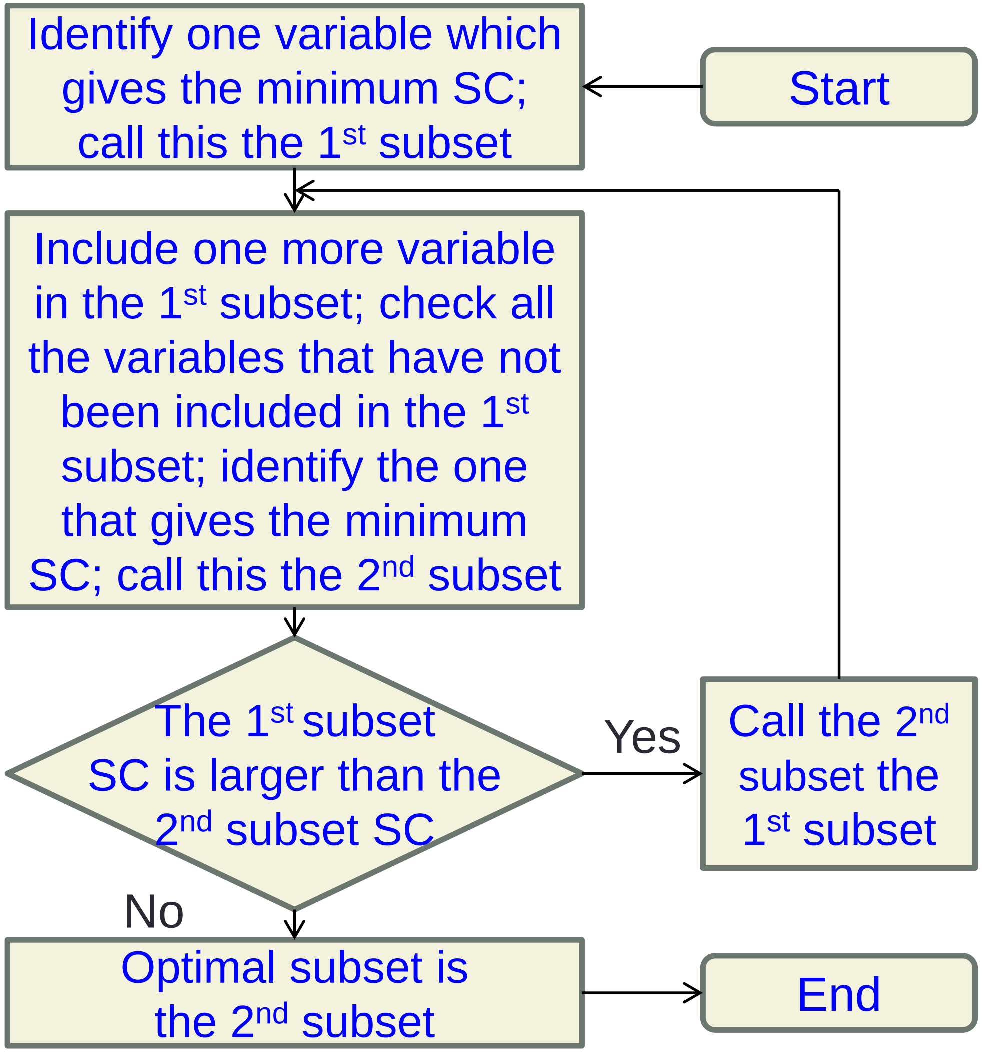
- Overfitting happens when the fitted model is too complex
- The degree of overfitting depends on model complexity and training data availability (why?)
- This means that overfitting is NOT a problem if there are infinitely many data points
- If a model overfits, it will be unstable – that means, removal part of the data will change the fit significantly

Tackle Overfitting – Variable Selection

- Variable selection – retain only the subset of variables that gives the “best fit“
- Direct greedy search of the best variable subset can take a long time of the number of variables is large
- Some typical variable selection search methods:
- Forward selections: starts with the intercept and add at each step the predictors that most improves the fit
- Backward elimination: starts with the full model and removes one by one the worst explanatory variable
- Stepwise selection: combines forward and backward to decide at each step which variable to remove and/or to add

Example: Forward Selection with Selection Criteria

- Choose a selection criteria (SC)
- The process stops when including further variables do not improve selection criteria



Variable Selection Criteria

- The variables are selected based on some methods:
  1. Cross-validation
  2. Information criteria
  3. Partial F-test

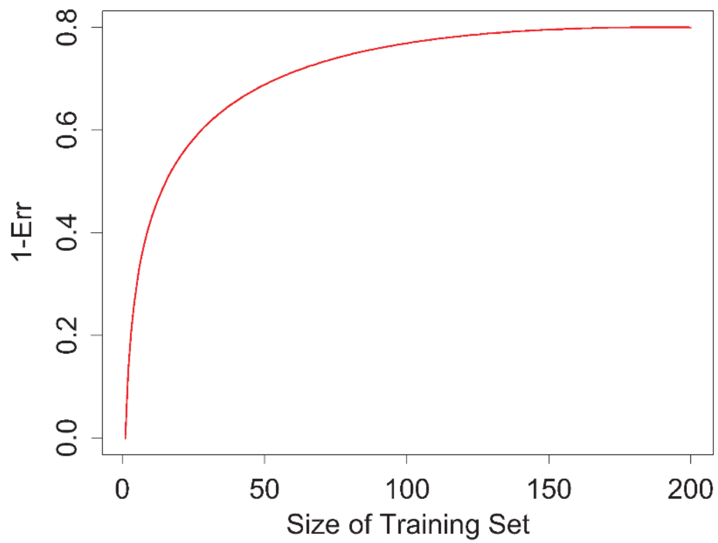
Method 1 – Cross-validation (CV)

- One of the most often used technique for model performance estimation
- k-fold cross-validation:
  1. Partition data into k roughly equal parts
  2. Train with all but jth part, test on the jth part
  3. The procedure is executed for a total of k times until all parts have been the test part
  4. The k error rates are averaged to yield an overall error estimate
- Leave-one-out cross-validation, i.e., $k = N$

Choice of k

- If $k = N$ then CV is approximately unbiased, but has high variance
- On the other hand, with $k = 5$, CV has low variance but more bias
- Typically $k = 10$ is chosen
- Increasing the number of k also increases the computational burden

Hypothetical Learning Curve with $k = 5$



Hastie, Tibshirani, and Friedman.
The Elements of Statistical Learning.

- How many samples do we need for cross validation?

Method 2 – Information Criteria

- The Akaike information criterion (AIC) and Bayesian information criterion (BIC) are defined as:

$$AIC = N \cdot \ln\left(\frac{RSS}{N}\right) + 2 \cdot k$$

Accuracy Complexity

$$BIC = N \cdot \ln\left(\frac{RSS}{N}\right) + \ln(N) \cdot k,$$

Accuracy Complexity

where RSS is the residual sum of squares from regression, and k denote the number of model parameters, i.e., $k = \text{size}(\boldsymbol{\beta})$

Information Criteria – AIC and BIC

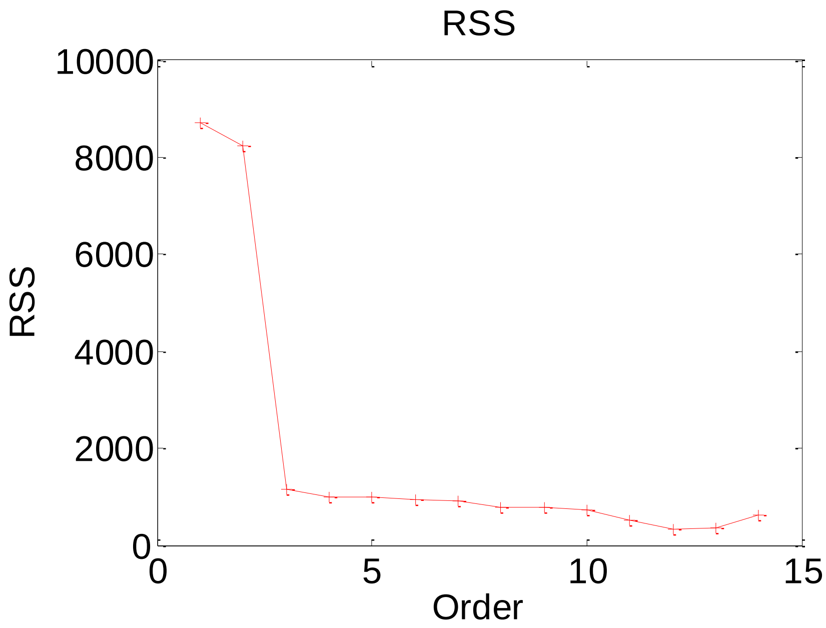
- A direct measure of training error with penalty of complexity
- A trade-off between model complexity and accuracy
- Information criteria tend to penalize complex models, giving preference to simpler models in selection
- A model associated with a smaller AIC or BIC value is preferred

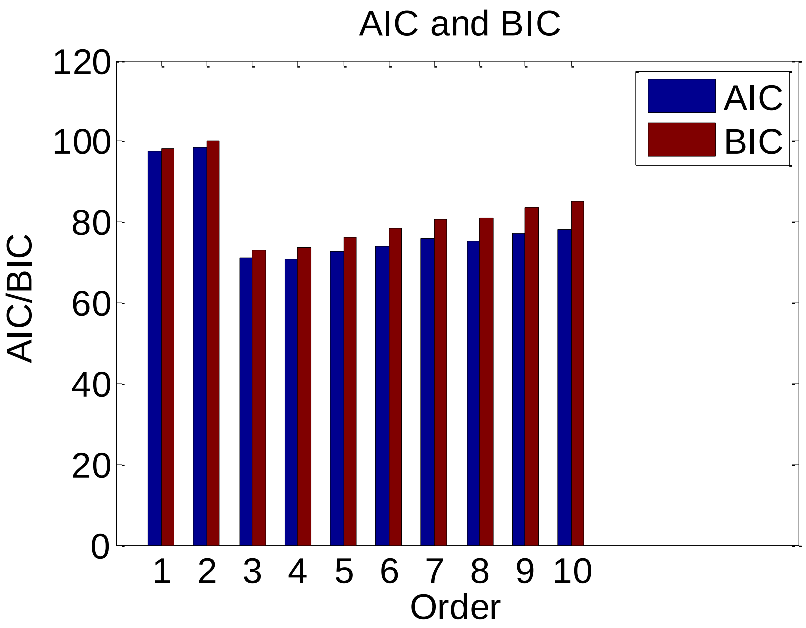
AIC or BIC?

- BIC is asymptotically consistent as a selection criterion – given a family of models including the true model, the probability that BIC will select the correct one approaches one as the sample size becomes large, i.e., $N \to \infty$
- AIC does not have the above property; instead, it tends to choose more complex models as $N \to \infty$
- For small or moderate samples, BIC often chooses models that are too simple, because of its heavy penalty on complexity

AIC and BIC of A Previous Example

- Higher order models are strongly penalized by AIC and BIC





Example MATLAB Code

```
% Calculate and plot AIC and BIC
for i=1:length(x)-1
    X(:,i)=power(x,i);
    [b,bint,r]=regress(y,[ones(length(x),1) X(:,1:i)]);
    RSS(i)=r'*r;
    AIC(i)=length(y)*log(RSS(i)/length(y))+2*i;
    BIC(i)=length(y)*log(RSS(i)/length(y))+log(length(y))*i;
end

figure; bar( [ AIC(1:10); BIC(1:10)]', 1);
title('AIC and BIC', 'FontSize', 16);
xlabel('Order', 'FontSize', 16); set(gca,'FontSize', 16);
ylabel('AIC/BIC', 'FontSize', 16);
set( gcf, 'Color', 'w'); legend({'AIC', 'BIC'});
```

Information Criteria – Mallows' C_p

- Mallows' C_p is defined as:

$$C_p = \frac{RSS_k}{\frac{RSS_{FULL}}{N}} - (N - k),$$

where RSS_k is the residual sum of squares for the model containing k explanatory variables, and RSS_{FULL} is the residual sum of squares for the model containing all the explanatory variables

- The model that has a C_p value closest to k is considered the best model

Criterion 3 – Partial F-test

- The partial F-test is used to test the significance of one or more variables in the presence of other variable(s) in the full model
- Suppose a $f$ull model: $\hat{y} = \beta_0 + \beta_1 x + \beta_2 x^2 + \cdots + \beta_M x^M$, and a $r$educed model: $\hat{y} = \beta_0 + \beta_2 x^2 + \cdots + \beta_{M-1} x^{M-1}$
- The null hypothesis is the change in sum of squares is not due to changes in model complexity
- Hypothesis: $H_0\!: \beta_M = 0,\ \ H_1\!: \beta_M \neq 0$
- F statistic: $F_{(q,n-p-1)} = \frac{\left(SSE_r - SSE_f\right)/q}{MSE_f}$, where the full model has p variables, and the reduced model has q variables

References

- T. Hastie, R. Tibshirani, and J. Friedman, The Elements of Statistical Learning, Chapter 3 and 7
- C. M. Bishop, Pattern Recognition and Machine Learning