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

- ☐ Understand the concept of model class and model order
- □ 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
- ☐ Understand the concept of bias, variance and the irreducible error for a model
 - Know how to compute each from synthetically generated data
- ☐ Understand the cross-validation process
 - Use it to assess the test error for a given model
 - Use it to select an optimal model order and for feature selection



Outline

Motivating example: What polynomial degree should a model use?

- ☐ Bias and variance
- ☐ Cross-validation
- ☐ Extension to feature selection

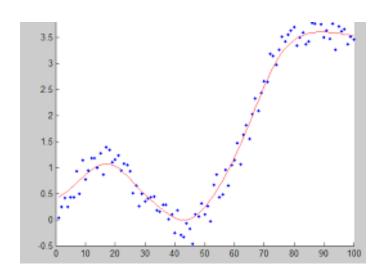


Polynomial Fitting

- ☐ Last lecture: polynomial regression
- □Given data (x_i, y_i) , i = 1, ..., N
- ☐ Learn a polynomial relationship:

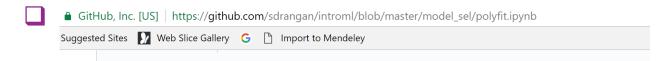
$$y = \beta_0 + \beta_1 x + \dots + \beta_d x^d + \epsilon$$

- \circ d = degree of polynomial. Called model order
- $\beta = (\beta_0, \cdots, \beta_d) = \text{coefficient vector}$
- \square Given d, can find β via least squares
- \square 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/unit03_model_sel/demo03_1_polyfit.ipynb



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:

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

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

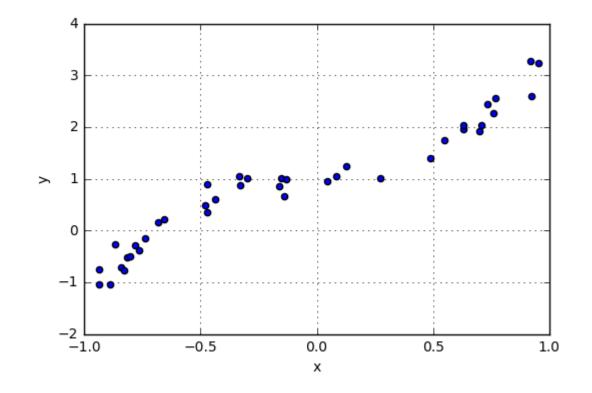


Example Question

- ☐ You are given some data.
- □ Want to fit a model: $y \approx f(x)$
- ☐ Decide to use a polynomial:

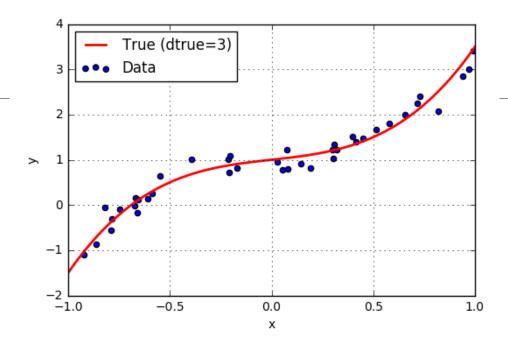
$$f(x) = \beta_0 + \beta_1 x + \dots + \beta_d x^d$$

- \square What model order d should we use?
- ☐Thoughts?



Synthetic Data

- ☐ Previous example is synthetic data
- $\square x_i$: 40 samples uniform in [-1,1]
- $\Box y = f(x) + \epsilon,$
 - $f(x) = \beta_0 + \beta_1 x + \dots + \beta_d x^d =$ "true relation"
 - $\circ d = 3, \ \epsilon \sim N(0, \sigma^2)$
- 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

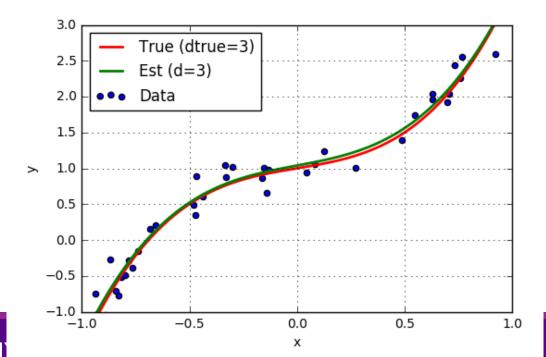
# Independent data
nsamp = 40
xdat = np.random.uniform(-1,1,nsamp)

# 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

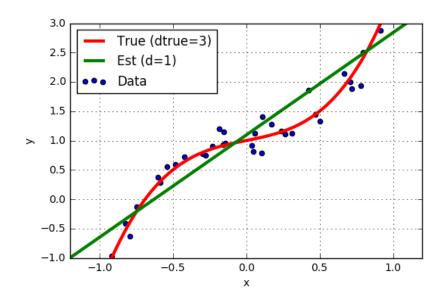


```
d = 3
beta hat = poly.polyfit(xdat,ydat,d)
# Plot true and estimated function
xp = np.linspace(-1,1,100)
yp = poly.polyval(xp,beta)
yp_hat = poly.polyval(xp,beta_hat)
plt.xlim(-1,1)
plt.ylim(-1,3)
plt.plot(xp,yp,'r-',linewidth=2)
plt.plot(xp,yp_hat,'g-',linewidth=2)
# Plot data
plt.scatter(xdat,ydat)
plt.legend(['True (dtrue=3)', 'Est (d=3)', 'Data'], loc='upper left')
plt.grid()
plt.xlabel('x')
plt.ylabel('y')
```

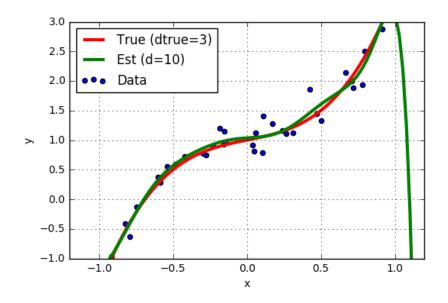


But, True Model Order not Known

□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?
- \square 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?

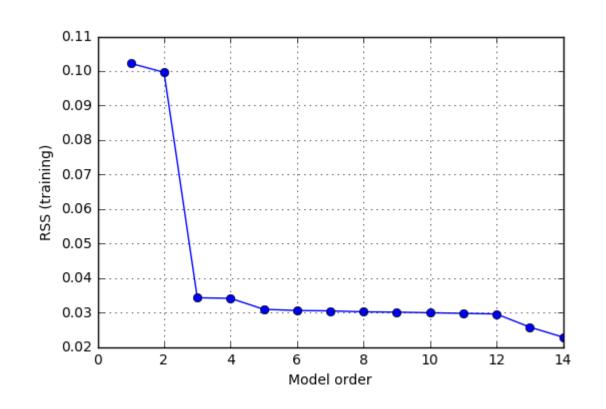
- ☐Simple (but bad) idea:
 - For each model order, d, find estimate $\widehat{\boldsymbol{\beta}}$
 - Compute predicted values on training data

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

Compute RSS

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

- \circ 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

☐ Cross-validation



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:

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

- \circ Set is parametrized by $\boldsymbol{\beta}$
- ☐ Many possible examples:
 - Linear model: $\hat{y} = \beta_0 + \beta_1 x_1 + \dots + \beta_k x_k$
 - Polynomial model: $\hat{y} = \beta_0 + \beta_1 x + \dots + \beta_k x^k$
 - Nonlinear: $\hat{y} = \beta_0 + \beta_1 e^{-\beta_2 x} + \beta_3 e^{-\beta_4 x}$
 - 0



Model Class and True Function

- ■Analysis set-up:
 - Learning algorithm assumes a model class: $\hat{y} = f(x, \beta)$
 - 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:
 - \circ A parameter estimate $\widehat{m{eta}}$ (computed from the learning algorithm for a fixed training set)
 - A test point x_{test}
 - Test point is generally different from training samples.
- \square Predicted value: $\hat{y} = f(x_{test}, \hat{\beta})$
- \square Actual value: $y = f_0(x_{test}) + \epsilon$
- □Output mean squared error:

$$MSE_{y}(\mathbf{x}_{test}, \widehat{\boldsymbol{\beta}}) \coloneqq E[y - \widehat{y}]^{2}$$

 \circ Expectation is over noise ϵ on the test sample.



Irreducible Error

☐ Rewrite output MSE:

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

 \square Since noise on test sample is independent of $\widehat{\boldsymbol{\beta}}$ and x_{test} :

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

- lacksquare Define irreducible error: σ_{ϵ}^2
 - Lower bound on $MSE_y(x_{test}, \widehat{\beta}) \ge \sigma_{\epsilon}^2$
 - Fundamental limit on ability to predict y
 - \circ Occurs since y is influenced by other factors than x



Under-Modeling

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

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

for some parameter β_0 .

 \circ β_0 called the true parameter

Under-modeling: When $f_0(x)$ 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

Analysis of Under-Modeling: Noise-Free Case

- \square Assume true relation has no noise: $y = f_0(x)$
 - Can model noise, but requires more probability theory
- \square Get training data: $(x_i, y_i), i = 1, ..., n$
- ☐ Fit model parameter from least-squares:

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

- □ Conclusions: With no noise
 - Minimizing training error finds best least squares fit of the true functions in the model class
 - If there is a unique true parameter, then $\widehat{\beta} = \beta_0$. Estimator identifies correct parameter



Bias: Noise-Free Case

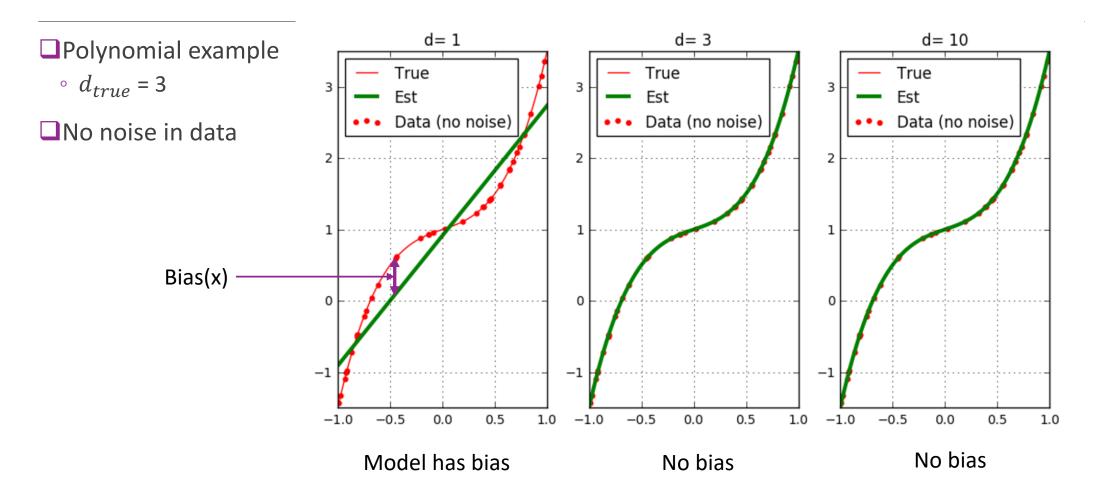
- \square Let x_{test} = some test point
 - Can be different from the training data set
- lacktriangle Definition: When there is no noise, the bias at a test point x_{test} is:

$$Bias(x_{test}) := f_0(x_{test}) - f(x_{test}, \widehat{\beta})$$

- ☐ Measures the difference between true and estimated relation in absence of noise
- ☐ Previous analysis shows:
 - Bias is small when true function is close to model class
 - When there is no under-modeling, $Bias(\mathbf{x}_{test}) = 0$ and true parameter can be found if there are sufficient training data.



Bias Visualized





Analysis with Noise (Advanced)

- □ Now assume noise: $y = f_0(x) + \epsilon$, $\epsilon \sim N(0, \sigma_{\epsilon}^2)$
- \square Get training data: $(x_i, y_i), i = 1, ..., n$
- ☐Fit parameter:

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

- \circ $\hat{\beta}$ will be random. Depends on particular noise realization for the selected training samples.
- Results may not be a good estimate for the true function!
- \square Take a new test point x_{test} : Error $y(x_{test}) f(x_{test}, \widehat{\beta})$ may be large!
- Solution: Multiple trials, each using a different training set.
 - \circ Compute mean and variance of estimated function $f(x_{test},\widehat{m{eta}})$ over $\widehat{m{eta}}$ from different training sets
 - Bias: Difference of true function from mean estimate
 - Variance: Variance of estimate around its mean



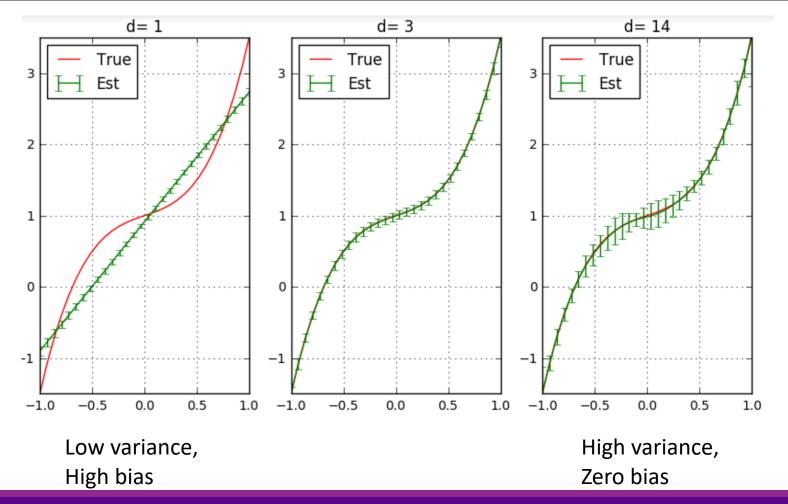
Bias-Variance Formula (Advanced)

 \square Consider test point x_{test} with noise. Observed value $y(x_{test}) = f_0(x_{test}) + \varepsilon$, Predicted value: $f(x_{test}, \hat{\beta})$ $MSE(x_{test}) \coloneqq E[y(x_{test}) - f(x_{test}, \widehat{\beta})]^2$ $= E[f_0(\mathbf{x}_{test}) + \varepsilon - f(\mathbf{x}_{test}, \widehat{\boldsymbol{\beta}})]^2 = E[f_0(\mathbf{x}_{test}) - f(\mathbf{x}_{test}, \widehat{\boldsymbol{\beta}})]^2 + \sigma_{\varepsilon}^2$ $E[f_0(\boldsymbol{x}_{test}) - f(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}})]^2 = E[f_0(\boldsymbol{x}_{test}) - E[f(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}})] + E[f(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}})] - f(\boldsymbol{x}_{test}, \widehat{\boldsymbol{\beta}})]^2$ $= (f_0(\mathbf{x}_{test}) - E[f(\mathbf{x}_{test}, \widehat{\boldsymbol{\beta}})])^2 + E[f(\mathbf{x}_{test}, \widehat{\boldsymbol{\beta}}) - E[f(\mathbf{x}_{test}, \widehat{\boldsymbol{\beta}})]]^2$ \square Bias: $Bias(\mathbf{x}_{test}) := f_0(\mathbf{x}_{test}) - E[f(\mathbf{x}_{test}, \widehat{\boldsymbol{\beta}})]$ \square Variance: $Var(x_{test}) \coloneqq E\left[f(x_{test}, \widehat{\beta}) - E[f(x_{test}, \widehat{\beta})]\right]^2$ \square Bias-Variance formula : $MSE(x_{test}) = Bias(x_{test})^2 + Var(x_{test}) + \sigma_{\varepsilon}^2$ (irreducible error) \square Note that expectation is taken over $\widehat{\beta}$ derived from different training samples \square Further averaging over test samples: $MSE = Bias^2 + Var + \sigma_{\varepsilon}^2$ (irreducible error)

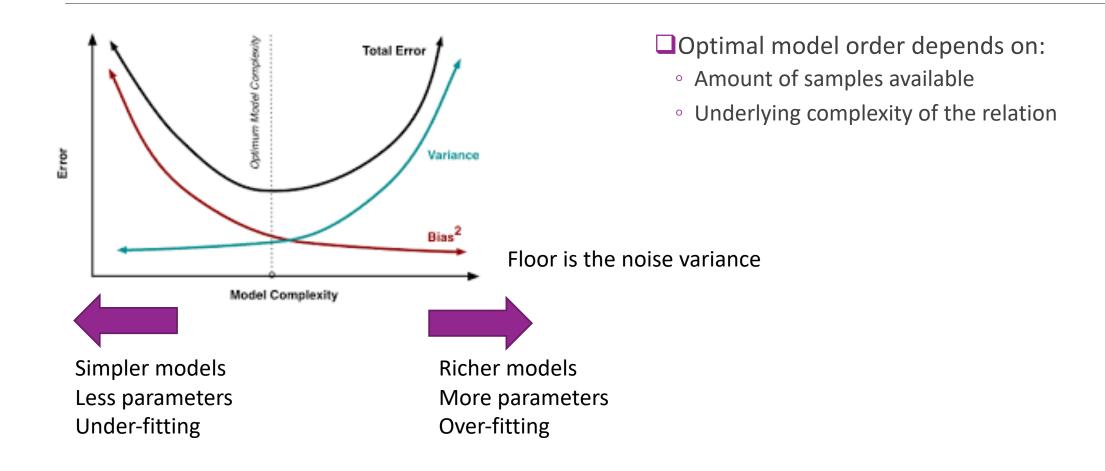


Bias and Variance Illustrated

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



Bias-Variance Tradeoff



Results for Linear Models

- \square Suppose model is linear with n = num samples, p = num parameters
- \blacksquare Result 1: When n < p, linear estimate is not unique
 - Need at least as many samples as parameters
- \square Now assume that $n \geq p$ and parameter estimate is unique
- ☐ Result 2: When there is no under-modeling, estimate is unbiased

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

Result 3: For $n \gg p$ and 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
- ☐ See textbook for proof: [Hastie] Hastie, Tibshirani, Friedman, The elements of statistical learning.



Outline

- ☐ Motivating Example: What polynomial degree should a model use?
- ☐Bias and variance

Cross-validation



Cross Validation

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

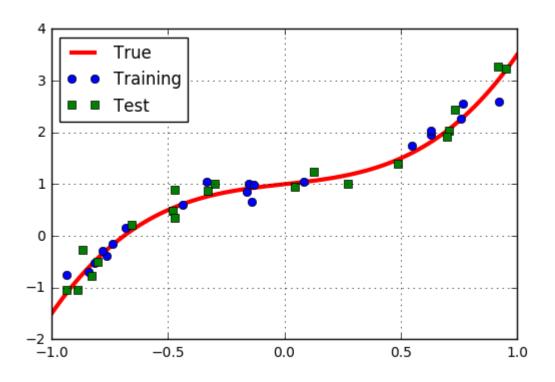
$$RSS_{test}(p) = \sum_{i \in test} (\hat{y}_i - y_i)^2$$

 \square 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



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

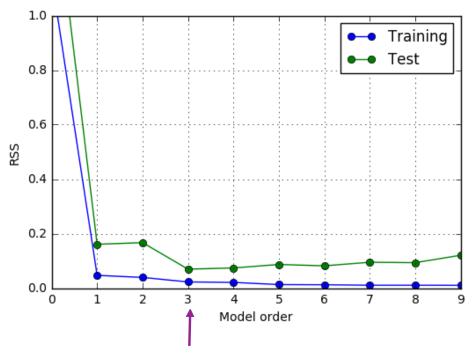
# Training
xtr = xdat[:ntr]
ytr = ydat[:ntr]

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



Finding the Model Order

☐ Estimated optimal model order = 3



RSS test minimized at d=3RSS 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')
```



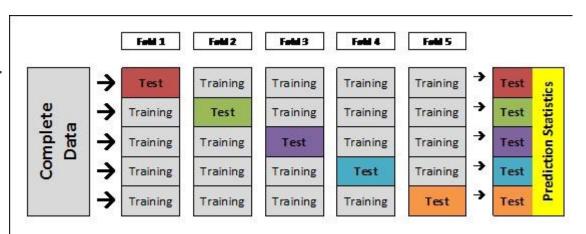
Problems with Simple Train/Test Split

- ☐ 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



K-Fold Cross Validation

- $\square K$ -fold cross validation
 - Divide data into *K* parts
 - Use K-1 parts for training. Use remaining for test.
 - Average over the *K* test choices
 - \circ 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/

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

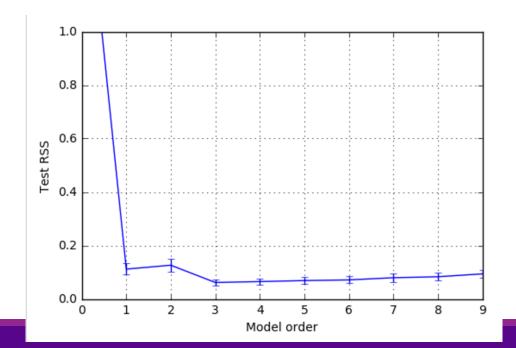
```
# Create a k-fold object
nfold = 20
kf = sklearn.model selection.KFold(n splits=nfold,shuffle=True)
# Model orders to be tested
dtest = np.arange(0,10)
nd = len(dtest)
# Loop over the folds
RSSts = np.zeros((nd,nfold))
for isplit, Ind in enumerate(kf.split(xdat)):
    # Get the training data in the 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 dev / $\sqrt{K-1}$
 - Mean and SE averaged over the K folds
- ☐ Simple model selection
 - Select d with lowest mean test RSS
- ☐ For this example
 - Estimate model order = 3

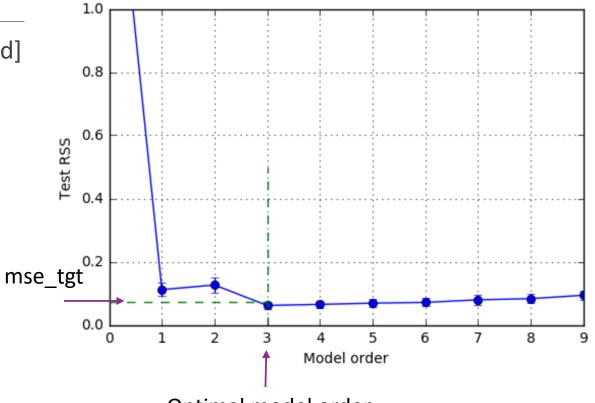
```
RSS_mean = np.mean(RSSts,axis=1)
RSS_std = np.std(RSSts,axis=1) / np.sqrt(nfold-1)
plt.errorbar(dtest, RSS_mean, yerr=RSS_std, fmt='-')
plt.ylim(0,1)
plt.xlabel('Model order')
plt.ylabel('Test RSS')
plt.grid()
```





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]
 - o Set mse_tgt = mse_mean[d0] + mse_std[d0]
 - Find minimal dopt s.t. mse_mean[dopt] <= mse_tgt</p>



Optimal model order



Feature selection as model selection

- □So far we discussed how to select the order of a fitting polynomial as a model selection problem.
- ☐ More generally, given many features, only a subset of the features may be useful for predicting the target. How do we select the useful features?
- ☐ With linear regression, each possible feature subset corresponds to a different model, and the feature number is the model order!
- ☐ Higher feature number leads to low bias but higher variance!
- ☐ We can use the approach for polynomial order selection to solve the feature selection problem.



Exhaustive search for feature selection

- \square Suppose you want to consider feature subset of size up to p
- \square For all possible feature subsets of size 1 to p: use cross validation to find mean RSS mean and standard deviation for each feature subset.
- ☐ Choose the subset with the minimal RSS mean, or use the one standard error rule.



Feature selection based on correlation with target

- Exhaustive search may be infeasible when the raw feature dimension is large!
- ■Suboptimal approach:
 - \circ For each candidate feature order $d \leq p$, choose d features with the highest correlation coefficients with the target
 - Use cross validation to determine the RSS mean and variance for this subset
 - Select the feature subset with minimal RSS mean or using the one standard error rule.
- ☐ Is using correlation with target a good idea?
 - Two features that are correlated could both be highly correlated with the target, but provide redundant information and ideally only one of them should be used.



Greedy feature selection

- ☐ Forward-Stepwise Selection
 - Select one feature from all features that provides the lowest RSS with cross validation
 - Select one new feature from all remaining features, so that previously chosen features plus the new feature provides the lowest RSS
 - Repeat until the maximum feature number is reached, or when the RSS starts to increase
- ☐ Backward-Stepwise
 - First use all features and find the RSS (using cross validation)
 - Remove one feature and find the new RSS. Go through all possible features to remove.
 - Find the one that leads to the least RSS increase. Remove this feature.
 - Repeat the above, remove one from the remaining features, to find the next most important feature.
- Except exhaustive search, can all lead to suboptimal solution
- ■We will discuss the method of LASSO in the next lecture for feature selection.



Comparison of feature selection methods

Figure from [Hastie2008]: Hastie, Tibshirani, Friedman, The elements of statistical learning.

For more on this subject, see Sec. 3.3

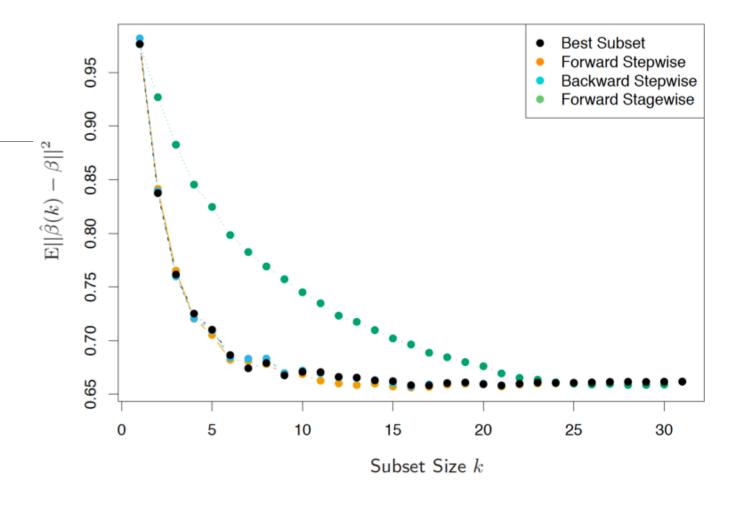
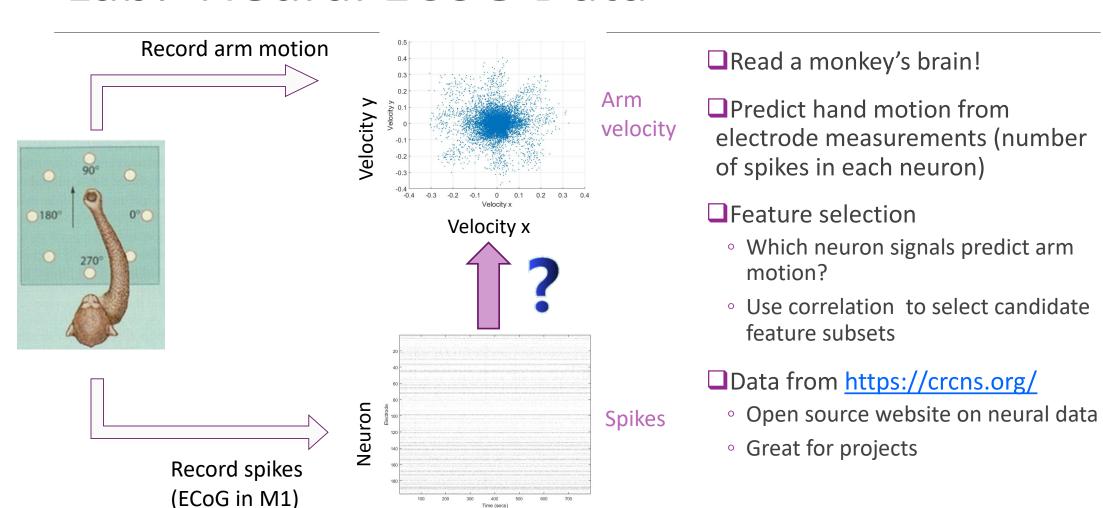


FIGURE 3.6. Comparison of four subset-selection techniques on a simulated linear regression problem $Y = X^T \beta + \varepsilon$. There are N = 300 observations on p = 31 standard Gaussian variables, with pairwise correlations all equal to 0.85. For 10 of the variables, the coefficients are drawn at random from a N(0,0.4) distribution; the rest are zero. The noise $\varepsilon \sim N(0,6.25)$, resulting in a signal-to-noise ratio of 0.64. Results are averaged over 50 simulations. Shown is the mean-squared error of the estimated coefficient $\hat{\beta}(k)$ at each step from the true β .



Lab: Neural ECoG Data





What you should know from this lecture

- ☐ Understand the concept of model class and model order
- □ 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
- ☐ Understand the concept of bias, variance and the irreducible error for a model
 - Know how to compute each from synthetically generated data
- ☐ Understand the cross-validation process
 - Use it to assess the test error for a given model
 - Use it to select an optimal model order and for feature selection

