

Unit 4

Model Order Selection

EL-GY 6143/CS-GY 6923: INTRODUCTION TO MACHINE LEARNING
PROF. PEI LIU



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Learning Objectives

- ☐ Compute the model order for a given model class
- ☐ Visually identify overfitting and underfitting of a model in a scatterplot
- ☐ Determine if there is under-modeling for a given true function and model class
- ☐ Compute the bias and variance for linear models (advanced)
- ☐ Perform cross-validation for selecting an optimal order selection



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Outline

 Motivating Example: What polynomial degree should a model use?

- ☐ Bias and variance
- ☐ Bias and variance for linear models (Advanced)
- ☐ Cross-validation



Polynomial Fitting

□ Last lecture: polynomial regression

□ Given data $(x_i, y_i), i = 1, \dots, N$

□ Learn a polynomial relationship:

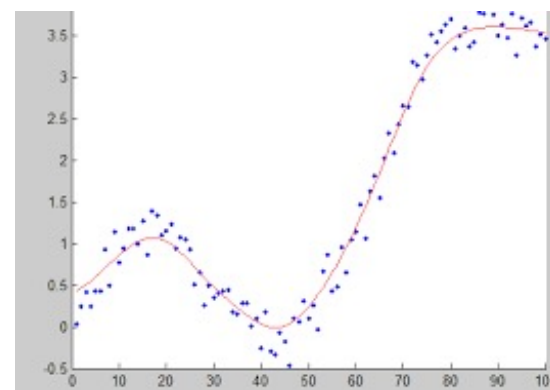
$$y = \beta_0 + \beta_1 x + \dots + \beta_d x^d + \epsilon$$

- d = degree of polynomial. Called **model order**
- $\boldsymbol{\beta} = (\beta_0, \dots, \beta_d)$ = coefficient vector

□ Given d , can find $\boldsymbol{\beta}$ via least squares

□ How do we select d from data?

□ This problem is called **model order selection**.



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Demo on Github

□ Demo on github:

https://github.com/pliugithub/MachineLearning/blob/master/unit04_model_sel/demo_polyfit.ipynb

GitHub, Inc. [US] | https://github.com/sdrangan/introml/blob/master/model_sel/polyfit.ipynb

□ Suggested Sites Web Slice Gallery Import to Mendeley

Demo: Polynomial Model Order Selection

In this demo, we will illustrate the process of cross-validation for model order selection. We derive data for a polynomial fit. The lab will demonstrate how to:

- Characterize the model order for a simple polynomial model
- Measure training and test error for a given model order
- Select a suitable model order using cross-validation
- Plot the results for the model order selection process

We first load the packages as usual.

```
In [2]: import numpy as np
import matplotlib
import matplotlib.pyplot as plt
from sklearn import datasets, linear_model, preprocessing
%matplotlib inline
```

Polynomial Data

To illustrate the concepts, we consider a simple polynomial model:

$$y = \beta_0 + \beta_1 x + \dots + \beta_d x^d + \epsilon,$$

where d is the polynomial degree. We first generate synthetic data for this model.



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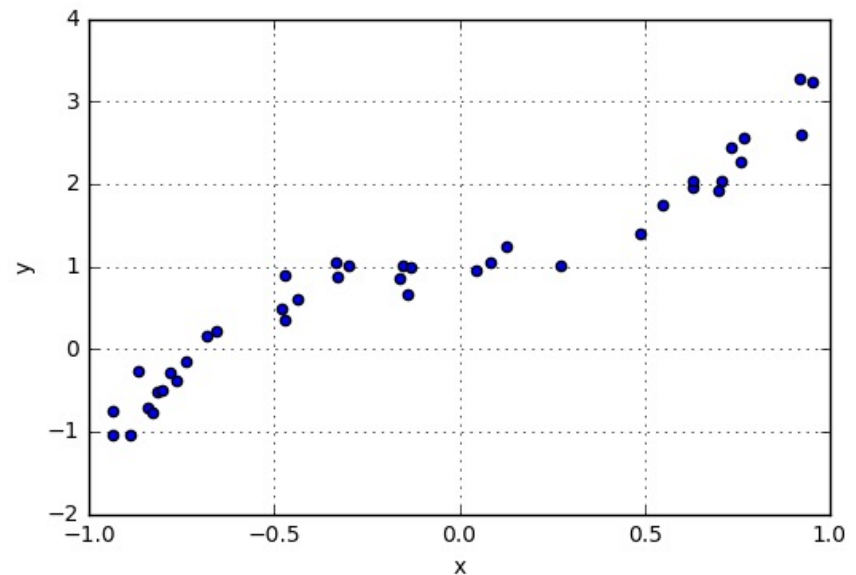
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Example Question

- ❑ You are given some data.
- ❑ Want to fit a model: $y \approx f(x)$
- ❑ Decide to use a polynomial:
$$f(x) = \beta_0 + \beta_1 x + \cdots + \beta_d x^d$$
- ❑ What model order d should we use?
- ❑ Thoughts?



Synthetic Data

□ Previous example is synthetic data

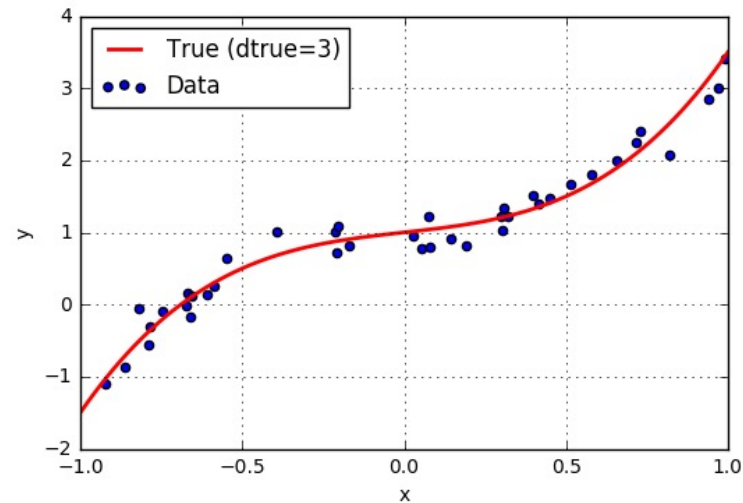
□ x_i : 40 samples uniform in $[-1,1]$

□ $y = f(x) + \epsilon$,

- $f(x) = \beta_0 + \beta_1 x + \dots + \beta_d x^d = \text{"true relation"}$
- $d = 3$, $\epsilon \sim N(0, \sigma^2)$

□ Synthetic data useful for analysis

- Know "ground truth"
- Can measure performance of various estimators



```
# Import useful polynomial library
import numpy.polynomial.polynomial as poly

# True model parameters
beta = np.array([1,0.5,0,2]) # coefficients
wstd = 0.2 # noise
dtrue = len(beta)-1 # true poly degree

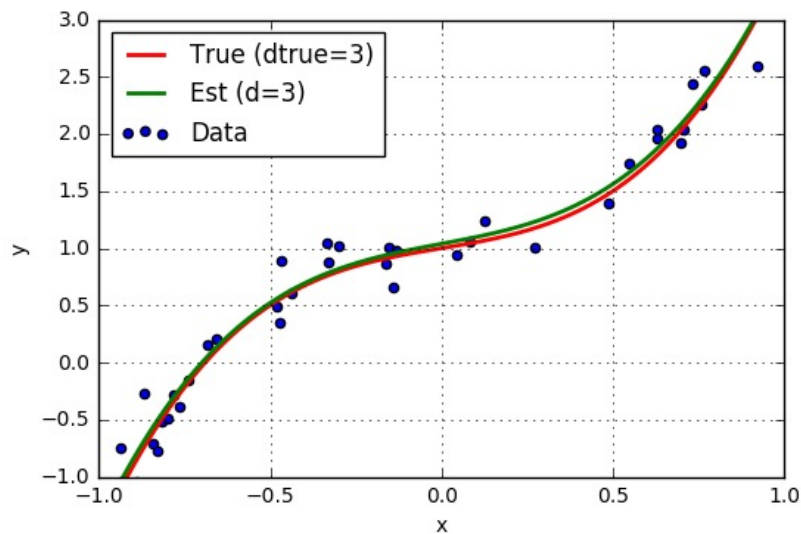
# Independent data
nsamp = 40
xdat = np.random.uniform(-1,1,nsamp)

# Polynomial
y0 = poly.polyval(xdat,beta)
ydat = y0 + np.random.normal(0,wstd,nsamp)
```



Fitting with True Model Order

- ❑ Suppose true polynomial order, $d=3$, is known
- ❑ Use linear regression
 - numpy.polynomial package
- ❑ Get very good fit



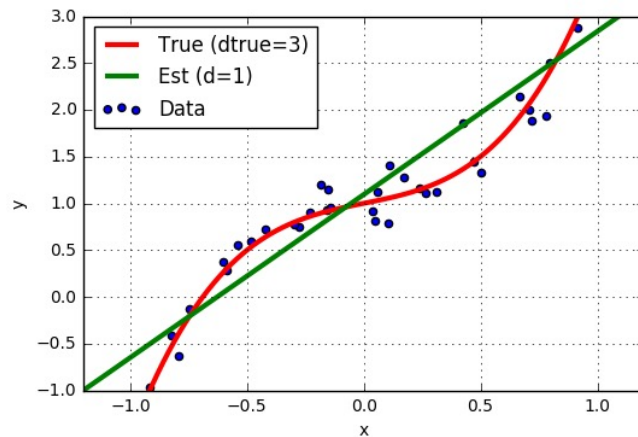
```
d = 3
beta_hat = poly.polyfit(xdat,ydat,d)

# Plot true and estimated function
xp = np.linspace(-1,1,100)
yp = poly.polyval(xp,beta)
yp_hat = poly.polyval(xp,beta_hat)
plt.xlim(-1,1)
plt.ylim(-1,3)
plt.plot(xp,yp,'r-',linewidth=2)
plt.plot(xp,yp_hat,'g-',linewidth=2)

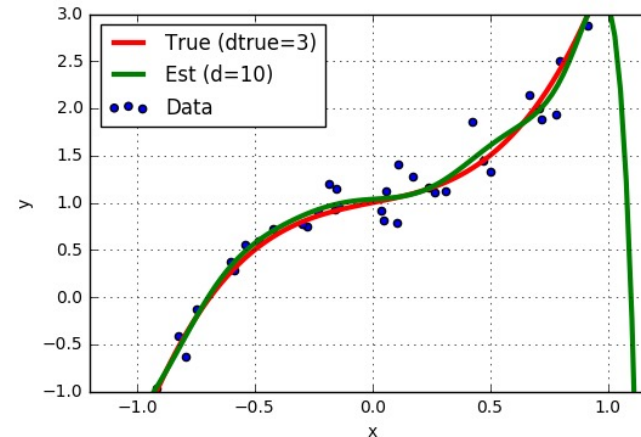
# Plot data
plt.scatter(xdat,ydat)
plt.legend(['True (dtrue=3)', 'Est (d=3)', 'Data'], loc='upper left')
plt.grid()
plt.xlabel('x')
plt.ylabel('y')
```


But, True Model Order not Known

□ Suppose we guess the wrong model order?



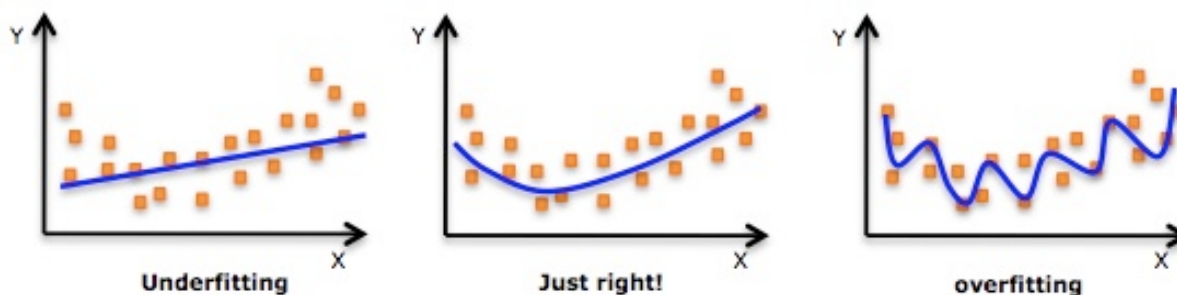
d=1 “Underfitting”



d=10 “Overfitting”



How Can You Tell from Data?



- ❑ Is there a way to tell what is the correct model order to use?
- ❑ Must use the data. Do not have access to the true d ?
- ❑ What happens if we guess:
 - d too big?
 - d too small?



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Using RSS on Training Data?

❑ Simple (but bad) idea:

- For each model order, d , find estimate $\hat{\beta}$
- Compute predicted values on training data

$$\hat{y}_i = \hat{\beta}^T x_i$$

- Compute RSS

$$RSS(d) = \sum_i (y_i - \hat{y}_i)^2$$

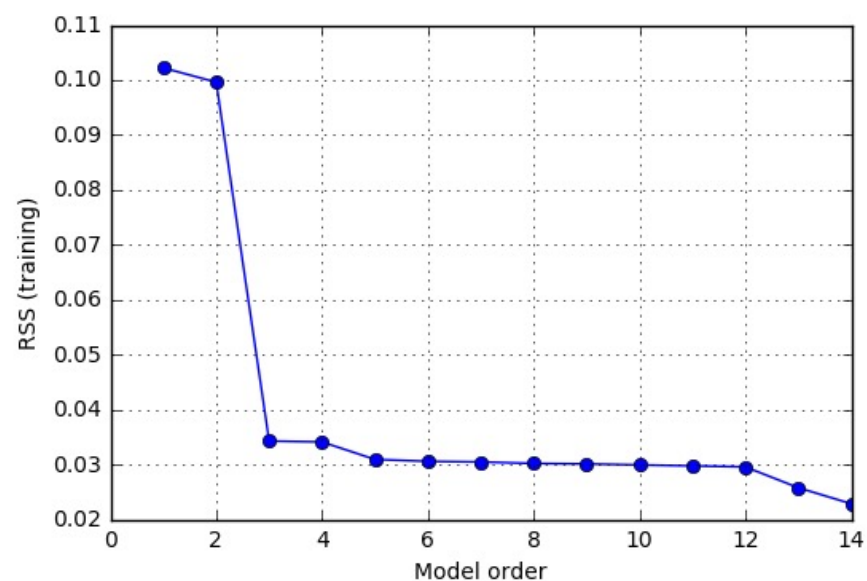
- Find d with lowest RSS

❑ This doesn't work

- $RSS(d)$ is always decreasing (Question: Why?)
- Minimizing $RSS(d)$ will pick d as large as possible
- Leads to overfitting


❑ What went wrong?

❑ How do we do better?



Outline

- ❑ Motivating Example: What polynomial degree should a model use?

- ❑ Bias and variance

- ❑ Bias and variance for linear models (Advanced)

- ❑ Cross-validation



Generalization

Machine learning:

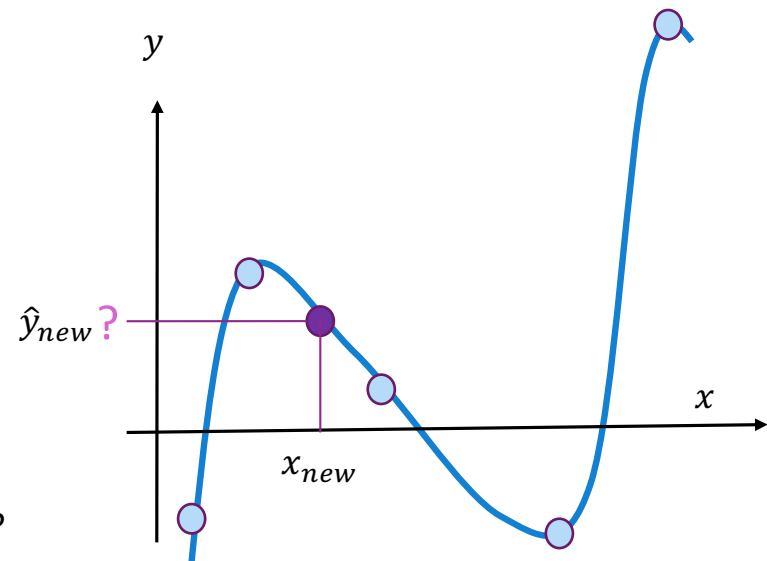
- Get **data** points $(x_i, y_i), i = 1, \dots, n$
- **Learn** some function $\hat{y} = f(x)$

Implicitly, we are

- **Inferring** the value of y at **new** values of x
- Called **generalization**

Basic question for all ML:

- *How well do models we train generalize to new samples?*



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A Model To Understand Generalization

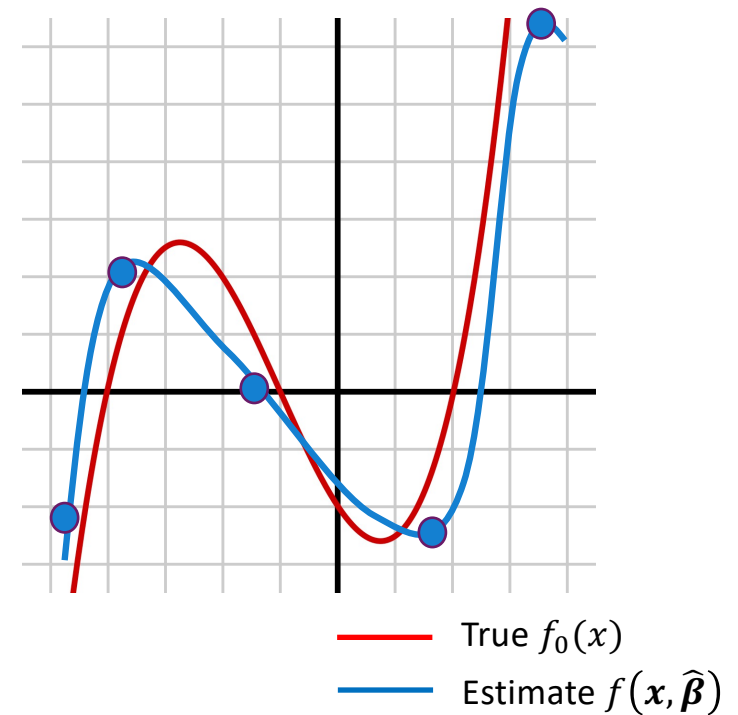
□ Assume a **true** relation: $y = f_0(x) + \epsilon$, $\epsilon \sim N(0, \sigma_\epsilon^2)$

□ Get **data** points $(x_i, y_i), i = 1, \dots, n$
 $y_i = f_0(x_i) + \epsilon_i$

□ Assume a **model** $\hat{y} = f(x, \beta)$
◦ Parameters β

□ **Fit** a parameter $\hat{\beta}$ from training data
◦ Results in estimated function $f(x, \hat{\beta})$

□ **Question**: How “good” is the estimated function?



Output Mean Squared Error

□ To evaluate generalization, suppose we are given:

- A **test point** \mathbf{x}_{test}
- New point, generally different from training samples.

□ Actual value: $y = f_0(\mathbf{x}_{test}) + \epsilon$

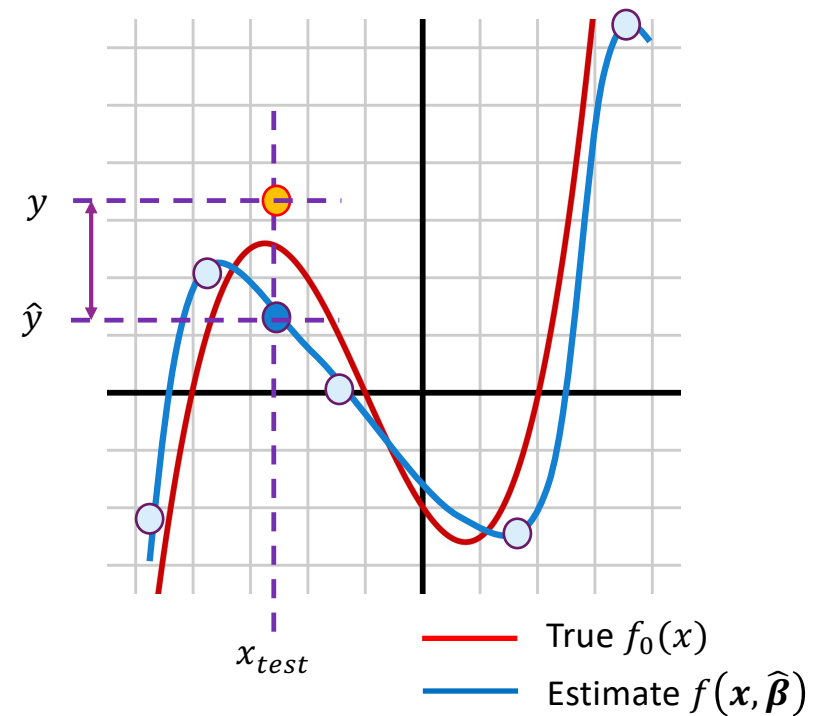
□ Predicted value: $\hat{y} = f(\mathbf{x}_{test}, \hat{\beta})$

- Note that $\hat{\beta}$ is random due to noise in training data

□ Define **output mean squared error** :

$$MSE_y(\mathbf{x}_{test}) := E[y - \hat{y}]^2$$

- Expectation is over noise ϵ on the training and test data.



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Function MSE and Irreducible Error

□ **Output MSE decomposition:** Output MSE, $MSE_y(\mathbf{x}_{test}) := E[y - \hat{y}]^2$, satisfies:

$$MSE_y(\mathbf{x}_{test}) = MSE_f(\mathbf{x}_{test}) + \sigma_\epsilon^2$$

□ **Function MSE:** $MSE_f(\mathbf{x}_{test}) = E[f_0(\mathbf{x}_{test}) - f(\mathbf{x}_{test}, \hat{\beta})]^2$

- Represents difference between estimated and true function

□ **Irreducible error:** $\sigma_\epsilon^2 = E(\epsilon^2)$ in output $y = f_0(x) + \epsilon$

- Occurs since y is influenced by other factors than x
- Fundamental limit on ability to predict y
- Lower bound on $MSE_y(\mathbf{x}_{test}, \hat{\beta}) \geq \sigma_\epsilon^2$



Proof of the MSE Decomposition

□ **Output MSE decomposition:** Output MSE $MSE_y(\mathbf{x}_{test}) := E[y - \hat{y}]^2$ is:

$$MSE_y(\mathbf{x}_{test}) = MSE_f(\mathbf{x}_{test}) + \sigma_\epsilon^2$$

□ **Proof:**

- $MSE_y(\mathbf{x}_{test}) := E[y - \hat{y}]^2 = E[f_0(\mathbf{x}_{test}) + \epsilon - f(\mathbf{x}_{test}, \hat{\boldsymbol{\beta}})]^2 = M_1 + M_2 + 2M_3$
- $M_1 = E[f_0(\mathbf{x}_{test}) - f(\mathbf{x}_{test}, \hat{\boldsymbol{\beta}})]^2 = MSE_f(\mathbf{x}_{test})$
- $M_2 = E[\epsilon^2] = \sigma^2$
- Noise on test sample is independent of $\hat{\boldsymbol{\beta}}$ and \mathbf{x}_{test} and $E(\epsilon) = 0$
- Therefore $M_3 = E[\epsilon(f_0(\mathbf{x}_{test}) - f(\mathbf{x}_{test}, \hat{\boldsymbol{\beta}}))] = E(\epsilon)E[f_0(\mathbf{x}_{test}) - f(\mathbf{x}_{test}, \hat{\boldsymbol{\beta}})] = 0$



Model Class and Under-Modeling

- ❑ **Model class:** The set of possible functions, $\hat{y} = f(x, \beta)$
 - Set is parametrized by β

- ❑ **Definition:** A true function $f_0(x)$ is in the model class $\hat{y} = f(x, \beta)$ if:

$$f_0(x) = f(x, \beta_0) \text{ for all } x$$

for some parameter β_0 .

- β_0 called the true parameter

- ❑ **Under-modeling:** When $f_0(x)$ is not in the model class



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Sample Questions 1 and 2

❑ For each pair, state if the true function is in the model class or not

- That is, is there under-modeling or not?
- If true function is in the model class, state the true parameter

❑ Ex 1:

- True function: $f_0(x) = 2 + 3x$ Model class: $f(x, \beta) = \beta_0 + \beta_1 x + \beta_2 x^2$
- **No under-modeling.** True parameter: $\beta = (2, 3, 0)$

❑ Ex 2:

- True function: $f_0(x) = 2 + 3x + 4x^2$ Model class: $f(x, \beta) = \beta_0 + \beta_1 x$
- **There is under-modeling.** Model class does not contain x^2 term



Sample Questions 3 and 4

□ For each pair, state if the true function is in the model class or not

- That is, is there under-modeling or not?
- If true function is in the model class, state the true parameter

□ Ex 3:

- True function: $f_0(x) = \sin(2\pi(5)x + 7)$ Model class: $f(x, \beta) = \beta_0 \sin(2\pi(5)x) + \beta_1 \cos(2\pi(5)x)$
- **No under-modeling.** $f_0(x) = \sin(2\pi(5)x + 7) = \sin(2\pi(5)x) \cos(7) + \cos(2\pi(5)x) \sin(7)$
- True parameter $\beta = (\cos 7, \sin 7)$

□ Ex 4:

- True function: $f_0(x) = \sin(2\pi(8)x + 7)$ Model class: $f(x, \beta) = \beta_0 \sin(2\pi(5)x) + \beta_1 \cos(2\pi(5)x)$
- **There is under-modeling.** Model class does not contain $\sin(2\pi(8)x)$ or $\cos(2\pi(8)x)$ terms



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Under-Modeling and Irreducible Error

□ Suppose that:

- There is no under-modeling: $f_0(\mathbf{x}) = f(\mathbf{x}, \boldsymbol{\beta}_0)$ for some “true” parameter $\boldsymbol{\beta}_0$; and
- Estimator selects the true parameter $\hat{\boldsymbol{\beta}} = \boldsymbol{\beta}_0$ (somehow?)

□ Then, function MSE is zero:

$$MSE_f(\mathbf{x}_{test}) = E[f_0(\mathbf{x}_{test}) - f(\mathbf{x}_{test}, \hat{\boldsymbol{\beta}})]^2 = E[f_0(\mathbf{x}_{test}) - f(\mathbf{x}_{test}, \boldsymbol{\beta}_0)]^2 = 0$$

□ Output MSE = irreducible error

$$MSE_y(\mathbf{x}_{test}) := MSE_f(\mathbf{x}_{test}) + \sigma_\epsilon^2 = \sigma_\epsilon^2$$



What We Have Learned So Far

□ If (A Big If!)

- There is no undermodeling (i.e. true function is in model class), and
- We can estimate the true parameter

□ Then:

- Output error = irreducible error
- We can achieve the same error as if we knew the true function $f_0(x)$

□ This suggests: *Select the model class large!*

- Guarantees to approximately contains true function
- Ex: Take model class = set of polynomials with very high degree

□ But, using large models has other problems...



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In-Class Exercise

Question

For each model and true function pair below: Determine if there is undermodeling (i.e. the true function is in the model class). If there is no undermodeling, find the true parameters

- (a) True function: $f_0(x) = (1 + 2x)(3 + 4x)$, Model: $f(x, \beta) = \beta_0 + \beta_1 x + \beta_2 x^2$
- (b) True function: $f_0(t) = 2(1 - e^{t-3})$ Model: $f(t, \beta) = a + be^{ct}, \beta = (a, b, c)$
- (c) True function: $f_0(t) = 2(1 - e^{t-3})$ Model: $f(t, \beta) = a + be^{-t}, \beta = (a, b)$



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Bias and Variance

□ To understand potential problem of using a large model class introduce two key quantities:

□ **Bias:** $Bias(\mathbf{x}_{test}) := E[f(\mathbf{x}_{test}, \hat{\boldsymbol{\beta}})] - f_0(\mathbf{x}_{test})$

- How much the average value of the estimate differs from the true function

□ **Variance:** $Var(\mathbf{x}_{test}) := E \left[f(\mathbf{x}_{test}, \hat{\boldsymbol{\beta}}) - E[f(\mathbf{x}_{test}, \hat{\boldsymbol{\beta}})] \right]^2$

- How much the estimate varies around its average

□ Bias and variance are (conceptually) measured as follows:

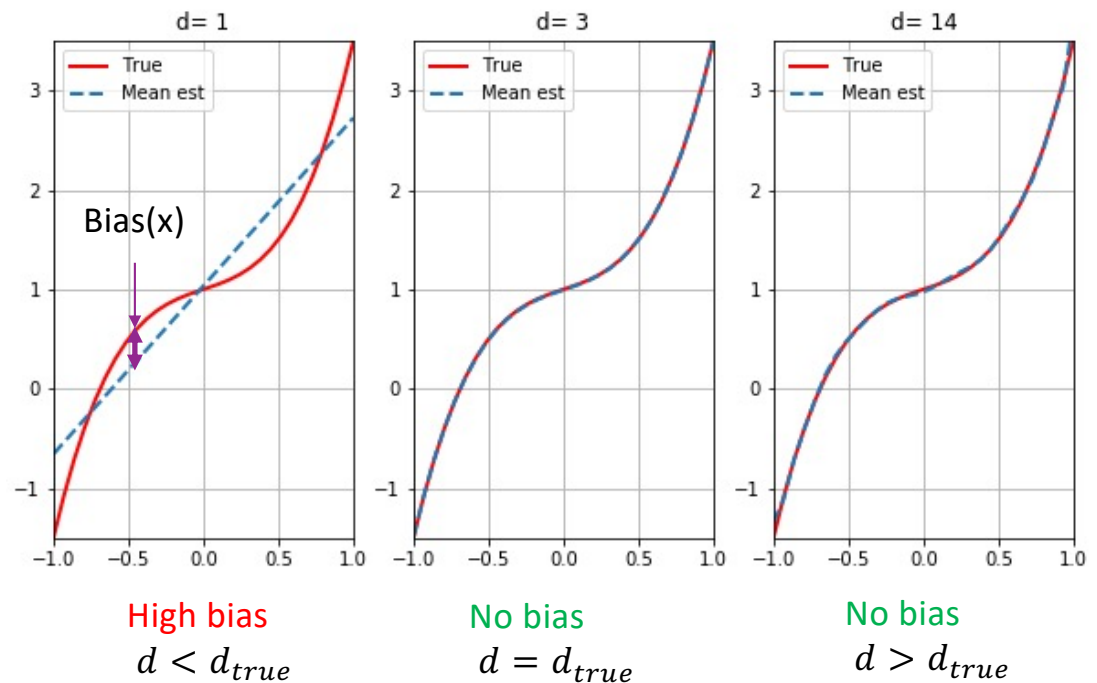
- Get many independent training data sets, each with same size N and input values \mathbf{x}_i
- Each dataset has different output values y_i because of independent noise in the training data
- Obtain $\hat{\boldsymbol{\beta}}$ for each training data set
- Bias and variances are computed over the different sets

□ Of course, in reality, we have only one training dataset

- Used to study theoretical averages over different experiments

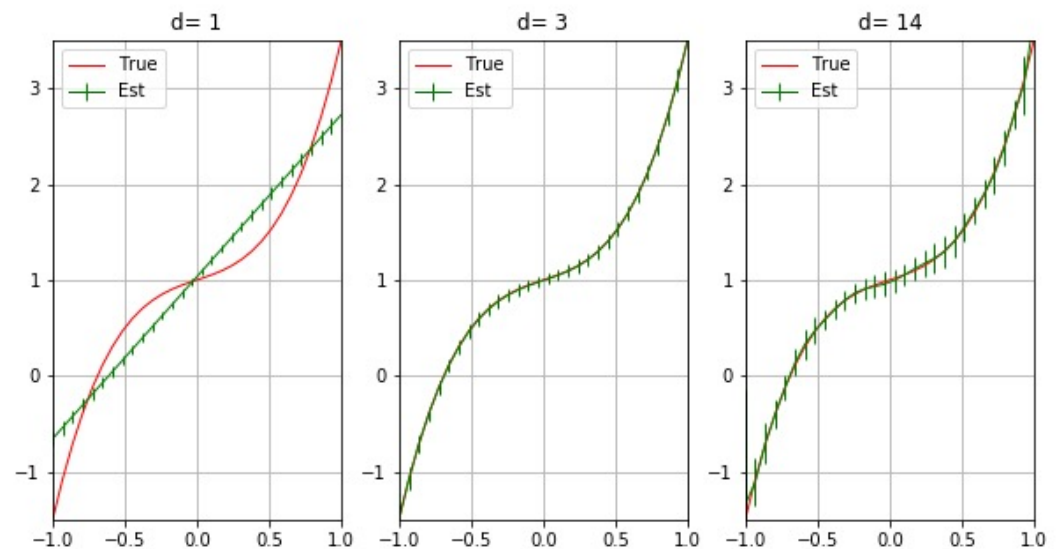
Bias Illustrated

- Red: True function
- Repeat 100 trials
 - Each trial has independent data
 - Obtain estimate for each trial
- Dashed line: Mean estimate among all trials
- Bias = True – Mean estimate
- Conclusions:
 - Low model orders \Rightarrow bias high
 - High model orders \Rightarrow bias low



Variance Illustrated

- Red: True function
- Repeat 100 trials
 - Each trial has independent data
 - Obtain estimate for each trial
- Variance=STD around mean
- Conclusions:
 - Low model orders \Rightarrow low variance
 - High model orders \Rightarrow high variance



High bias

Low variance

No bias

Med variance

No bias

High variance



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Bias-Variance Formula

□ Recall definitions:

- **Function MSE:** $\text{MSE}_f(\mathbf{x}_{test}) := E[f_0(\mathbf{x}_{test}) - f(\mathbf{x}_{test}, \hat{\boldsymbol{\beta}})]$:
- **Bias:** $\text{Bias}(\mathbf{x}_{test}) := E[f(\mathbf{x}_{test}, \hat{\boldsymbol{\beta}})] - f_0(\mathbf{x}_{test})$
- **Variance:** $\text{Var}(\mathbf{x}_{test}) := E[f(\mathbf{x}_{test}, \hat{\boldsymbol{\beta}}) - E[f(\mathbf{x}_{test}, \hat{\boldsymbol{\beta}})]]^2$

□ Bias-Variance formula : $\text{MSE}_f(\mathbf{x}_{test}) = \text{Bias}(\mathbf{x}_{test})^2 + \text{Var}(\mathbf{x}_{test})$

- Will be proved below

□ Bias-Variance tradeoff

□ Bias due to under-modeling

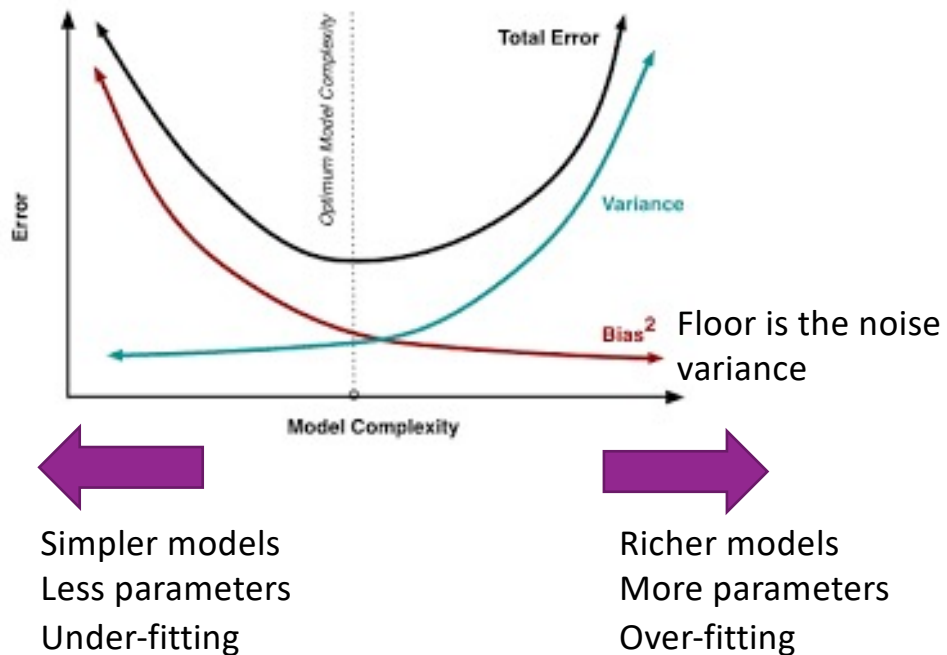
- Reduced with high model order

□ Variance is due to noise in training data and number of parameters to estimate

- Increases with higher model order



Bias-Variance Tradeoff



□ Bias:

- Due to under-modeling
- Reduced with high model order

□ Variance:

- Increases with noise in training data
- Increase with high model order

□ Optimal model order depends on:

- Amount of samples available
- Underlying complexity of the relation



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Bias-Variance Formula Proof

□ Define $\bar{f}(\mathbf{x}_{test}) = E[f(\mathbf{x}_{test}, \hat{\beta})]$ = average value of estimated function

$$\square \text{MSE}_f(\mathbf{x}_{test}) = E[f_0(\mathbf{x}_{test}) - f(\mathbf{x}_{test}, \hat{\beta})]^2 = E[f_0(\mathbf{x}_{test}) - \bar{f}(\mathbf{x}_{test}) + \bar{f}(\mathbf{x}_{test}) - f(\mathbf{x}_{test}, \hat{\beta})]^2$$

□ Three components: $\text{MSE}_f(\mathbf{x}_{test}) = M_1 + M_2 - 2M_3$

- $M_1 = E[f_0(\mathbf{x}_{test}) - \bar{f}(\mathbf{x}_{test})]^2 = [f_0(\mathbf{x}_{test}) - \bar{f}(\mathbf{x}_{test})]^2 = \text{Bias}(\mathbf{x}_{test})^2$
- $M_2 = E[f(\mathbf{x}_{test}, \hat{\beta}) - \bar{f}(\mathbf{x}_{test})]^2 = \text{Var}(\mathbf{x}_{test})$
- $M_3 = E[(f_0(\mathbf{x}_{test}) - \bar{f}(\mathbf{x}_{test}))(f(\mathbf{x}_{test}, \hat{\beta}) - \bar{f}(\mathbf{x}_{test}))]$
 $= (f_0(\mathbf{x}_{test}) - \bar{f}(\mathbf{x}_{test}))E[f(\mathbf{x}_{test}, \hat{\beta}) - \bar{f}(\mathbf{x}_{test})]$
 $= (f_0(\mathbf{x}_{test}) - \bar{f}(\mathbf{x}_{test}))(f(\mathbf{x}_{test}) - \bar{f}(\mathbf{x}_{test})) = 0$



Summary of Results for Linear Models

□ Suppose model is linear with N = num samples, p = num parameters

□ Can show the following results (need some math, see next section)

□ Result 1: When $N < p$, linear estimate is not unique

- Need at least as many samples as parameters

□ Now assume that $N \geq p$ and parameter estimate is unique

□ Result 2: When there is no under-modeling, estimate is unbiased

$$E[f(\mathbf{x}_{test}, \hat{\boldsymbol{\beta}})] = f_0(\mathbf{x}_{test}).$$

□ Result 3: If test point drawn randomly from the training data:

$$Var = \frac{p}{N} \sigma_{\epsilon}^2$$

- Variance increases linearly with number of parameters and inversely with number of samples



In-Class Exercise

Question

A teacher tries to model the score of a child on a test as follows:

$$\text{Test score} \approx \beta_0 + \beta_1[\text{Hours studied}] + \beta_2[\text{Hours sleep before test}]$$

Below are three possible shortcomings of the model. For each shortcoming, indicate whether it would lead to (i) High irreducible error, (ii) High bias error or (iii) High variance error


- (a) The relation between test score and hours studied is not linear. After some amount of studying, the students test score will no longer improve.
- (b) The model should also include the age of the child.
- (c) The model was fit with data from one class with only 15 children.



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Outline

- ☐ Motivating Example: What polynomial degree should a model use?
- ☐ Bias and variance
-  ☐ Bias and variance for linear models (Advanced)
- ☐ Cross-validation



Linear Models

- Consider linear model in general transformed feature space:

$$\hat{y} = f(x, \beta) = \phi(x)^T \beta = \beta_1 \phi_1(x) + \cdots + \beta_p \phi_p(x)$$

- See previous lecture

- Assume true data relation is: $y = f_0(x) + \epsilon$, $E(\epsilon) = 0$, $E(\epsilon^2) = \sigma^2$

- When there is no under-modeling: $f_0(x) = f(x, \beta^0) = \phi(x)^T \beta^0$

- $\beta^0 = (\beta_0^0, \dots, \beta_k^0)$ True parameter

- Get data $(x_i, y_i), i = 1, \dots, N$

- Least squares fit $\hat{\beta} = (A^T A)^{-1} A^T y$

$$A = \begin{bmatrix} \phi_1(x_1) & \cdots & \phi_p(x_1) \\ \vdots & \vdots & \vdots \\ \phi_1(x_N) & \cdots & \phi_p(x_N) \end{bmatrix}$$



Minimum Number of Samples

- ❑ LS estimate requires $A^T A$ is invertible.
- ❑ Linear algebra fact: Since $A \in R^{N \times p}$, we need $\text{Rank}(A) \geq p$
 - Otherwise solution is not unique
- ❑ Since $\text{Rank}(A) \leq \min(N, p)$ we need $N \geq p$.
- ❑ Recall:
 - N = number of data samples
 - p = number of parameters
- ❑ **Conclusion:** Number of samples \geq number of parameters
- ❑ This places a basic limit on the model complexity that you can use



Random Vectors Review

□ To analyze bias and variance in linear models, we need to review random vectors

□ **Random vectors:** $\mathbf{x} = (x_1, \dots, x_d)^T$: Each component x_j is a random variable

□ **Mean:** The vector of means of the components

$$\boldsymbol{\mu} = E\mathbf{x} = (Ex_1, \dots, Ex_d)^T = (\mu_1, \dots, \mu_d)^T$$

□ **Covariance components:** $\text{Cov}(x_i, x_j) = E[(x_i - \mu_i)(x_j - \mu_j)]$

□ **Variance matrix ($d \times d$):**

$$\text{Var}(\mathbf{x}) := E[(\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^T] = \begin{bmatrix} \text{Cov}(x_1, x_1) & \cdots & \text{Cov}(x_1, x_d) \\ \vdots & \vdots & \vdots \\ \text{Cov}(x_d, x_1) & \cdots & \text{Cov}(x_d, x_d) \end{bmatrix}$$



Linear Transforms of Random Vectors

- A linear transform is a map: $y = Ax + b$
- $A \in R^{M \times N}$ maps input $x \in R^N$ to $Ax \in R^M$
- Mean and variance matrix under linear map given by
 - Mean: $E(y) = AE(x) + b$
 - Variance: $Var(y) = AVar(x)A^T$



Bias With No Under-Modeling

- Suppose that there is no undermodeling: $f_0(x) = \phi(x)^T \beta^0$
- Then each training sample output is: $y_i = \phi(x_i)^T \beta^0 + \epsilon_i$
- Hence: true data vector $y = A\beta^0 + \epsilon$
- Parameter estimate is:
$$\hat{\beta} = (A^T A)^{-1} A^T y = (A^T A)^{-1} A^T (A\beta^0 + \epsilon) = \beta^0 + (A^T A)^{-1} A^T \epsilon$$
- Since $E\epsilon = 0$, $E\hat{\beta} = \beta^0$. Average of parameter estimate matches true parameter
- $E f(x_{test}, \hat{\beta}) = \phi(x_{test})^T E\hat{\beta} = \phi(x_{test})^T \beta^0 = f_0(x_{test})$
- Therefore $Bias(x_{test}) := E f(x_{test}, \hat{\beta}) - f_0(x_{test}) = 0$
- **Conclusion:** When the model is linear and there is no under-modeling, there is no bias



Variance of the Parameters in Linear Models

- Since ϵ_i are independent for different samples with $E\epsilon_i = 0$, $E\epsilon_i^2 = \sigma^2$

$$\text{Cov}(\epsilon_i, \epsilon_j) = \begin{cases} 0 & i \neq j \\ \sigma^2 & i = j \end{cases}$$

- Therefore variance matrix is: $\text{Var}(\epsilon) = \sigma^2 I$

- From last slide: $\hat{\beta} = \beta^0 + (A^T A)^{-1} A^T \epsilon$.

- Applying variance formula of a linear transformation of ϵ

$$\begin{aligned} E \left((\hat{\beta} - \beta^0)(\hat{\beta} - \beta^0)^T \right) &= (A^T A)^{-1} A^T \text{Var}(\epsilon) A (A^T A)^{-1} \\ &= \sigma^2 (A^T A)^{-1} A^T A (A^T A)^{-1} = \sigma^2 (A^T A)^{-1} \end{aligned}$$



Variance in Linear Estimate

- To compute variance use trick: Suppose \mathbf{a} and \mathbf{z} are vectors, \mathbf{a} is non-random, \mathbf{z} is random:

$$E|\mathbf{a}^T \mathbf{z}|^2 = E(\mathbf{a}^T \mathbf{z} \mathbf{z}^T \mathbf{a}) = \mathbf{a}^T E(\mathbf{z} \mathbf{z}^T) \mathbf{a}$$

- From earlier: $E f(\mathbf{x}_{test}, \hat{\boldsymbol{\beta}}) = \phi(\mathbf{x}_{test})^T E \hat{\boldsymbol{\beta}} = \phi(\mathbf{x}_{test})^T \boldsymbol{\beta}^0$

- Therefore variance of linear model:

$$\begin{aligned} \text{Var}(\mathbf{x}_{test}) &= E[f(\mathbf{x}_{test}, \hat{\boldsymbol{\beta}}) - E f(\mathbf{x}_{test}, \hat{\boldsymbol{\beta}})]^2 = E[\phi(\mathbf{x}_{test})^T (\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}^0)]^2 \\ &= \phi(\mathbf{x}_{test})^T E[(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}^0)(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}^0)^T] \phi(\mathbf{x}_{test}) \\ &= \sigma^2 \phi(\mathbf{x}_{test})^T (\mathbf{A}^T \mathbf{A})^{-1} \phi(\mathbf{x}_{test}) \end{aligned}$$

- Above calculation is for the case of no under-modeling
- But, similar calculation shows variance expression is the same when there is under-modeling



Case with Equal Test & Training Distributions

□ Suppose that test point is distributed identically to training data

- Training data inputs $\mathbf{x}_i, i = 1, \dots, N$
- $\mathbf{x}_{test} = \mathbf{x}_i$ with probability $\frac{1}{N}$

□ Since rows of A are $\phi(\mathbf{x}_i)^T$: $A^T A = \sum_{i=1}^N \phi(\mathbf{x}_i) \phi(\mathbf{x}_i)^T$

□ Now use trick: For random vectors \mathbf{u}, \mathbf{v} : $E(\mathbf{u}^T \mathbf{v}) = \text{Tr } E(\mathbf{v} \mathbf{u}^T)$

- $\text{Tr}(A) = \sum_i A_{ii}$ = sum of diagonals

□ Therefore, variance averaged over \mathbf{x}_{test} is:

$$E \text{Var}(\mathbf{x}_{test}) = \sigma^2 E[\phi(\mathbf{x}_{test})^T (A^T A)^{-1} \phi(\mathbf{x}_{test})] = \sigma^2 \text{Tr}\{E[\phi(\mathbf{x}_{test}) \phi(\mathbf{x}_{test})^T (A^T A)^{-1}]\}$$

$$= \frac{\sigma^2}{N} \text{Tr}\left\{E\left[\sum_i \phi(\mathbf{x}_i) \phi(\mathbf{x}_i)^T (A^T A)^{-1}\right]\right\} = \frac{\sigma^2}{N} \text{Tr}\{E[(A^T A)(A^T A)^{-1}]\} = \frac{\sigma^2}{N} \text{Tr}\{I_p\} = \frac{\sigma^2 p}{N}$$



Case with Equal Test & Training Distributions

- Assumption on previous slide: Test point \mathbf{x}_{test} is randomly selected from training data
- Then, average variance is given by

$$E \text{Var}(\mathbf{x}_{test}) = \frac{\sigma^2 p}{N}$$

- Increases with number of parameters p
 - Shows that increasing model complexity increases variance error
- Decreases with number of samples N
- What if test data point is distributed differently from training data?
 - Then variance may be much larger $\frac{\sigma^2 p}{N}$
 - If test data is not like training data, we are extending model to regions not seen in training data
 - Often leads to high error



Summary of Results for Linear Models

□ Suppose model is linear with N = num samples, p = num parameters

□ Result 1: When $N < p$, linear estimate is not unique

- Need at least as many samples as parameters

□ Now assume that $N \geq p$ and parameter estimate is unique

□ Result 2: When there is no under-modeling, estimate is unbiased

$$E[f(\mathbf{x}_{test}, \hat{\boldsymbol{\beta}})] = f_0(\mathbf{x}_{test}).$$

□ Result 3: If test point drawn from same distribution as training data:

$$Var = \frac{p}{n} \sigma_{\epsilon}^2$$

- Variance increases linearly with number of parameters and inversely with number of samples



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Outline

- ❑ Motivating Example: What polynomial degree should a model use?
- ❑ Bias and variance
- ❑ Bias and variance for linear models (Advanced)

 Cross-validation



Cross Validation

❑ **Key idea:** Evaluate on samples different from training

❑ Get data X, y

❑ Split into training X_{tr}, y_{tr} and test X_{ts}, y_{ts}

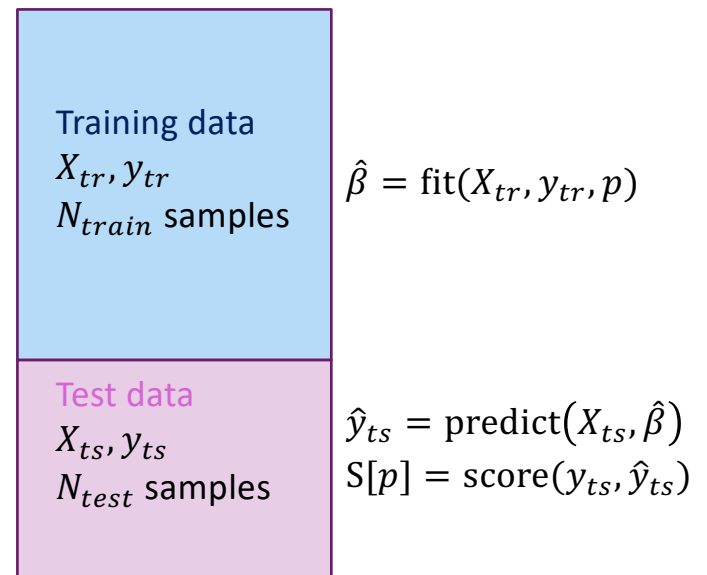
❑ For $p = 1$ to p_{max} // Loop over model order

- **Fit** on training data with model order p
- **Predict** values on test data
- **Score** fit on test data (e.g. measure RSS)

❑ Select model order with smallest score:

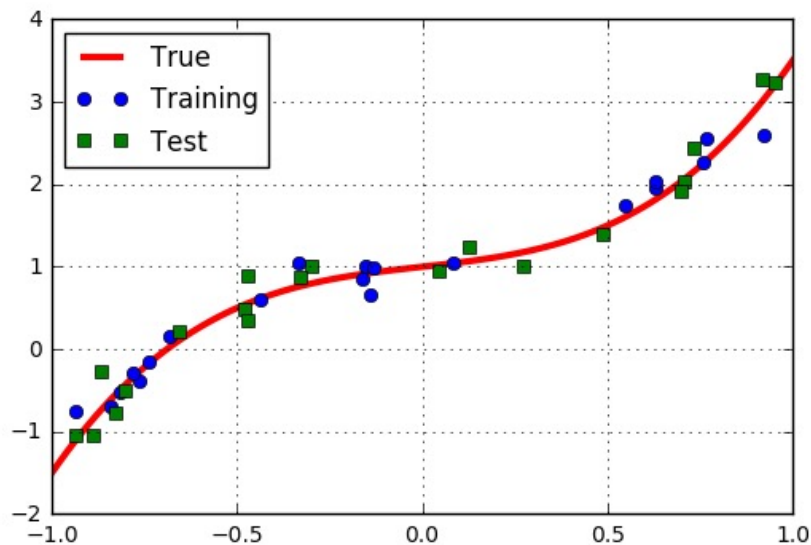
$$\hat{p} = \arg \min_p S[p]$$

- Maximize if higher score is better



Polynomial Example: Training Test Split

□ Example: Split data into 20 samples for training, 20 for test



```
# Number of samples for training and test
ntr = nsamp // 2
nts = nsamp - ntr

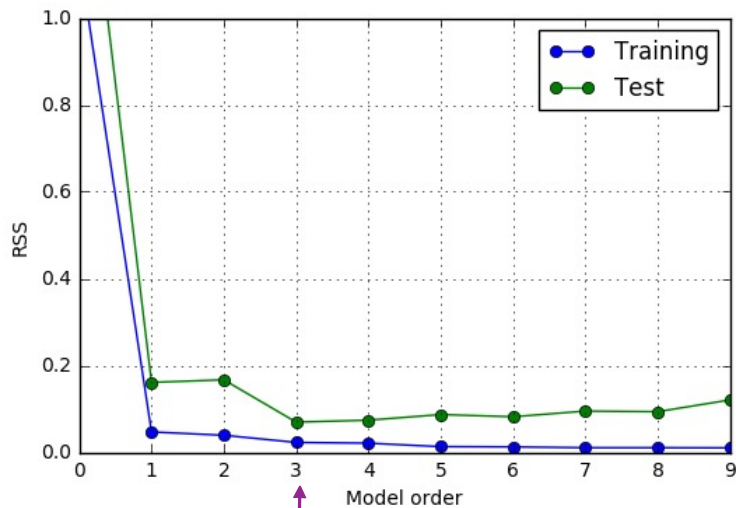
# Training
xtr = xdat[:ntr]
ytr = ydat[:ntr]

# Test
xts = xdat[ntr:]
yts = ydat[ntr:]
```



Finding the Model Order

Estimated optimal model order = 3



RSS test minimized at $d = 3$
RSS training always decreases

```
dtest = np.array(range(0,10))
RSStest = []
RSStr = []
for d in dtest:

    # Fit data
    beta_hat = poly.polyfit(xtr,ytr,d)

    # Measure RSS on training data
    # This is not necessary, but we do it just to show the training error
    yhat = poly.polyval(xtr,beta_hat)
    RSSd = np.mean((yhat-ytr)**2)
    RSStr.append(RSSd)

    # Measure RSS on test data
    yhat = poly.polyval(xts,beta_hat)
    RSSd = np.mean((yhat-yts)**2)
    RSStest.append(RSSd)

plt.plot(dtest,RSStr,'bo-')
plt.plot(dtest,RSStest,'go-')
plt.xlabel('Model order')
plt.ylabel('RSS')
plt.grid()
plt.ylim(0,1)
plt.legend(['Training','Test'],loc='upper right')
```



Problems with Simple Train/Test Split

- ❑ Test error could vary significantly depending on samples selected
- ❑ Only use limited number of samples for training
- ❑ Problems particularly bad for data with limited number of samples



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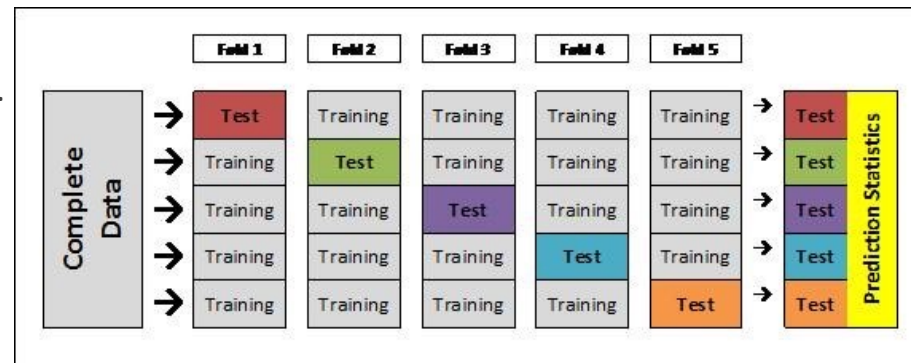
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K-Fold Cross Validation

□ K-fold cross validation

- Divide data into K parts
- Use $K - 1$ parts for training. Use remaining for test.
- Average over the K test choices
- More accurate, but requires K fits of parameters
- Typical choice: $K=5$ or 10
- Average MSE over K folds estimates the total MSE
- $(= \text{Bias}^2 + \text{Variance} + \text{irreducible error})$



□ Leave one out cross validation (LOOCV)

- Take $K = N$ so one sample is left out.
- Most accurate, but requires N model fittings
- Necessary when N is small.

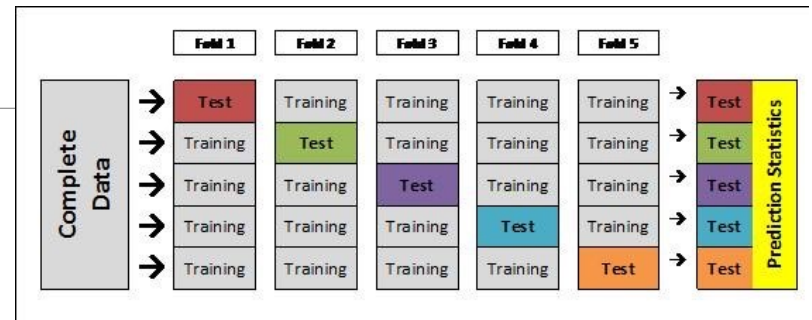
From

<http://blog.goldenhelix.com/goldenadmin/cross-validation-for-genomic-prediction-in-svs/>



K-Fold Pseudo-Code

- ❑ Get data X, y
- ❑ For $i = 1$ to K // Loop over folds
 - Split into training X_{tr}, y_{tr} and test X_{ts}, y_{ts} for fold i
 - For $p = 1$ to p_{max} // Loop over model order
 - **Fit** on training data with model order p : $\hat{\beta} = \text{fit}(X_{tr}, y_{tr}, p)$
 - **Predict** values on test data: $\hat{y}_{ts} = \text{predict}(X_{ts}, \hat{\beta})$
 - **Score** the fit on test data: $S[p, i] = \text{score}(y_{ts}, \hat{y}_{ts})$
- ❑ Find **average score** for each model order: $\bar{S}[p] = \frac{1}{K} \sum_{i=1}^K S[p, i]$
- ❑ Select model order with lowest average score: $\hat{p} = \arg \min_p \bar{S}[p]$



Polynomial Example

❑ Use sklearn Kfold object

❑ Loop

- Outer loop: Over K folds
- Inner loop: Over D model orders
- Measure test error in each fold and order
- Averaging test errors from K folds for each model order
- Find the model order with the minimal average test errors
- Can be time-consuming

```
# Create a k-fold object
nfold = 20
kf = sklearn.model_selection.KFold(n_splits=nfold,shuffle=True)

# Model orders to be tested
dtest = np.arange(0,10)
nd = len(dtest)

# Loop over the folds
RSSs = np.zeros((nd,nfold))
for isplit, Ind in enumerate(kf.split(xdat)):

    # Get the training data in the split
    Itr, Its = Ind
    xtr = xdat[Itr]
    ytr = ydat[Itr]
    xts = xdat[Its]
    yts = ydat[Its]

    for it, d in enumerate(dtest):

        # Fit data on training data
        beta_hat = poly.polyfit(xtr,ytr,d)

        # Measure RSS on test data
        yhat = poly.polyval(xts,beta_hat)
        RSSs[it,isplit] = np.mean((yhat-yts)**2)
```



Polynomial Example CV Results

□ For each model order d

- Compute mean test RSS over K folds
- Compute standard error (SE) of test RSS
- $SE = \text{STD of mean RSS} = \text{RSS std} / \sqrt{K - 1}$
- (expectation over different realizations of data in each fold)

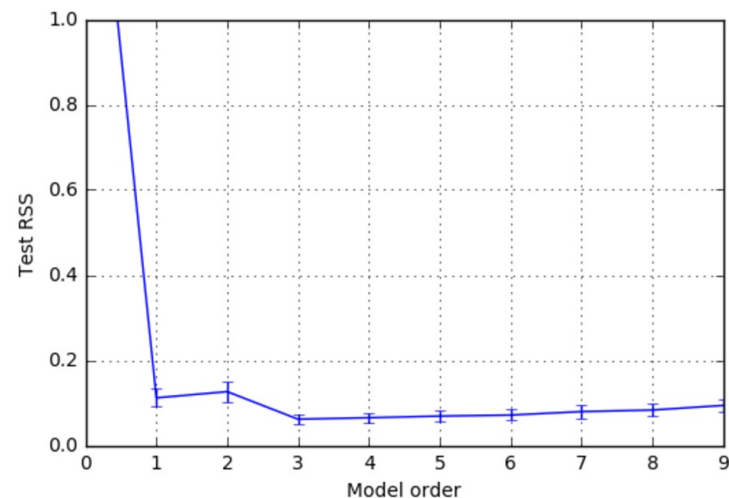
□ Simple model selection

- Select d with lowest mean test RSS

□ For this example

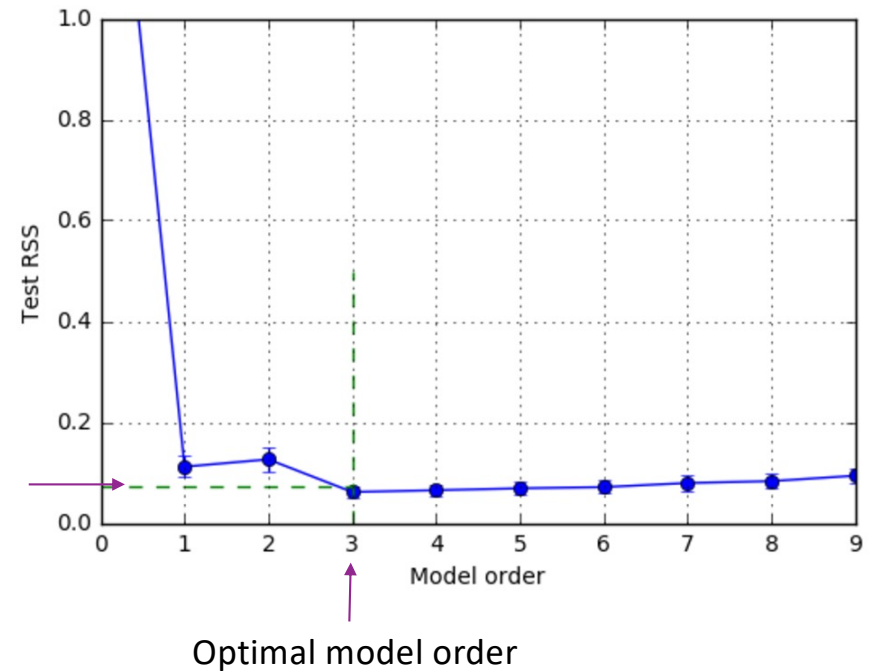
- Estimate model order = 3

```
RSS_mean = np.mean(RSSsts,axis=1)
RSS_std = np.std(RSSsts,axis=1) / np.sqrt(nfold-1)
plt.errorbar(dtest, RSS_mean, yerr=RSS_std, fmt='--')
plt.ylim(0,1)
plt.xlabel('Model order')
plt.ylabel('Test RSS')
plt.grid()
```



One Standard Error Rule

- Previous slide: Select d to minimize $RSS_mean[d]$
 - Average RSS across the folds and select lowest average
- Problem: Often over-predicts model order
- One standard deviation rule
 - Use simplest model “within one SE of minimum”



One SE Rule Pseudo-Code

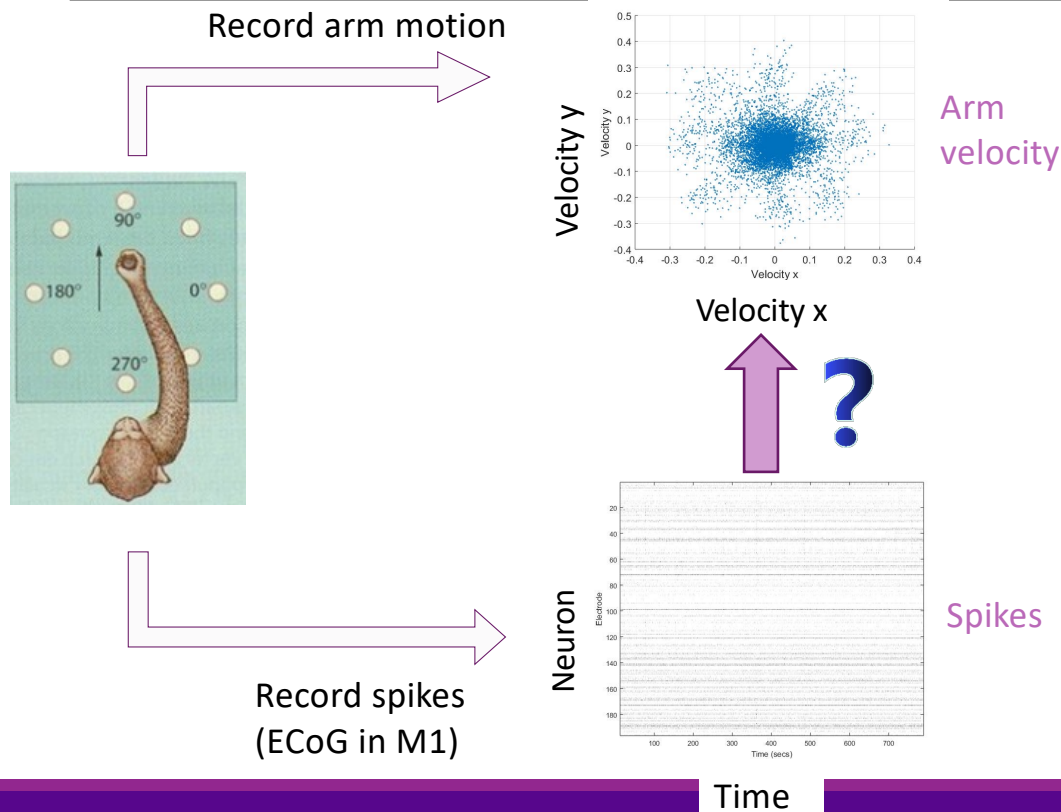
- ❑ Get data X, y
- ❑ Compute score as before: $S[p, i] = \text{score for model order } p \text{ on fold } i$
- ❑ Compute average, std deviation and standard error of the scores:
 - $\bar{S}[p] = \frac{1}{K} \sum_{i=1}^K S[p, i]$, $\sigma^2[p] = \frac{1}{K} \sum_{i=1}^K (S[p, i] - \bar{S}[p])^2$, $SE[p] = \frac{\sqrt{K}}{\sqrt{K-1}} \sigma[p]$
- ❑ Find model order via **normal rule**: $\hat{p}_0 = \arg \min_p \bar{S}[p]$ (lowest average score)
- ❑ Compute target score: $S_{tgt} = \bar{S}[p_0] + SE[p_0]$
- ❑ **One SE rule**: Find simplest model with score lower than target:

$$\hat{p} = \min\{p \mid \bar{S}[p] \leq S_{tgt}\}$$

- ❑ Note that one SE rule always produce a model order \leq normal rule ($\hat{p} \leq \hat{p}_0$)



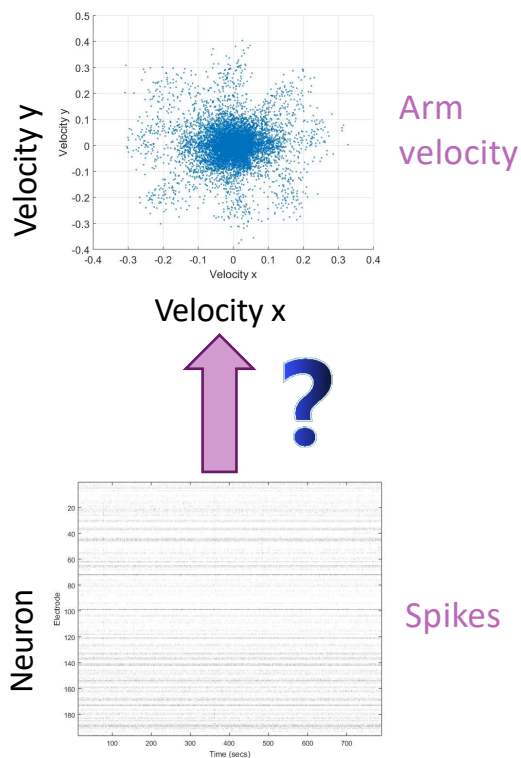
Lab: Neural ECoG Data



- ☐ Read a monkey's brain!
- ☐ Predict hand motion from electrode measurements (number of spikes in each neuron)
- ☐ Data from <https://crcns.org/>
 - Open source website on neural data
 - Great for projects



Lab: Neural ECoG Data



□ Linear filter model:

$$y[t, k] = \sum_{\ell=0}^d \sum_{j=0}^{p-1} X[t - \ell, j] W[\ell, j, k] + b[k]$$

- $X[t, j]$ = spikes from neuron j at time t
- $y[t, k]$ = Output k at time t (two outputs for x and y motion)
- $W[\ell, j, k]$ = weight from neuron j to output k at time delay ℓ

□ Linear fitting: Find W and b from X and y

□ Model order selection:

- Find optimal maximum delay d
- Higher d allows better fit, but uses more parameters



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