Lecture 4
Model Order Selection

EE-UY 4563/EL-GY 9123: INTRODUCTION TO MACHINE LEARNING

PROF. SUNDEEP RANGAN (WITH MODIFICATION BY YAO WANG)

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

Outline

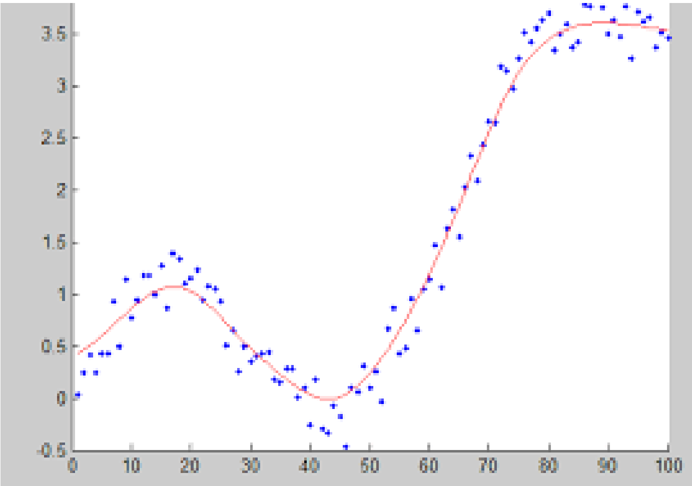
- Motivating Example: What polynomial degree should a model use?
- Bias and variance
- Bias and variance for linear models (Advanced)
- Cross-validation

Polynomial Fitting

- Last lecture: polynomial regression
- Given data $(x_i, y_i), i = 1, \ldots, N$
- Learn a polynomial relationship:

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

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



Demo on Github

- Demo on github: https://github.com/sdrangan/introml/blob/master/unit04_model_sel/demo1_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 der
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

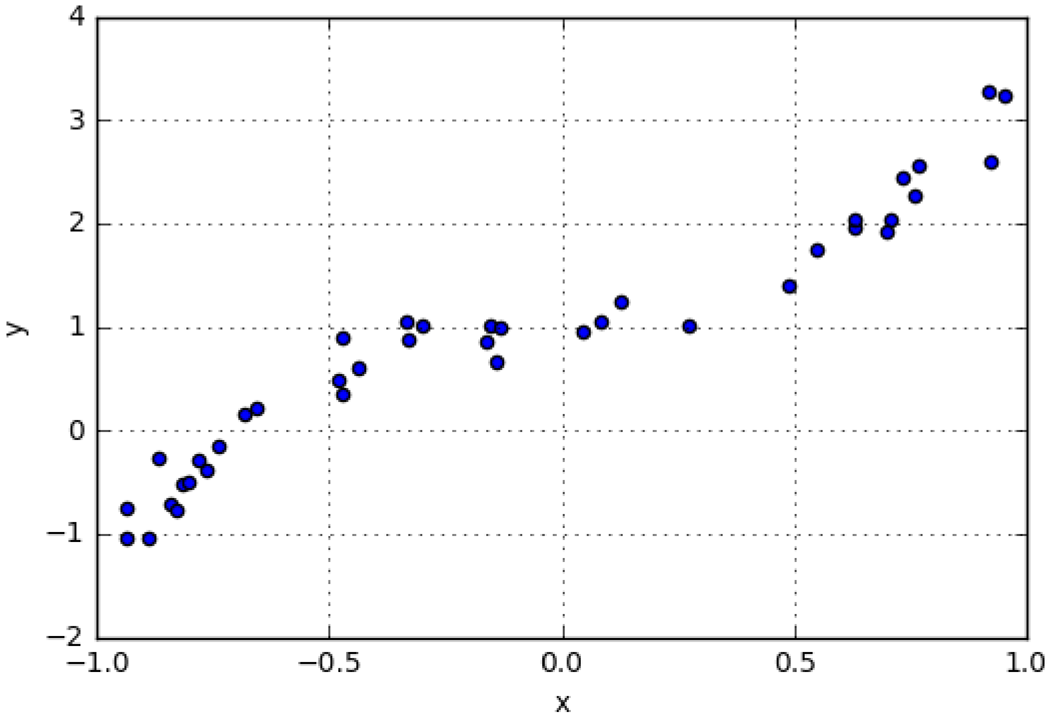
To illustrate the concepts, we consider a simple polynomial model:

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

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

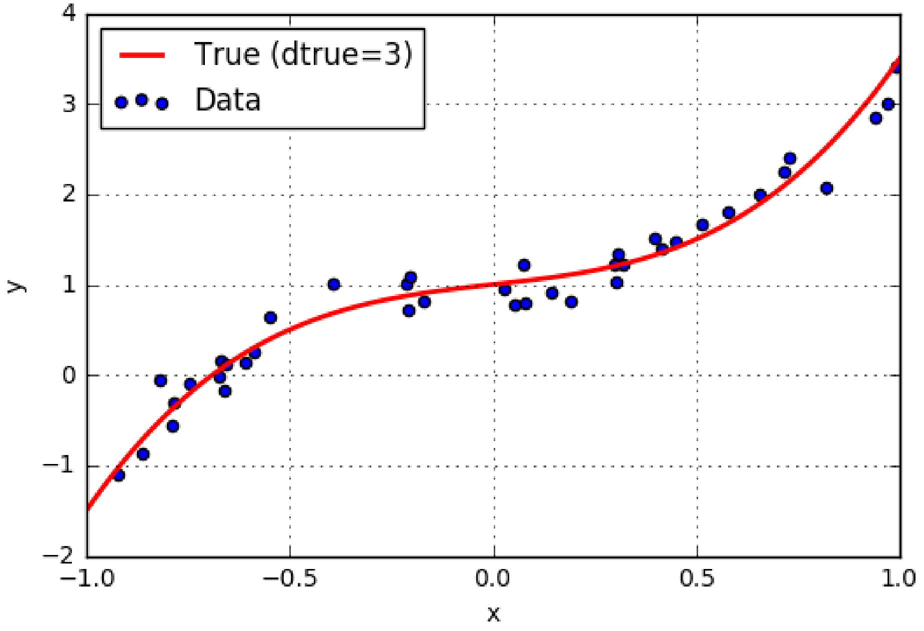
Example Question

- 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

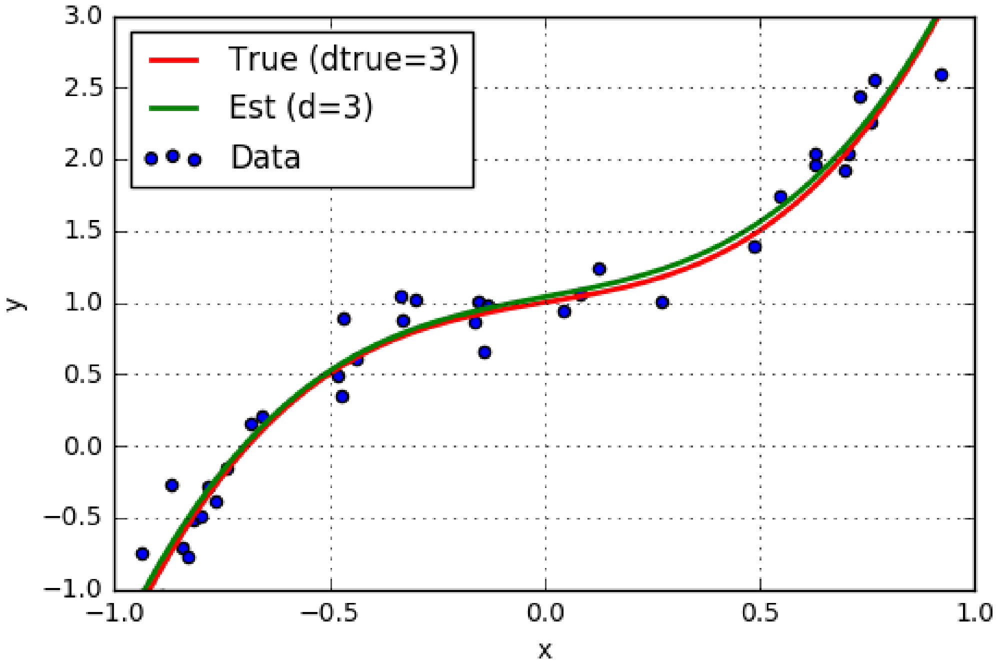
- Previous example is synthetic data
- x_i: 40 samples uniform in [-1,1]
- $y = f(x) + \epsilon$,
  - $f(x) = \beta_0 + \beta_1 x + \cdots + \beta_d x^d$ = "true relation"
  - $d = 3,\ \epsilon \sim N(0, \sigma^2)$
- Synthetic data useful for analysis
  - Know "ground truth"
  - Can measure performance 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

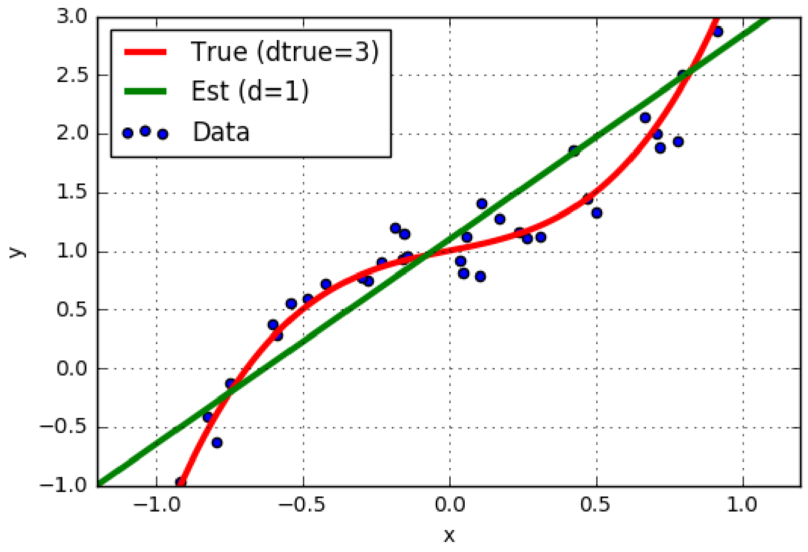
- Suppose true polynomial order, d=3, is known
- Use linear regression
  - numpy.polynomial package
- Get very good fit



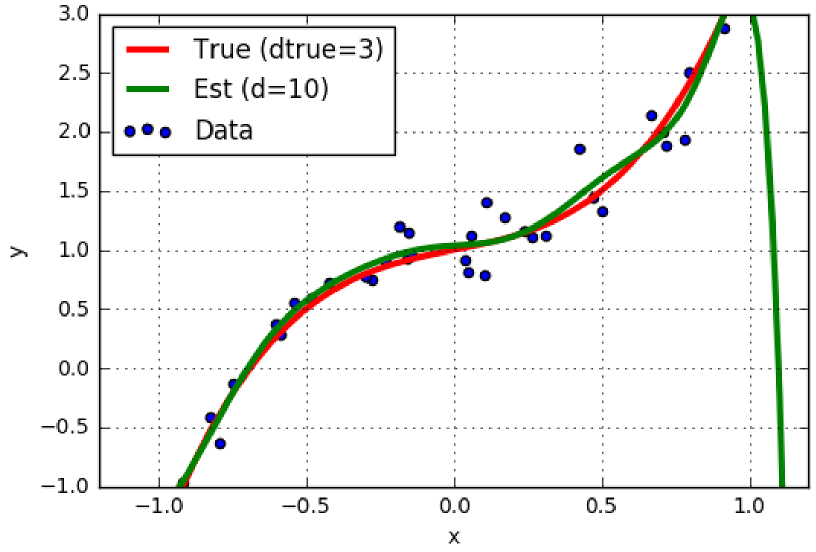

```
d = 3
beta_hat = poly.polyfit(xdat,ydat,d)

# 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?

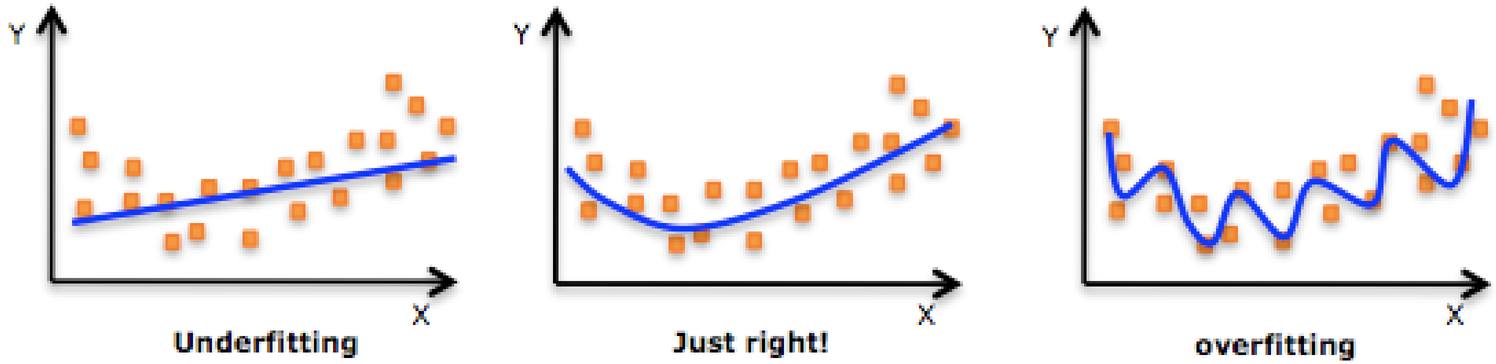


d=1 “Underfitting”



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?

Using RSS on Training Data?

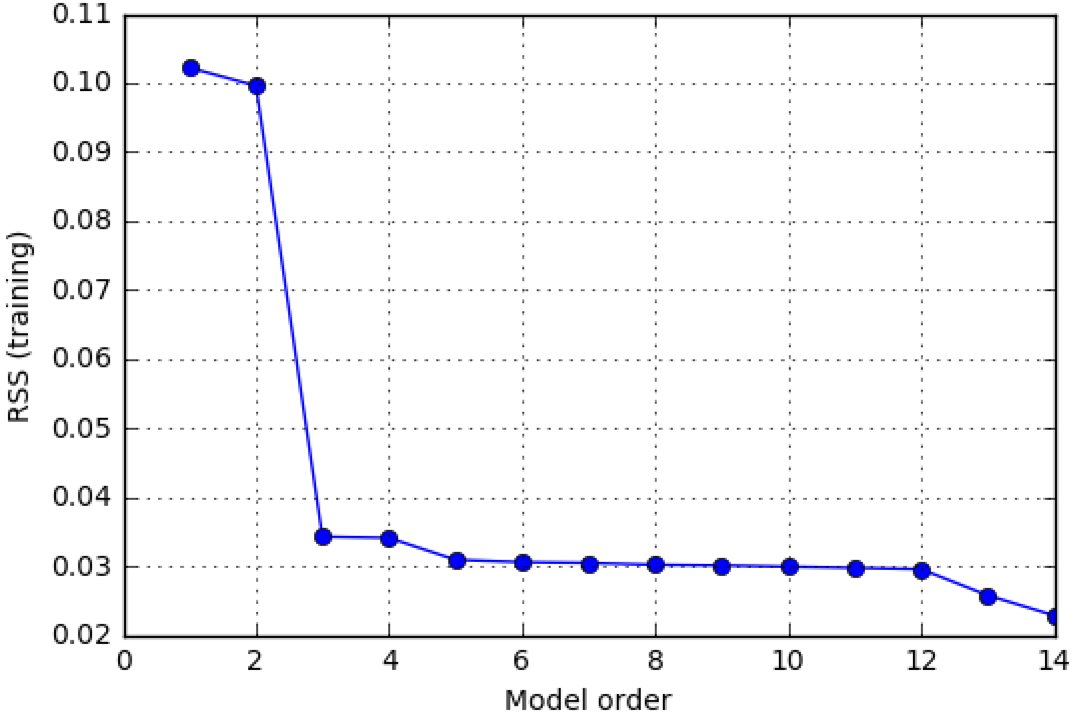
- Simple (but bad) idea:
  - For each model order, d, find estimate $\widehat{\boldsymbol{\beta}}$
  - Compute predicted values on training data

$$\hat{y}_i = \widehat{\boldsymbol{\beta}}^T \boldsymbol{x}_i$$

  - 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
- Feature selection

Model Class

- Consider general estimation problem
  - Given data (x_i, y_i) want to learn a functional relation: $y \approx \hat{y} = f(x)$
- Model class: The set of possible estimates:

$$\hat{y} = f(\boldsymbol{x}, \boldsymbol{\beta})$$

  - Set is parametrized by $\boldsymbol{\beta}$
- Many possible examples:
  - Linear model: $\hat{y} = \beta_0 + \beta_1 x_1 + \cdots + \beta_k x_k$
  - Polynomial model: $\hat{y} = \beta_0 + \beta_1 x + \cdots + \beta_k x^k$
  - Nonlinear: $\hat{y} = \beta_0 + \beta_1 e^{-\beta_2 x} + \beta_3 e^{-\beta_4 x}$
  - …

Model Class and True Function

- Analysis set-up:
  - Learning algorithm assumes a model class: $\hat{y} = f(\boldsymbol{x}, \boldsymbol{\beta})$
  - But, data has true relation: $y = f_0(x) + \epsilon,\ \epsilon \sim N(0, \sigma_\epsilon^2)$

- Will quantify three key effects:
  - Irreducible error
  - Under-modeling
  - Over-fitting

Output Mean Squared Error

- To evaluate prediction error suppose we are given:
  - A parameter estimate $\widehat{\boldsymbol{\beta}}$ (computed from the learning algorithm for a fixed training set)
  - A test point $\boldsymbol{x}_{test}$
  - Test point is generally different from training samples.
- Predicted value: $\hat{y} = f\left(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}}\right)$
- Actual value: $y = f_0(\boldsymbol{x}_{test}) + \boldsymbol{\epsilon}$
- Define output mean squared error given $\widehat{\boldsymbol{\beta}}$:

$$MSE_y\left(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}}\right) := E[y - \hat{y}]^2$$

  - Expectation is over noise $\boldsymbol{\epsilon}$ on the test sample.

Irreducible Error

- Rewrite output MSE:

$$MSE_y(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}}) \coloneqq E[y - \hat{y}]^2 = E\left[f_0(\boldsymbol{x}_{test}) + \epsilon - f(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}})\right]^2$$

- Since noise on test sample is independent of $\widehat{\boldsymbol{\beta}}$ and $\boldsymbol{x}_{test}$:

$$MSE_y(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}}) \coloneqq \left[f_0(\boldsymbol{x}_{test}) - f(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}})\right]^2 + \mathrm{E}(\epsilon^2) = \left[f_0(\boldsymbol{x}_{test}) - f(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}})\right]^2 + \sigma_\epsilon^2$$

- Define irreducible error: σ_ϵ^2
  - Lower bound on $MSE_y(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}}) \geq \sigma_\epsilon^2$
  - Fundamental limit on ability to predict y
  - Occurs since y is influenced by other factors than $\boldsymbol{x}$

Under-Modeling

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

$$f_0(\boldsymbol{x}) = f(\boldsymbol{x}, \boldsymbol{\beta}_0) \text{ for all } \boldsymbol{x}$$

  for some parameter $\boldsymbol{\beta}_0$.
    - $\boldsymbol{\beta}_0$ called the true parameter

- Under-modeling: When $f_0(\boldsymbol{x})$ is not in the model class

Sample Question

- 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

- Examples:
  - True function: $f_0(x) = 2 + 3x$ Model class: $f(x, \beta) = \beta_0 + \beta_1 x + \beta_2 x^2$
  - True function: $f_0(x) = 2 + 3x + 4x^2$ Model class: $f(x, \beta) = \beta_0 + \beta_1 x$
  - True function: $f_0(x) = \sin(2\pi(5)x + 7)$ Model class: $f(x, \beta) = \beta_0 \sin(2\pi(5)x) + \beta_1 \cos(2\pi(5)x)$
  - True function: $f_0(x) = \sin(2\pi(8)x + 7)$ Model class: $f(x, \beta) = \beta_0 \sin(2\pi(5)x) + \beta_1 \cos(2\pi(5)x)$

- Solutions in class

Under-Modeling and Irreducible Error

- Suppose that:
  - There is no under-modeling: $f_0(\boldsymbol{x}) = f(\boldsymbol{x}, \boldsymbol{\beta}_0)$ for some "true" parameter $\boldsymbol{\beta}_0$; and
  - Estimator selects the true parameter $\widehat{\boldsymbol{\beta}} = \boldsymbol{\beta}_0$
- Then, output error is:

$$MSE_y\left(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}}\right) \coloneqq \left[f_0(\boldsymbol{x}_{test}) - f\left(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}}\right)\right]^2 + \sigma_\epsilon^2 = \sigma_\epsilon^2$$

- Conclusion: If there is no undermodeling and we can estimate the true parameter:
  - We can get output error = irreducible error
  - We can achieve the same error as if we knew the true function $f_0(\boldsymbol{x})$

Bias of an Estimator

- Suppose training data $(\boldsymbol{x}_i, y_i)$ is generated as follows:
  - Fix data input points $\boldsymbol{x}_i, i = 1, \ldots, N$ (Treat as non-random)
  - Generate data output points $y_i = f_0(\boldsymbol{x}_i) + \epsilon_i$ with random i.i.d. noise ϵ_i with some distribution
- Then estimate $\widehat{\boldsymbol{\beta}}$ is a random vector
  - Depends on the noise ϵ_i in the training data
- Definition: The bias at a test point $\boldsymbol{x}_{test}$ is:

$$\text{Bias}(\boldsymbol{x}_{test}) := f_0(\boldsymbol{x}_{test}) - E\left[f\left(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}}\right)\right]$$

- Measures the difference between:
  - True function $f_0(\boldsymbol{x}_{test})$
  - Expected value of estimated $f\left(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}}\right)$, averaged over the noise in the training data

Bias: Noise-Free Case

- Suppose true relation has no noise: $y = f_0(\boldsymbol{x})$
  - Will handle noise later
- Get training data: $(\boldsymbol{x}_i, y_i), i = 1, \ldots, n$
- Fit model parameter from least-squares:

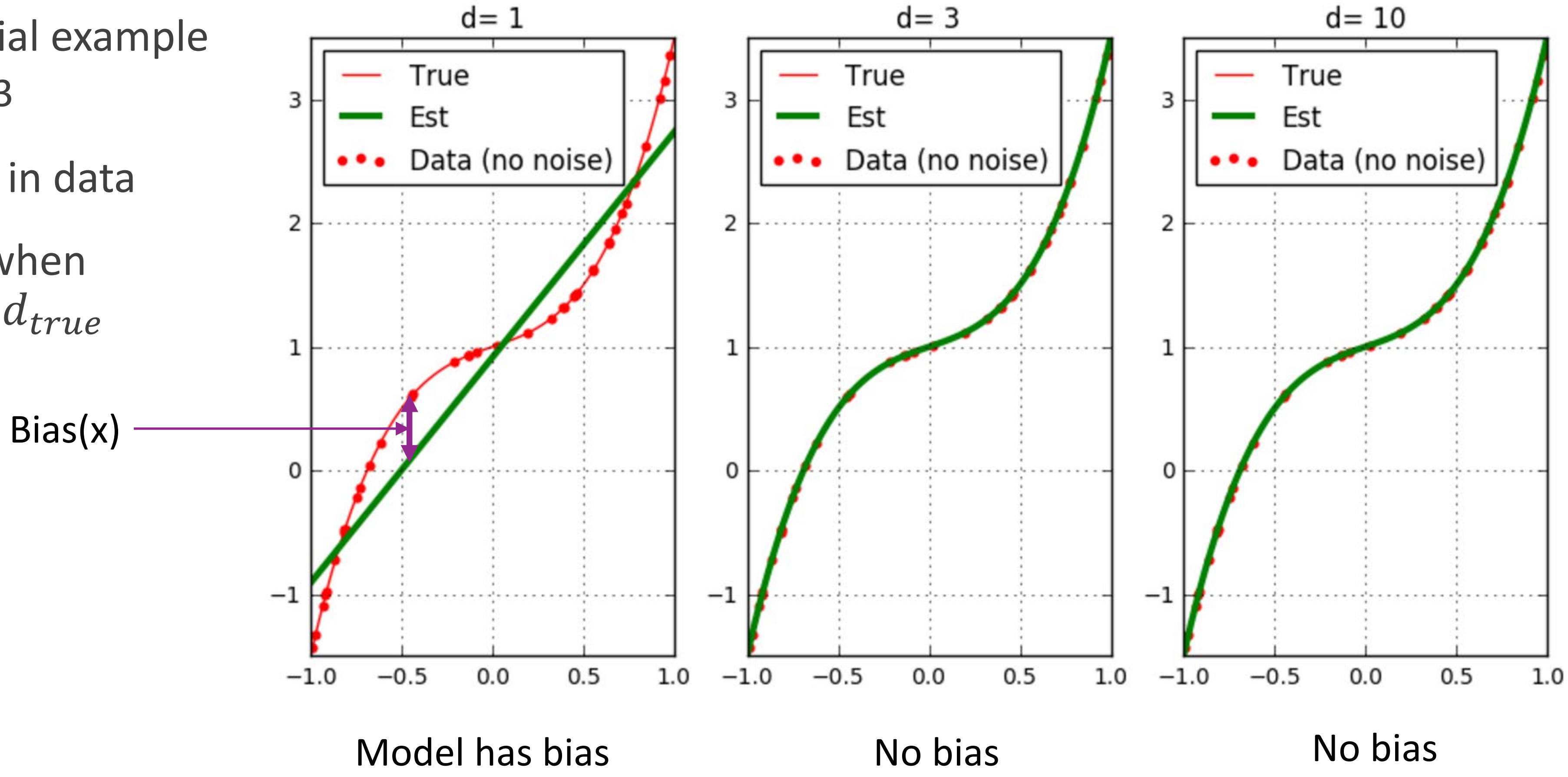
$$\hat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}} \sum_{i=1}^{n} \left(y_i - f(\boldsymbol{x}_i, \boldsymbol{\beta})\right)^2 = \arg\min_{\boldsymbol{\beta}} \sum_{i=1}^{n} \left(f_0(\boldsymbol{x}_i) - f(\boldsymbol{x}_i, \boldsymbol{\beta})\right)^2$$

  - Minimizing training error finds best least squares fit of the true functions in the model class
- Conclusions: If
  - There is no under-modeling: $f_0(\boldsymbol{x}_i) = f(\boldsymbol{x}_i, \boldsymbol{\beta}_0)$ for some true parameter $\boldsymbol{\beta}_0$
  - Minimization for $\hat{\boldsymbol{\beta}}$ is unique

Then $\hat{\boldsymbol{\beta}}$= $\boldsymbol{\beta}_0$ and $\mathrm{Bias}(\boldsymbol{x}_{test}) = 0$ for all $\boldsymbol{x}_{test}$:
  - No bias when there is no under-modeling and no noise
- Will show later that for linear models, there is no bias even when there is no noise

Bias Visualized

- Polynomial example
  - $d_{true} = 3$
- No noise in data
- No bias when $d \geq d_{true}$



MSE of an Estimator

- Data model: $y = f_0(\boldsymbol{x}) + \epsilon, \epsilon \sim N(0, \sigma_\epsilon^2)$
- Get training data: $(\boldsymbol{x}_i, y_i), i = 1, \ldots, n$
- Fit parameter $\widehat{\boldsymbol{\beta}}$ from data (e.g. via least squares)
  - $\widehat{\boldsymbol{\beta}}$ will be random. Depends on particular noise realization for the selected training samples.
- Take a new test point $\boldsymbol{x}_{test}$
- Define two mean square errors:
  - Output MSE: $\mathrm{MSE}_y(\boldsymbol{x}_{test}) \coloneqq E\left[y - f\left(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}}\right)\right]$: Error on the predicted value
  - Function MSE: $\mathrm{MSE}_f(\boldsymbol{x}_{test}) \coloneqq E\left[f_0(\boldsymbol{x}_{test}) - f\left(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}}\right)\right]$: Error on the underlying function
- Expectation is over both:
  - Noise in the training data : $y_i = f_0(\boldsymbol{x}_i) + \epsilon_i$
  - Noise on the test sample: $y = f_0(\boldsymbol{x}_{test}) + \epsilon$

MSE and the and Irreducible Error

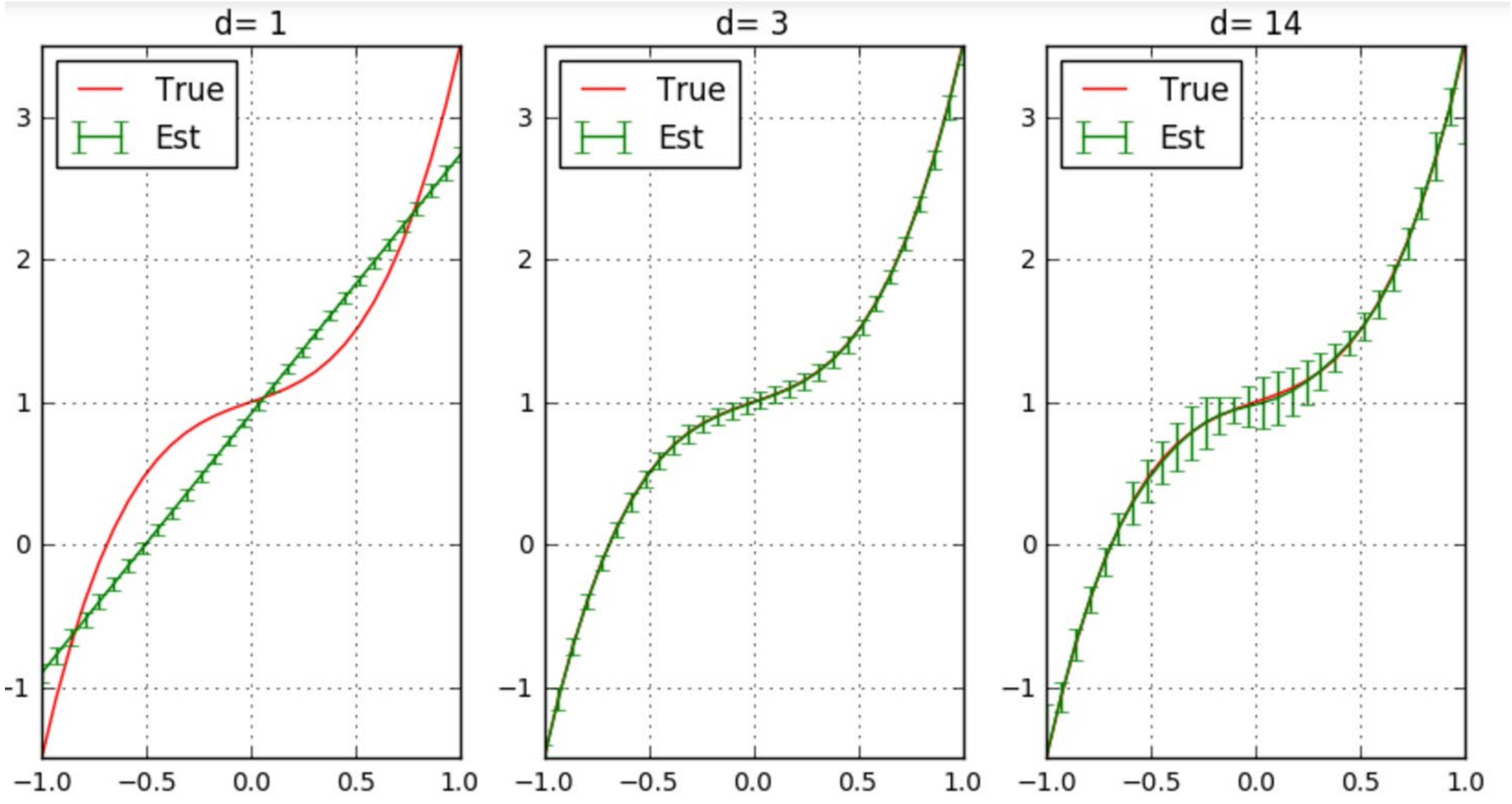
- From previous slide:
  - Output MSE: $\mathrm{MSE}_y(\boldsymbol{x}_{test}) \coloneqq E\left[y - f\left(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}}\right)\right]$: Error on the predicted value
  - Function MSE: $\mathrm{MSE}_f(\boldsymbol{x}_{test}) \coloneqq E\left[f_0(\boldsymbol{x}_{test}) - f\left(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}}\right)\right]$: Error on the underlying function
- Theorem: $\mathrm{MSE}_y(\boldsymbol{x}_{test}) = \mathrm{MSE}_f(\boldsymbol{x}_{test}) + \epsilon^2$
  - Recall ϵ^2 is the irreducible error
- Proof: Similar to before:
  - We know $y = f_0(x_{test}) + \epsilon$
  - $MSE_y(\boldsymbol{x}_{test}) = E\left[y - f\left(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}}\right)\right]^2 = E\left[f_0(\boldsymbol{x}_{test}) + \epsilon - f\left(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}}\right)\right]^2$
  - But, ϵ is independent of $f_0(\boldsymbol{x}_{test})$ and $f\left(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}}\right)$
  - Therefore $MSE_y(\boldsymbol{x}_{test}) = E\left[f_0(\boldsymbol{x}_{test}) - f\left(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}}\right)\right]^2 + \mathrm{E}(\epsilon^2) = MSE_f(\boldsymbol{x}_{test}) + \sigma_\epsilon^2$

Bias and Variance

- We will show that function MSE can be related to two key quantities
- Bias: $Bias(\boldsymbol{x}_{test}) := f_0(\boldsymbol{x}_{test}) - E\left[f\left(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}}\right)\right]$
  - How much the average value of the estimate differs from the true function
- Variance: $Var(\boldsymbol{x}_{test}) \coloneqq E\left[f\left(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}}\right) - E\left[f\left(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}}\right)\right]\right]^2$
  - 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 x_i
  - Each dataset has different output values y_i because of independent noise in the training data
  - Obtain $\widehat{\boldsymbol{\beta}}$ for each training data set
  - Bias and variances are computed over the different sets
- Of course, in reality, we have only one training dataset
- But, bias and variance are used to study theoretical averages over different experiments

Bias and Variance Illustrated

- Polynomial ex
- Mean and std dev of estimated functions
- 100 trials
- Solid line: mean estimate among all trials
- Error bars: 1 STD



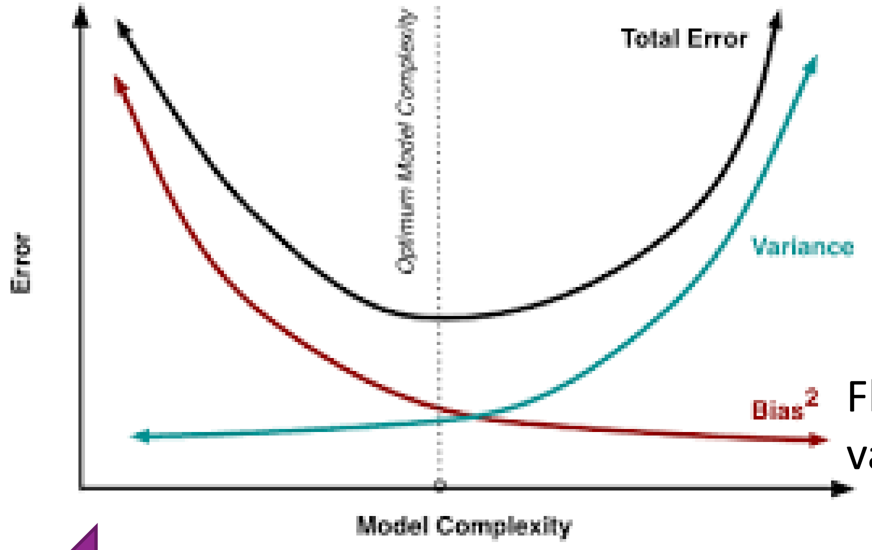
Low variance,
High bias

High variance,
Zero bias

Bias-Variance Formula

- Recall definitions:
  - Function MSE: $\mathrm{MSE}_f(\boldsymbol{x}_{test}) \coloneqq E\left[f_0(\boldsymbol{x}_{test}) - f\left(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}}\right)\right]$:
  - Bias: $Bias(\boldsymbol{x}_{test}) := f_0(\boldsymbol{x}_{test}) - E\left[f\left(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}}\right)\right]$
  - Variance: $Var(\boldsymbol{x}_{test}) \coloneqq E\left[f\left(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}}\right) - E\left[f\left(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}}\right)\right]\right]^2$
- Bias-Variance formula : $MSE_f(\boldsymbol{x}_{test}) = Bias(\boldsymbol{x}_{test})^2 + Var(\boldsymbol{x}_{test})$
  - 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



Floor is the noise variance

Simpler models
Less parameters
Under-fitting

Richer models
More parameters
Over-fitting

- 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

Bias-Variance Formula Proof

- Define $\bar{f}(\boldsymbol{x}_{test}) = E[f(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}})]$ = average value of estimated function
- $\mathrm{MSE}_f(\boldsymbol{x}_{test}) = E[f_0(\boldsymbol{x}_{test}) - f(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}})]^2 = E\left[f_0(\boldsymbol{x}_{test}) - \bar{f}(\boldsymbol{x}_{test}) + \bar{f}(\boldsymbol{x}_{test}) - f(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}})\right]^2$
- Three components: $\mathrm{MSE}_f(\boldsymbol{x}_{test}) = M_1 + M_2 - 2M_3$
  - $M_1 = E\left[f_0(\boldsymbol{x}_{test}) - \bar{f}(\boldsymbol{x}_{test})\right]^2 = \left[f_0(\boldsymbol{x}_{test}) - \bar{f}(\boldsymbol{x}_{test})\right]^2 = Bias(x_{test})$
  - $M_2 = E\left[f(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}}) - \bar{f}(\boldsymbol{x}_{test})\right]^2 = Var(x_{test})$
  - $M_3 = E\left[(f_0(\boldsymbol{x}_{test}) - \bar{f}(\boldsymbol{x}_{test}))(f(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}}) - \bar{f}(\boldsymbol{x}_{test}))\right]$
    $= (f_0(\boldsymbol{x}_{test}) - \bar{f}(\boldsymbol{x}_{test}))E\left[f(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}}) - \bar{f}(\boldsymbol{x}_{test})\right]$
    $= (f_0(\boldsymbol{x}_{test}) - \bar{f}(\boldsymbol{x}_{test}))(\bar{f}(\boldsymbol{x}_{test}) - \bar{f}(\boldsymbol{x}_{test})) = 0$

Outline

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

This Section is Advanced

- This section requires more advanced probability and linear algebra
- Means and variances of random vectors
- Undergraduates: Skip to final slide for final conclusions
- Graduate students: We will cover this
  - You should review your multi-variable probability and linear algebra

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: $y = f_0(x) + \epsilon, E(\epsilon) = 0, \quad E(\epsilon^2) = \sigma^2$
- When there is no under-modeling: $f_0(x) = f(x, \beta^0) = \phi(x)^T \beta^0$
  - $\beta^0 = (\beta_0^0, \cdots, \beta_k^0)$ True parameter
- Get data $(x_i, y_i), i = 1, \ldots, N$
- 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 $Rank(A) \geq p$
  - Otherwise solution is not unique
- Since $Rank(A) \leq \min(N, p)$ we need $N \geq p$.
- Recall:
  - N = number of data samples
  - p = number of parameters
- Conclusion: Number of samples ≥ 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: $\boldsymbol{x} = (x_1, \ldots, x_d)^T$: Each component x_j is a random variable
- Mean: The vector of means of the components

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

- Covariance components: $\mathrm{Cov}(x_i, x_j) = E\left[(x_i - \mu_i)(x_j - \mu_j)\right]$
- Variance matrix ($d \times d$):

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

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
- $Ef\left(x_{test}, \hat{\beta}\right) = \phi(x_{test})^T E\hat{\beta} = \phi(x_{test})^T \beta^0 = f_0(x_{test})$
- Therefore $Bias(x_{test}) := f_0(x_{test}) - Ef\left(x_{test}, \hat{\beta}\right) = 0$
- 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 $E\epsilon_i = 0, E\epsilon_i^2 = \sigma^2$

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

- Therefore variance matrix is: $\mathrm{Var}(\epsilon) = \sigma^2 I$
- From last slide: $\hat{\beta} = \beta^0 + (A^T A)^{-1} A^T \epsilon$.
- Applying variance formula of a linear transformation of ϵ

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

Variance in Linear Estimate

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

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

- From earlier: $Ef\left(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}}\right) = \phi(\boldsymbol{x}_{test})^T E\widehat{\boldsymbol{\beta}} = \phi(\boldsymbol{x}_{test})^T\boldsymbol{\beta}^0$

- Therefore variance of linear model:

$$\begin{aligned}\mathrm{Var}(\boldsymbol{x}_{test}) &= E\left[f\left(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}}\right) - Ef\left(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}}\right)\right]^2 = E\left[\phi(\boldsymbol{x}_{test})^T(\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}^0)\right]^2 \\ &= \phi(\boldsymbol{x}_{test})^T E\left[\left(\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}^0\right)\left(\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}^0\right)^T\right]\phi(\boldsymbol{x}_{test}) \\ &= \sigma^2\phi(\boldsymbol{x}_{test})^T(\boldsymbol{A}^T\boldsymbol{A})^{-1}\phi(\boldsymbol{x}_{test})\end{aligned}$$

- 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 $\boldsymbol{x}_i, i = 1, \ldots, N$
  - $\boldsymbol{x}_{test} = \boldsymbol{x}_i$ with probability $\frac{1}{N}$
- Since rows of A are $\phi(\boldsymbol{x}_i)^T$: $A^T A = \sum_{i=1}^{N} \phi(\boldsymbol{x}_i)\phi(\boldsymbol{x}_i)^T$
- Now use trick: For random vectors $\boldsymbol{u}, \boldsymbol{v}$: $E(\boldsymbol{u}^T \boldsymbol{v}) = Tr\, E(\boldsymbol{v}\boldsymbol{u}^T)$
  - $Tr(A) = \sum_i A_{ii}$ = sum of diagonals
- Therefore, variance averaged over $\boldsymbol{x}_{test}$ is:
  $E\, Var(\boldsymbol{x}_{test}) = \sigma^2 E[\phi(\boldsymbol{x}_{test})^T (\boldsymbol{A}^T\boldsymbol{A})^{-1} \phi(\boldsymbol{x}_{test})] = \sigma^2 Tr\{E[\phi(\boldsymbol{x}_{test})\phi(\boldsymbol{x}_{test})^T](\boldsymbol{A}^T\boldsymbol{A})^{-1}\}$

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

Case with Equal Test & Training Distributions

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

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

- 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

$$E\left[f\left(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}}\right)\right] = f_0\ (\boldsymbol{x}_{test},).$$

- 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

Outline

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

Cross Validation

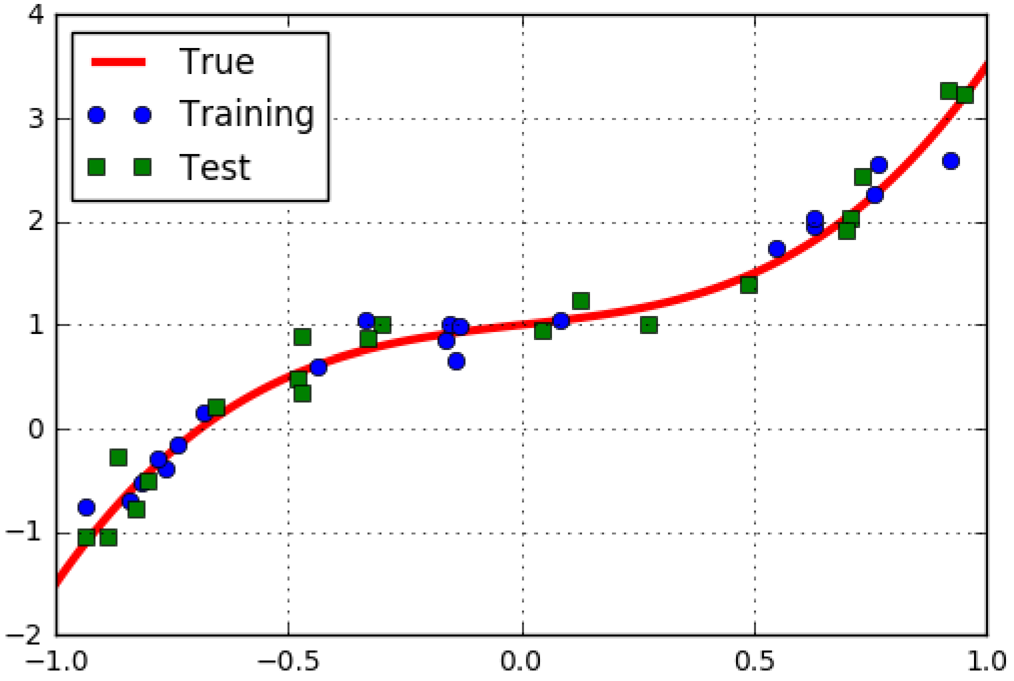
- Concept: Need to fit on test data independent of training data
- Divide data into two sets:
  - N_{train} training samples, N_{test} test samples
- For each model order, p, learn parameters $\hat{\beta}$ from training samples
- Measure RSS on test samples.

$$RSS_{test}(p) = \sum_{i \in \text{test}} (\hat{y}_i - y_i)^2$$

- Select model order p that minimizes $RSS_{test}(p)$

Polynomial Example: Training Test Split

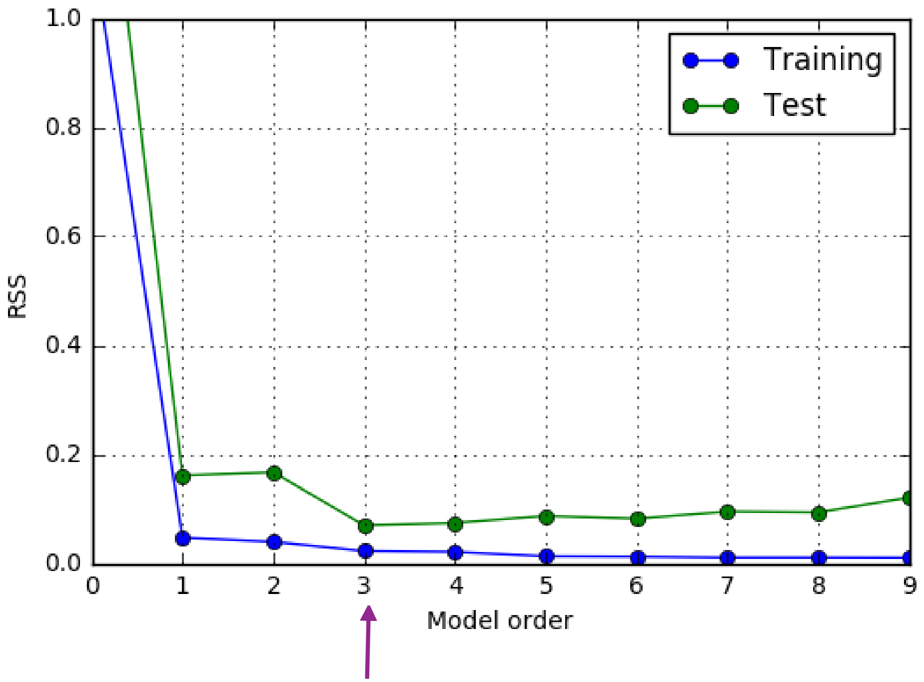
- Example: Split data into 20 samples for training, 20 for test




```python
# 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

```python
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')
```

General Procedure

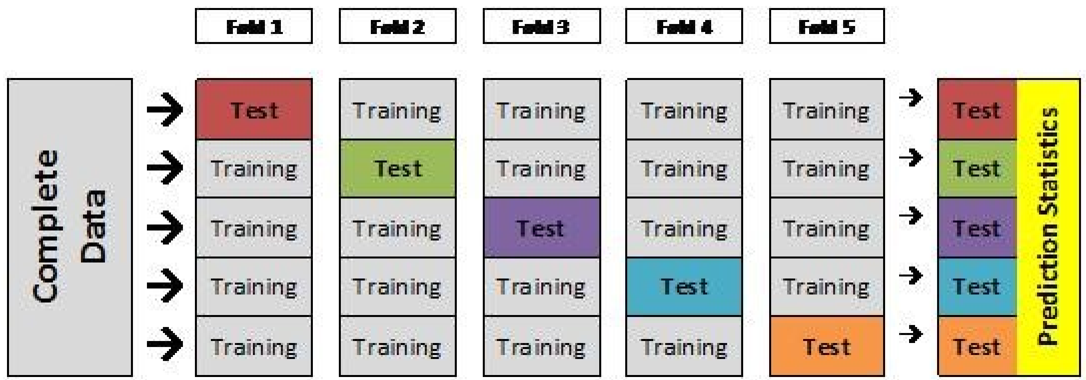
- Get data X, y
- Split into training X_{tr}, y_{tr} and test X_{ts}, y_{ts}
- For $p = 1$ to p_{max} // Loop over model order
  - Fit on training data with model order p : $\hat{\beta} = \text{fit}(X_{tr}, y_{tr}, p)$
  - Predict values on test data: $\hat{y}_{ts} = \text{predict}(X_{ts}, \hat{\beta})$
  - Score fit on test data: $\text{S}[p] = \text{score}(y_{ts}, \hat{y}_{ts})$
- Select model order with smallest score: $\hat{p} = \arg\min_{p} S[p]$
  - Or, use highest score if we want to maximize score instead of minimizing

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

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
  - (=Bias^2+Variance+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 : $\hat{\beta} = \mathrm{fit}(X_{tr}, y_{tr}, p)$
    - Predict values on test data: $\hat{y}_{ts} = \mathrm{predict}(X_{ts}, \hat{\beta})$
    - Score the fit on test data: $\mathrm{S}[p, i] = \mathrm{score}(y_{ts}, \hat{y}_{ts})$
- Find average score for each model order: $\bar{S}[\mathrm{p}] = \frac{1}{K} \sum_{i=1}^{K} S[p, i]$
- Select model order with lowest average score: $\hat{p} = \arg\min_{p} \bar{S}[p]$

Polynomial Example

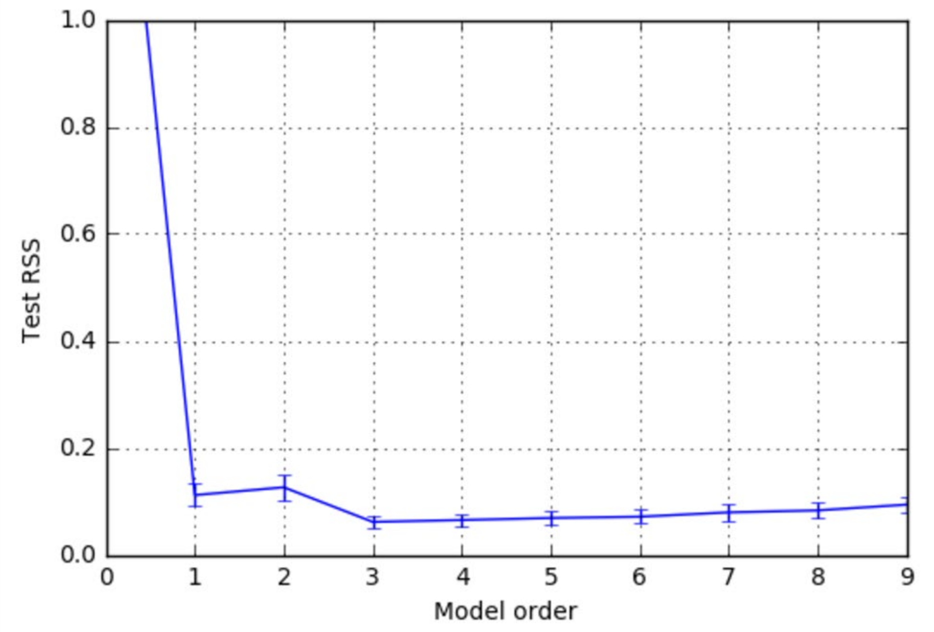
- ❑ Use sklearn Kfold object
- ❑ Loop
  - Outer loop: Over K folds
  - Inner loop: Over D model orders
  - Measure test error in each fold and order
  - Averaging test errors from K folds for each model order
  - Find the model order with the minimal average test errors
  - Can be time-consuming

```python
# 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
RSSts = 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)
        RSSts[it,isplit] = np.mean((yhat-yts)**2)
```

Polynomial Example CV Results

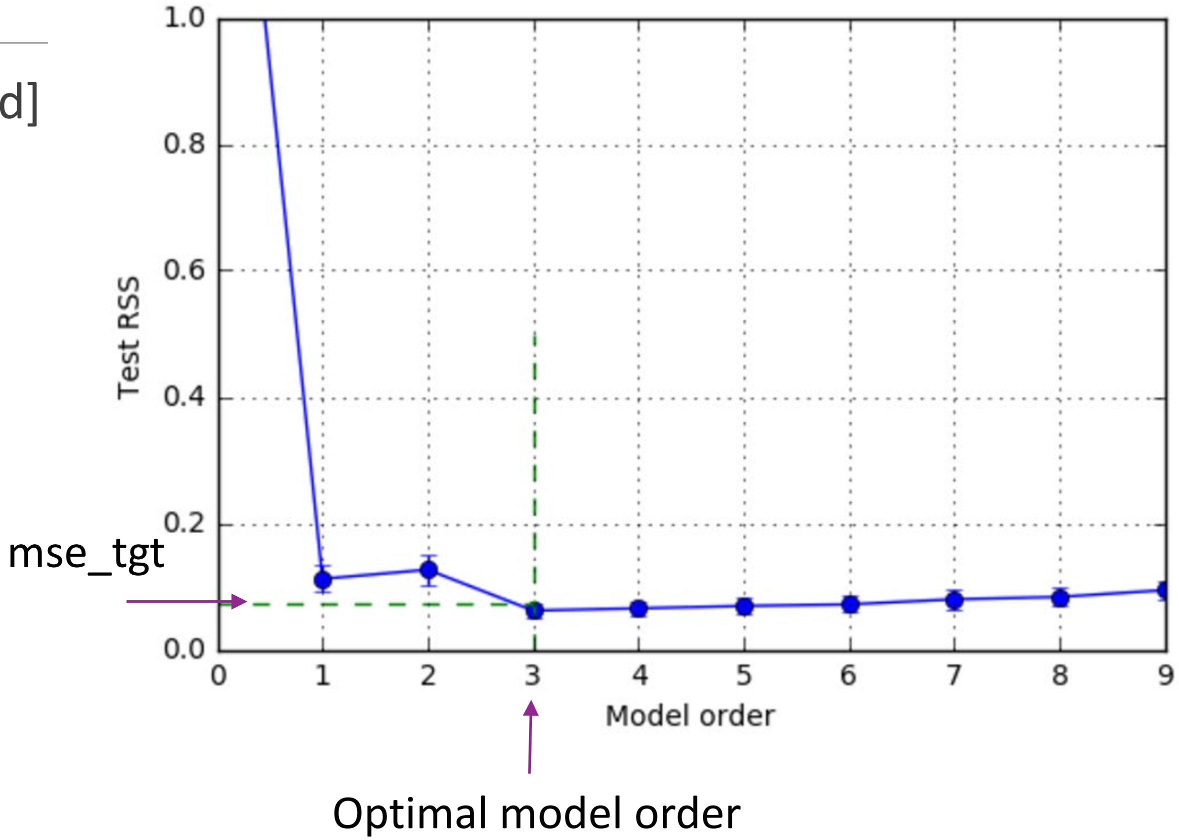
- For each model order d
  - Compute mean test RSS over K folds
  - Compute standard error (SE) of test RSS
  - SE=STD of mean RSS=RSS std/ $\sqrt{K-1}$
  - (expectation over different realizations of data in each fold)
- Simple model selection
  - Select d with lowest mean test RSS
- For this example
  - Estimate model order = 3

```
RSS_mean = np.mean(RSSts,axis=1)
RSS_std  = np.std(RSSts,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 mse_mean[d]
- Problem: Often over-predicts model order
- One standard deviation rule
  - Use simplest model within one SE of minimum
- Detailed procedure:
  - Find d0 to minimize mse_mean[d]
  - Set mse_tgt = mse_mean[d0] + mse_std[d0]
  - Find minimal dopt s.t. mse_mean[dopt] <= mse_tgt



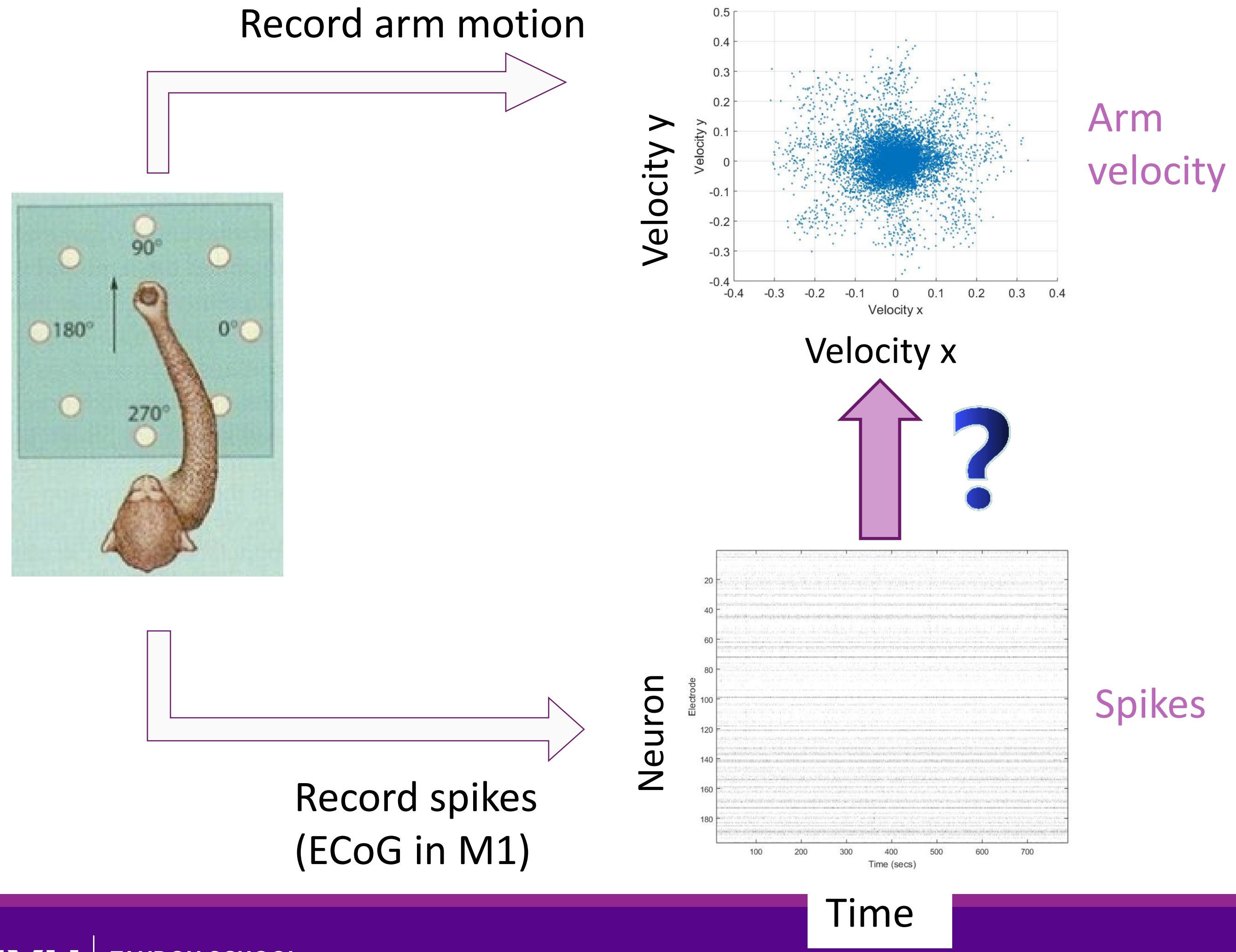
One SE Rule Pseudo-Code

- Get data X, y
- Compute score as before: $S[p, i]$ = score for model order p on fold i
- Compute average, std deviation and standard error of the scores:
  - $\bar{S}[\mathrm{p}] = \frac{1}{K}\sum_{i=1}^{K} S[p,i]$, $\sigma^2[p] = \frac{1}{K}\sum_{i=1}^{K} S[p,i]$, $SE[p] = \frac{\sigma[p]}{\sqrt{K-1}}$
- 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:

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

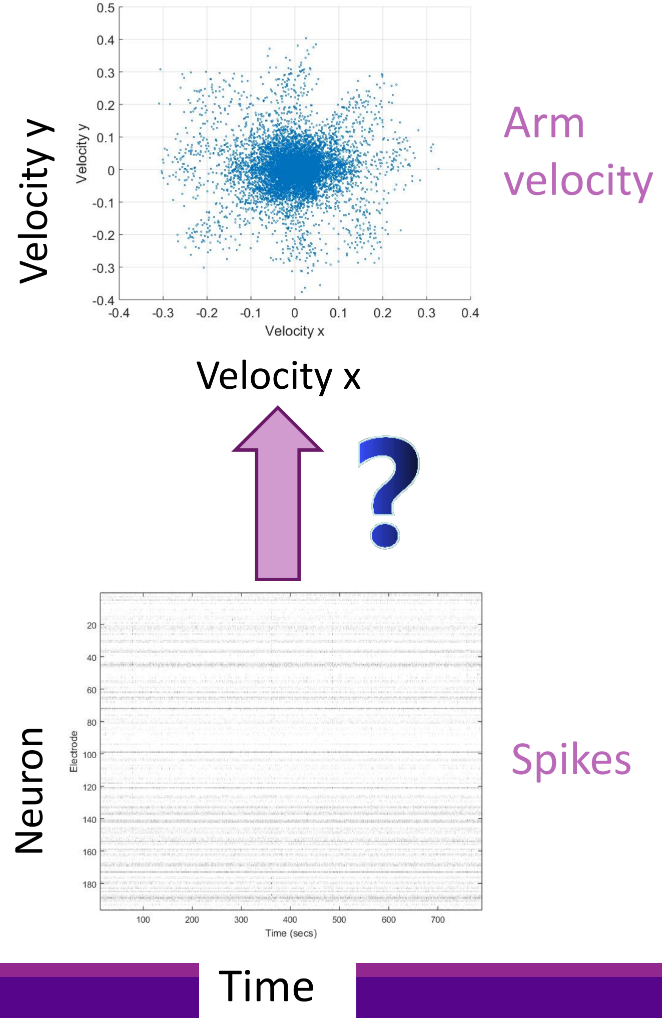
- Note that one SE rule always produce a model order $\le$ normal rule ($\hat{p} \le \hat{p}_0$)

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