

# Lecture 7: Regression Part 2

*Leap into the 21st century*

**ADDO AI**

2018

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# Theory of Generalization

# Agenda

- Prerequisite Self Check
- Generalization
- Recap of Overfitting
- Bias-Variance Decomposition
- Expectation
- Expectation Math
- Polynomial Curve fitting
- Expectation and Bias Variance Decomposition
- Variance, Bias, Noise
- Guess the best model?
- Bias-Variance tradeoff
- K-cross validation
- Data Splitting
- Hyperparameters Tuning
- Coefficient of Determination  $R^2$
- Jupyter Notebook

# Generalization

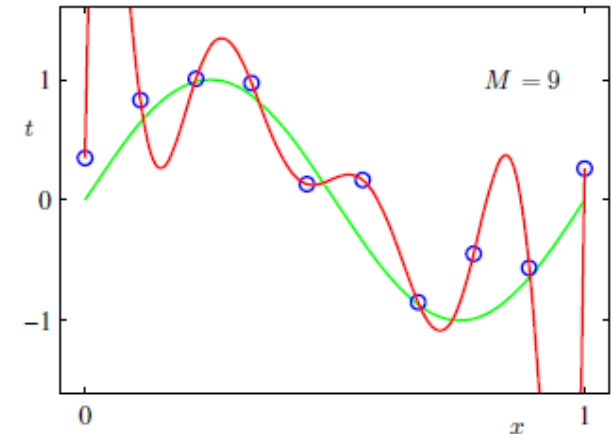
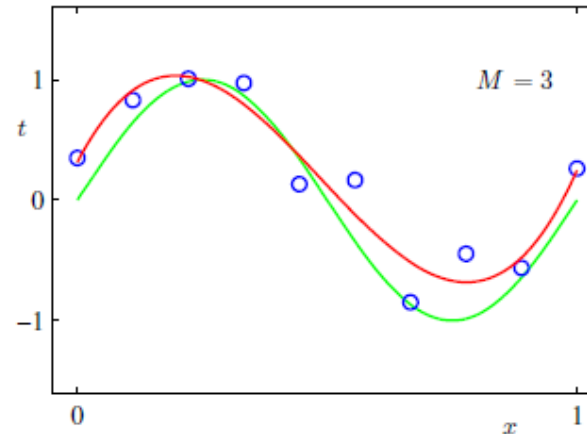
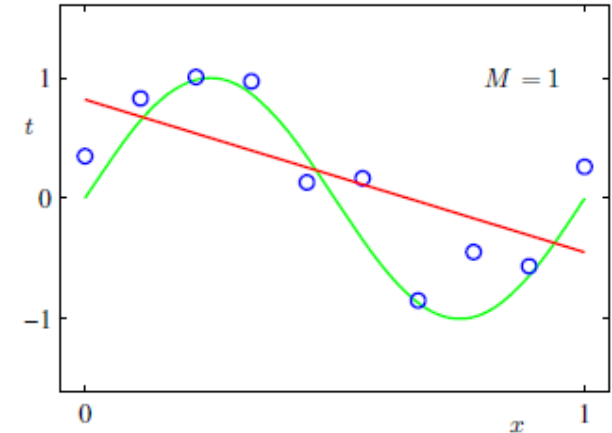
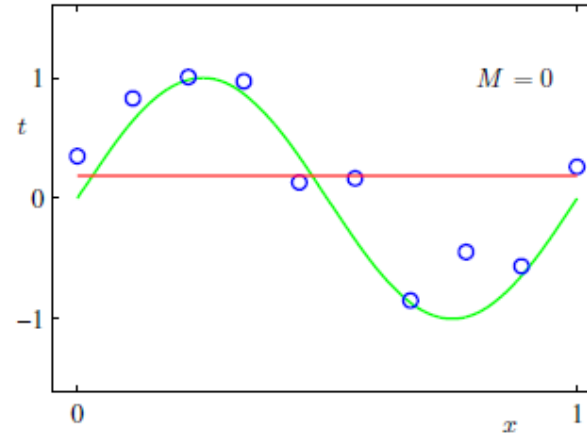
- Refers to model's ability to handle unseen data
- To best describe the unseen data
- In other words, model should not "Overfit"
- Overfitting can be expressed using another concept
  - Bias-variance tradeoff

# Recap

- True function  $y = f(x) + \epsilon$
- Our approximate function:  $\hat{y} = \hat{w}_0 + \hat{w}_1 \cdot x$
- Error at data-tuple  $(x_i, y_i)$  :  $e_i = \text{actual} - \text{predicted} = y_i - \hat{y}_i$
- Goal:  $\operatorname{argmin}_{w_0, w_1} \sum_{i=1}^n e_i^2 = \operatorname{argmin}_{w_0, w_1} \sum_{i=1}^n (y_i - \hat{y}_i)^2$

# Recap

- Again, taking example from last lecture
- $M$  refers to the no. of polynomial degree
- $x$ -axis represents input/independent variables
- $y$ -axis represents dependent/output variable
- The problem presented in the figure is called polynomial curve fitting

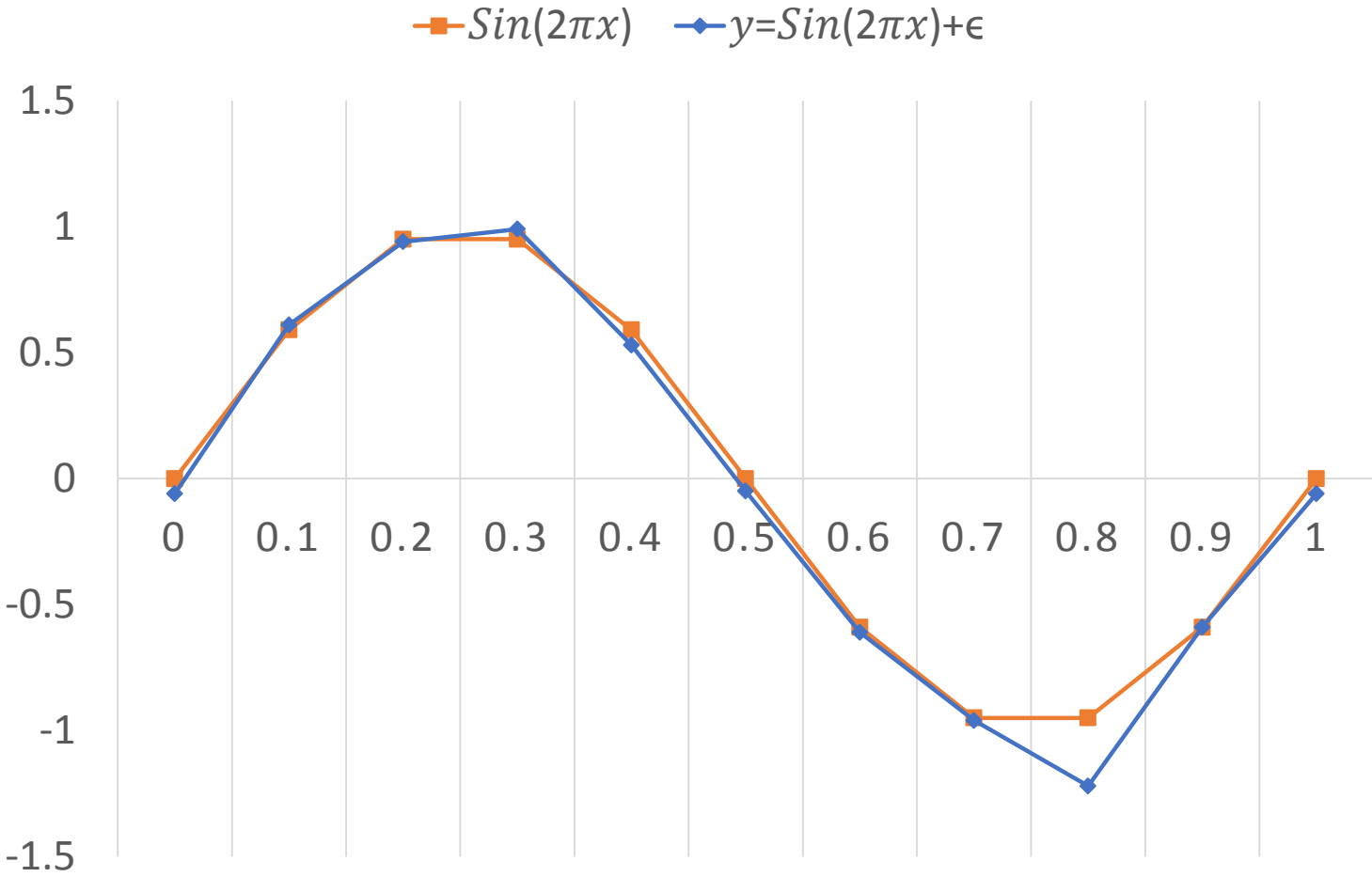


# Polynomial Curve Fitting

- So far, we've discussed linear regression
- If we are to model a non-linear relationship using regression
  - Kernel Trick
- Lets assume that underlying function is of sin i.e.  $y = \sin(2\pi x) + \epsilon$
- $\epsilon$  is noise, so assume, noise follows normal distribution with zero-mean and some standard deviation  $\sigma$ .

# Polynomial Curve Fitting

x	$2\pi x$	$\text{Sin}(2\pi x)$	$\epsilon$	y
0	0	0	0.16	0.16
0.1	0.63	0.59	0.11	0.7
0.2	1.26	0.95	-0.06	0.89
0.3	1.88	0.95	-0.11	0.84
0.4	2.51	0.59	-0.08	0.51
0.5	3.14	0	-0.14	-0.14
0.6	3.77	-0.59	0.04	-0.55
0.7	4.4	-0.95	0.17	-0.78
0.8	5.03	-0.95	-0.04	-0.99
0.9	5.65	-0.59	0.04	-0.55
1	6.28	0	0.12	0.12





# Polynomial Curve Fitting

- Regression function learnt so far:

$$\hat{y} = \hat{w}_0 + \hat{w}_1 \cdot x \text{ (Simple linear regression)}$$

$$\hat{y} = \hat{w}_0 + \hat{w}_1 \cdot x + \hat{w}_2 \cdot x_2 + \dots + \hat{w}_M \cdot x_M \text{ (Multiple linear regression)}$$

- In case of multiple linear regression, we have m-dimensional input data i.e. input features are M in total
- In current case of polynomial curve fitting:
  - Input is 1-Dimensional
  - Transform into Polynomial

# Polynomial Curve Fitting

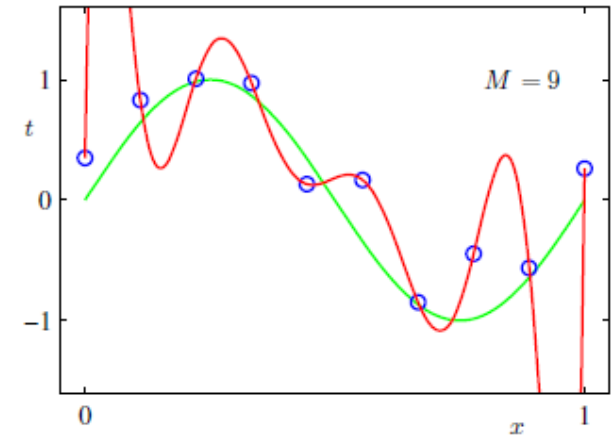
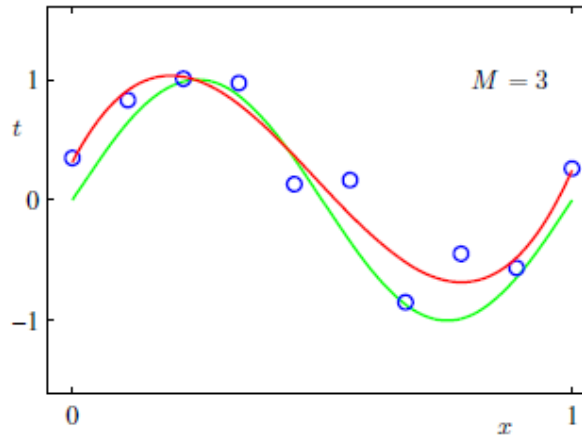
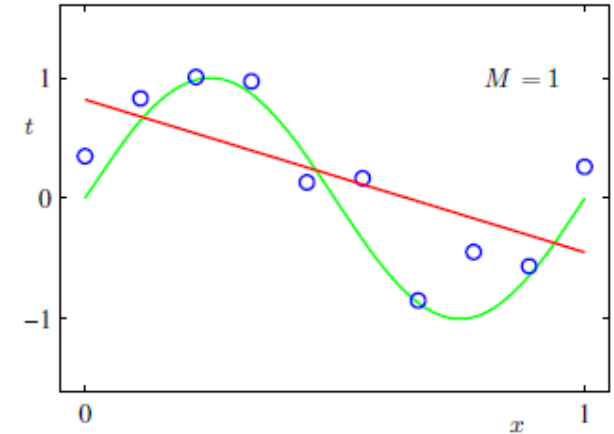
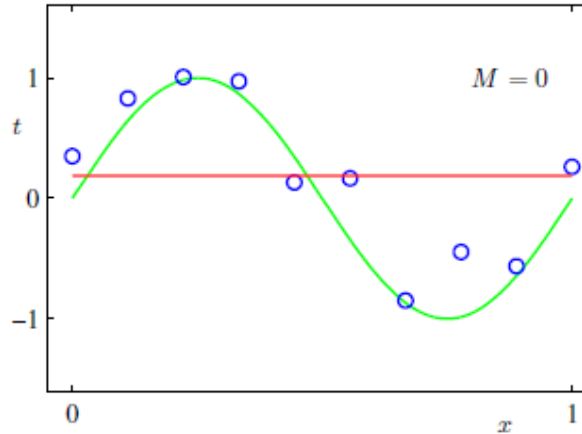
- Lets transform our function:

$$\hat{y} = \hat{w}_0 + \hat{w}_1 \cdot x + \hat{w}_2 \cdot x^2 + \hat{w}_3 \cdot x^3 + \dots + \hat{w}_M \cdot x^M$$

- Here, we are using only x but has transformed existing model into a non-linear model
- Primary thing to note is that this function is:
  - Polynomial in terms of input variable
  - Linear in terms of parameters
- This function now has capability to model non-linear relationships using regression
- Varying value of M can result in various models

# Polynomial Curve Fitting

- This figure contains four models with varied  $M$  values
- As error used is still SSR, hence
  - $\operatorname{argmin}_{\vec{w}} \sum_{i=1}^n (y_i - \hat{y}_i)^2$
- Recall that previously:
  - $\frac{\partial E}{\partial \hat{w}_i} = -2 \sum_{n=1}^N (y_n - \hat{y}_n) (x_n)$
- It now becomes:
  - $\frac{\partial E}{\partial \hat{w}_i} = -2 \sum_{n=1}^N (y_n - \hat{y}_n) (x_n)^i$



# Polynomial Curve Fitting

- $E = \sum_{n=1}^N (y_n - \hat{y}_n)^2$
- $E = \sum_{n=1}^N (y_i - (\hat{w}_0 + \hat{w}_1 \cdot x_n + \hat{w}_2 \cdot x_n^2 + \hat{w}_3 \cdot x_n^3 + \dots + \hat{w}_M \cdot x_n^M))^2$

$x_n^0 = 1$  for  $\hat{w}_0$ , Hence, expression can be summarized as:

$$\begin{aligned} E &= \sum_{n=1}^N (y_n - \sum_{j=0}^M \hat{w}_j x_n^j)^2 \\ \frac{\partial E}{\partial \hat{w}_0} &= \frac{\partial}{\partial \hat{w}_0} \sum_{n=1}^N (y_n - \sum_{j=0}^M \hat{w}_j x_n^j)^2 \\ \frac{\partial E}{\partial \hat{w}_0} &= -2 \sum_{n=1}^N (y_n - \sum_{j=0}^M \hat{w}_j x_n^j) \frac{\partial E}{\partial \hat{w}_0} (\sum_{j=0}^M \hat{w}_j x_n^j) \\ \frac{\partial E}{\partial \hat{w}_0} &= -2 \sum_{n=1}^N (y_n - \sum_{j=0}^M \hat{w}_j x_n^j) * [\frac{\partial E}{\partial \hat{w}_0} (\hat{w}_0 * x_n^0) + \frac{\partial E}{\partial \hat{w}_0} (\hat{w}_1 * x_n^1) \\ &+ \frac{\partial E}{\partial \hat{w}_0} (\hat{w}_2 * x_n^2) + \dots + \frac{\partial E}{\partial \hat{w}_0} (\hat{w}_i * x_n^i) + \dots + \frac{\partial E}{\partial \hat{w}_0} (\hat{w}_M * x_n^M)] \end{aligned}$$

# Polynomial Curve Fitting

$$\frac{\partial E}{\partial \hat{w}_0} = -2 \sum_{n=1}^N (y_n - \sum_{j=0}^M \hat{w}_j x_n^j) * \left[ \frac{\partial E}{\partial \hat{w}_0} (\hat{w}_0 * x_n^0) + 0 + \dots + \dots + 0 \right]$$

$$\frac{\partial E}{\partial \hat{w}_0} = -2 \sum_{n=1}^N (y_n - \sum_{j=0}^M \hat{w}_j x_n^j) * x_n^0$$

Hence, for any  $\hat{w}_i$

$$\frac{\partial E}{\partial \hat{w}_i} = -2 \sum_{n=1}^N (y_n - \sum_{j=0}^M \hat{w}_j x_n^j) * x_n^i$$

Equating gradient to zero yields:

$$\frac{\partial E}{\partial \hat{w}_i} = -2 \sum_{n=1}^N (y_n - \sum_{j=0}^M \hat{w}_j x_n^j) * x_n^i = 0$$

# Polynomial Curve Fitting

$$\frac{\partial E}{\partial \hat{w}_i} = \sum_{n=1}^N (y_n - \sum_{j=0}^M \hat{w}_j x_n^j) * x_n^i = 0$$

$$\frac{\partial E}{\partial \hat{w}_i} = \sum_{n=1}^N (y_n x_n^i - \sum_{j=0}^M \hat{w}_j x_n^j x_n^i) = 0$$

$$\frac{\partial E}{\partial \hat{w}_i} = \sum_{n=1}^N (y_n x_n^i) - \sum_{n=1}^N (\sum_{j=0}^M \hat{w}_j x_n^j x_n^i) = 0$$

$$\begin{aligned} \Rightarrow \sum_{n=1}^N (y_n x_n^i) &= \sum_{n=1}^N \left( \sum_{j=0}^M \hat{w}_j x_n^j x_n^i \right) \\ \Rightarrow \sum_{n=1}^N (x_n^i) y_n &= \sum_{j=0}^M \left( \sum_{n=1}^N \hat{w}_j x_n^{i+j} \right) \\ \Rightarrow \sum_{n=1}^N (x_n^i) y_n &= \sum_{j=0}^M \hat{w}_j \left( \sum_{n=1}^N x_n^{i+j} \right) \end{aligned}$$

# Polynomial Curve Fitting

$$\Rightarrow \sum_{n=1}^N (x_n^i) y_n = \sum_{j=0}^M \left( \sum_{n=1}^N x_n^{i+j} \right) \hat{w}_j$$

$$\text{If } A_{ij} = \sum_{n=1}^N x_n^{i+j}; T_i = \sum_{n=1}^N (x_n^i) y_n$$

$$\Rightarrow T_i = \sum_{j=0}^M A_{ij} \hat{w}_j$$

- Solution to these equations provide optimal value for  $\hat{w}_i$

$$T_i = \sum_{j=0}^M A_{ij} \hat{w}_j$$

- This is similar to the system of equation form:  $B = AX$
- Hence solving these systems of simultaneous equations provides optimal parameter values during training.

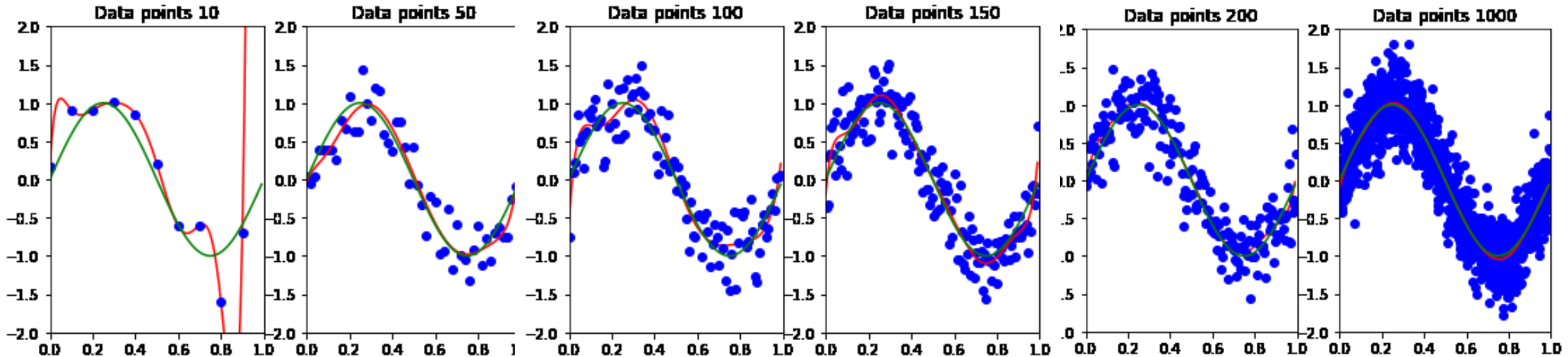
# Polynomial Curve Fitting

$$f(x) = \sin(2\pi x)$$

$$y = f(x) + \epsilon$$

$$\hat{y} = \sum_{j=0}^M \hat{w}_j x_n^j$$

- Solution system discussed just now can result in overfitting
- Overfitting can be avoided if training dataset is huge
- These figures show model performance with degree of 9 using variety of datasets.
- With increase in training data points, overfitting is greatly reduced.





# Evaluation of Model Generalization

- There are various ways to evaluate the GOOD FIT of any model
- Some of these include
  - Bias-Variance Tradeoff
  - Error Graphs
  - Coefficient of Determination  $R^2$
- We'll discuss each one by one

# Bias-Variance Decomposition

- To understand the concept of overfitting:
  - Break down the error function
  - Error function studied so far can be broken down:
    - Reducible Error
    - Irreducible Error
  - Reducible error can be further broken down:
    - Bias Error
    - Variance Error

# Bias-Variance Decomposition

- Notation
  - For an unseen data point  $x'$ 
    - $y'$  will represent the actual value
    - $\hat{y}'$  will represent the predicted value
- Goal:
  - To find the expected performance of our model
  - In other words, expected error on unseen instances

# Expectation

- Expectation is also known as Expected Value.
- It can be defined as weighted average of a function
  - $E(x) = \sum_{i=1}^n x_i * p(x_i)$   *$p(x_i)$  shows probability when  $x = x_i$*
- If weight is equally distributed among all
  - Expectation would be equal to standard mean or average.
- Hence, average or mean values are also expected values

# Expectation

- For example, when a six-sided unbiased die is rolled, then:
  - As it is unbiased die, probability of each number is equal
  - Hence  $p(x_1) = p(x_2) = p(x_3) = p(x_4) = p(x_5) = p(x_6) = \frac{1}{6}$
- Hence, Expectation becomes:

$$E(x) = 1 * p(x_1) + 2 * p(x_2) + 3 * p(x_3) + 4 * p(x_4) + 5 * p(x_5) + 6 * p(x_6)$$

$$E(x) = 1 * \frac{1}{6} + 2 * \frac{1}{6} + 3 * \frac{1}{6} + 4 * \frac{1}{6} + 5 * \frac{1}{6} + 6 * \frac{1}{6}$$

$$E(x) = \frac{1}{6} * (1 + 2 + 3 + 4 + 5 + 6) = \frac{1}{6} * (21) = 3.5$$

# Expectation

- Assume an investor who likes to determine his rate of return on three investments. Assume the investments are proportioned according to following probability distributions: 25% in investment A, 25% in investment B, and 50% in investment C. The rate of return is 5% for investment A, 6% for investment B, and 2% for investment C.
- Find the expected rate of return.

# Expectation

- In this example,  $x$  = Rate of Return
- Probability of  $x$  is determined here by the proportions of investment performed.
- Hence Expected Rate of Return becomes:
  - $E(x) =$   
 $\text{Rate of return of investment A} * \text{prob}(A) +$   
 $\text{Rate of return of investment A} * \text{prob}(B) +$   
 $\text{Rate of return of investment A} * \text{prob}(C)$
  - $E(x) = 5 * 0.25 + 6 * 0.25 + 2 * 0.50 = 3.75$
- Hence, Expected Rate of Return is 3.75%

# Background Math

Let  $Z$  be a random variable with probability distribution  $P(Z)$

Let  $\bar{Z} = E[Z]$  be the average value of  $Z$ .

• Lemma:  $E[(Z - \bar{Z})^2] = E[Z^2] - \bar{Z}^2$

**Proof:**  $E[(Z - \bar{Z})^2] = E[(Z^2 - 2Z\bar{Z} + \bar{Z}^2)]$

$$E[(Z - \bar{Z})^2] = E[Z^2] - 2E[Z]\bar{Z} + \bar{Z}^2 \quad E[\bar{Z}] = \bar{Z}$$

$$E[(Z - \bar{Z})^2] = E[Z^2] - 2\bar{Z}\bar{Z} + \bar{Z}^2$$

$$E[(Z - \bar{Z})^2] = E[Z^2] - 2\bar{Z}^2 + \bar{Z}^2$$

$$E[(Z - \bar{Z})^2] = E[Z^2] - \bar{Z}^2$$

$$\Rightarrow E[Z^2] = E[(Z - \bar{Z})^2] + \bar{Z}^2$$



# Expectation and Bias Variance Decomposition

- Error Function is:
  - $(y - \hat{y})^2$  where  $y = f(x) + \epsilon$  and  $\hat{y} = \hat{f}(x)$
- Hence, expectation for a new data point  $x'$  and corresponding  $y'$  would become:
  - $E[(y' - \hat{y}')^2]$  where  $y' = f(x') + \epsilon$  and  $\hat{y}' = \hat{f}(x')$
- For a given problem, there could be infinite training samples and distributions to which a data could belong
- Hence, assume, that training sample belongs to some Probability Distribution  $P$
- Then, our goal is to find:
  - $E_P[(y' - \hat{y}')^2]$  # For simplicity,  $E_P$  would be written as  $E$

# Expectation and Bias Variance Decomposition

$$\begin{aligned}E_P[(y' - \hat{y}')^2] &= E[(y' - \hat{y}')^2] \\&= E[(y'^2 + \hat{y}'^2 - 2y'\hat{y}')] \\&= E[y'^2] + E[\hat{y}'^2] - E[2y'\hat{y}']\end{aligned}$$

Using lemma we derived earlier:  $E[\mathbf{Z}^2] = E[(\mathbf{Z} - \bar{\mathbf{Z}})^2] + \bar{\mathbf{Z}}^2$

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

As  $y = f(x) + \epsilon$ , hence input dependent factor contributes towards mean:

$$\begin{aligned}&= E[(y' - f(x'))^2] + f(x')^2 + E[(\hat{y}' - \bar{\hat{y}}')^2] + \bar{\hat{y}}'^2 - 2 E[y'] E[\hat{y}'] \\&= E[(y' - f(x'))^2] + f(x')^2 + E[(\hat{y}' - \bar{\hat{y}}')^2] + \bar{\hat{y}}'^2 - 2\bar{y}' E[\hat{y}'] \\&= E[(y' - f(x'))^2] + f(x')^2 + E[(\hat{y}' - \bar{\hat{y}}')^2] + \bar{\hat{y}}'^2 - 2f(x') \bar{\hat{y}}'\end{aligned}$$

# Expectation and Bias Variance Decomposition

After rearranging the terms:

$$\begin{aligned} &= E[(y' - f(x'))^2] + E[(\hat{y}' - \bar{\hat{y}}')^2] + f(x')^2 + \bar{\hat{y}}'^2 - 2f(x') \bar{\hat{y}}' \\ &= E[(y' - f(x'))^2] + E[(\hat{y}' - \bar{\hat{y}}')^2] + (f(x') - \bar{\hat{y}}')^2 \end{aligned}$$

- $E(y' - \hat{y}')^2 = E[\epsilon^2] + \text{Variance}(\hat{y}') + \text{Bias}(\bar{\hat{y}}')^2$
- If we assume irreducible noise to follow a normal Gaussian distribution with zero mean and standard deviation of  $\sigma$ :

$$\mathbf{E}(\mathbf{y}' - \hat{\mathbf{y}}')^2 = \boldsymbol{\sigma}^2 + \mathbf{Variance}(\hat{\mathbf{y}}') + \mathbf{Bias}(\bar{\hat{\mathbf{y}}}')^2$$

This equation is bias-variance decomposition of expected error.

# Variance $E[(\hat{y} - \bar{\hat{y}})^2]$

- Describes how much  $\hat{y}$  varies from one training set  $S$  to another
- Describes how much a single model deviates from the average model over multiple datasets
- It is the average squared difference between any single data-set-dependent estimate of  $\hat{y}$  and average value of  $\hat{y}$  estimated over all datasets
- Variance captures the degree to which model's predictions vary between multiple iterations.

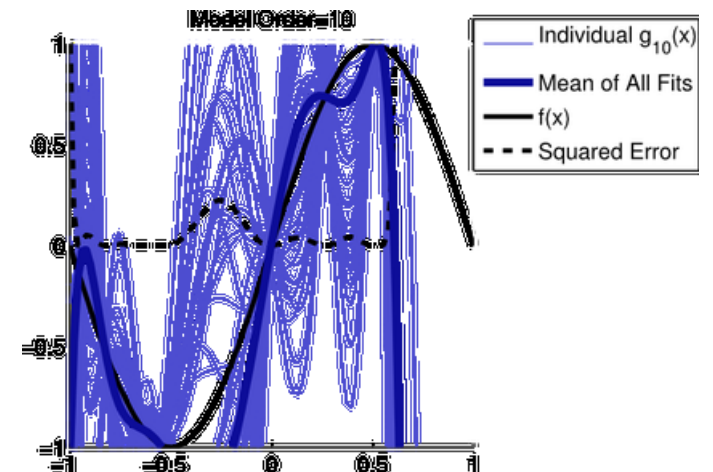
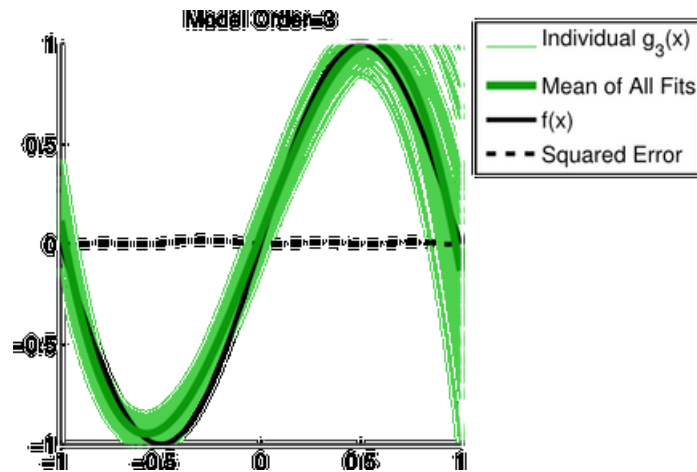
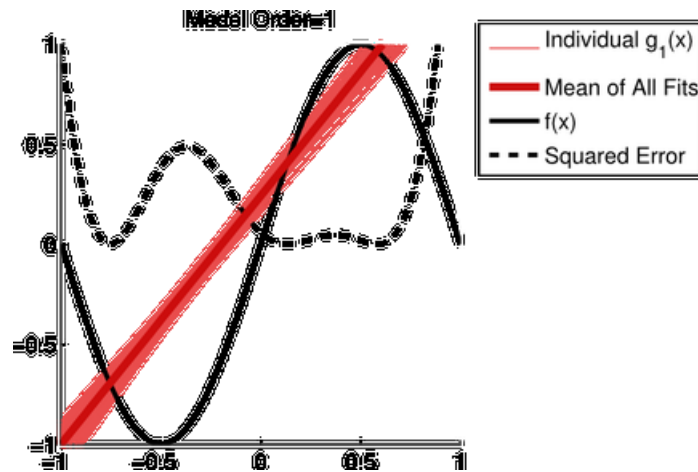
# Bias $(f(x) - \bar{\hat{y}})^2$

- Describes the average error of  $\hat{y}$  with respect to the actual function
- Assesses how a model approximates actual function
- It is based on behavior over multiple data sets, hence, difference between average model behavior is taken into account
- It describes how much the average estimator fit over datasets
- **bias** represents that how far a model's predictions are from correctness

Noise  $E[(y - f(x))^2]$

- Describes how much  $y$  varies from  $f(x)$
- It captures irreducible error
- For the sake of simplicity:
  - it can be assumed zero
  - It can be modeled using Normal distribution

# Guess the best model ?

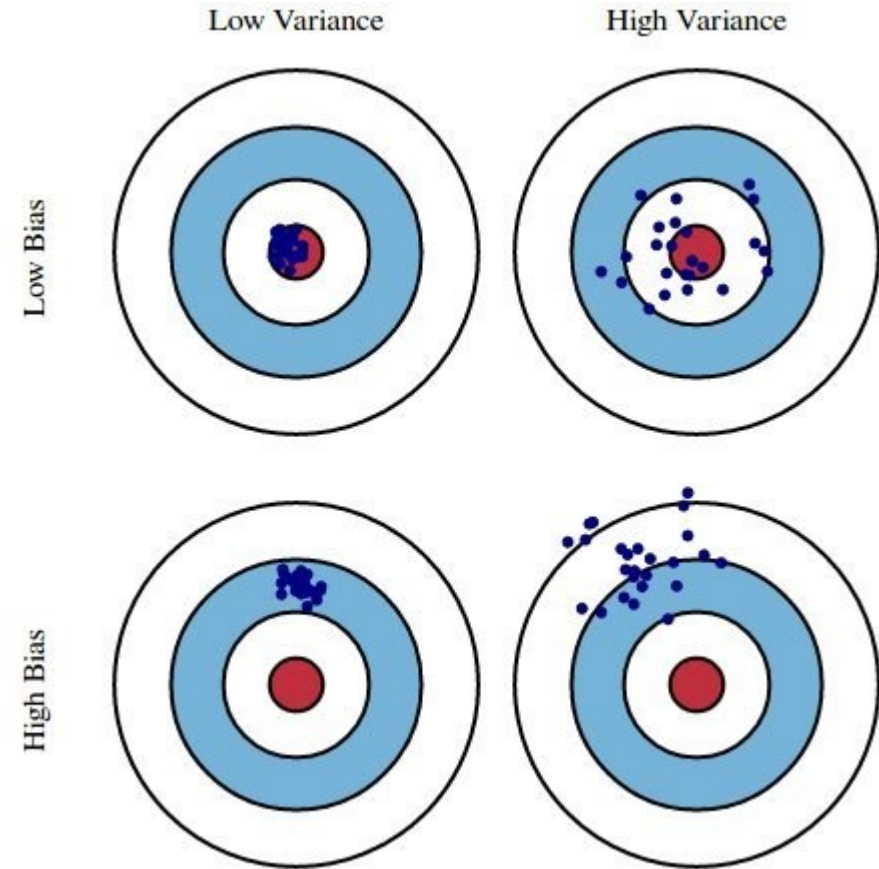


Which model has lowest bias?

Which model has highest Variance ?

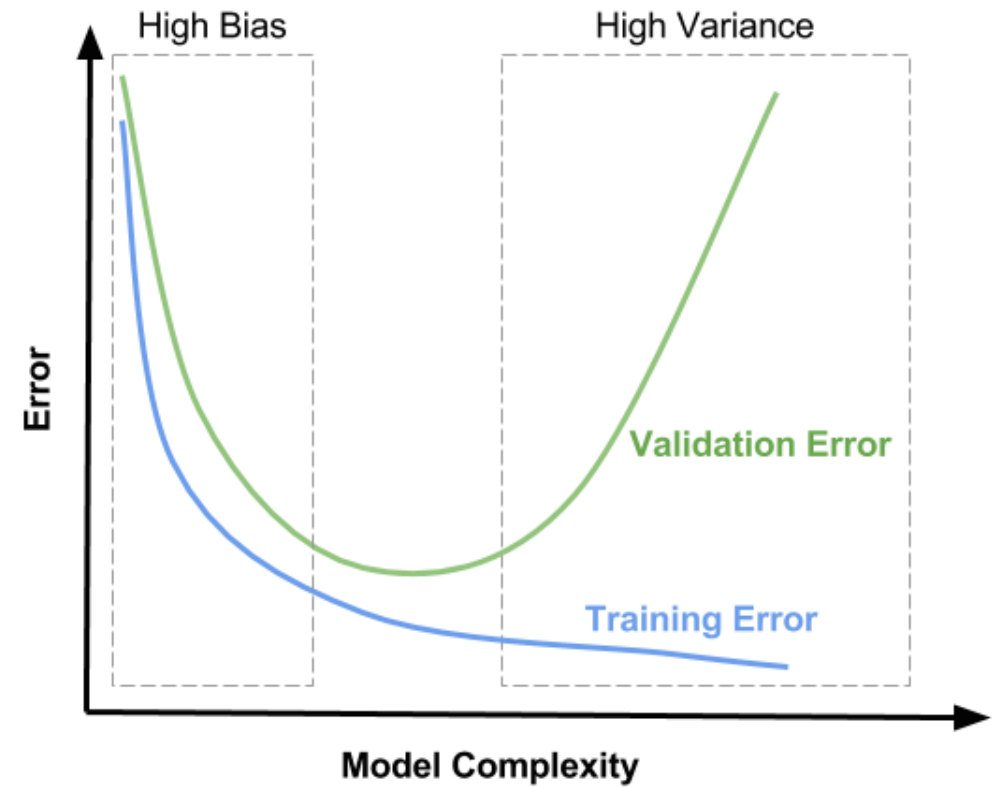
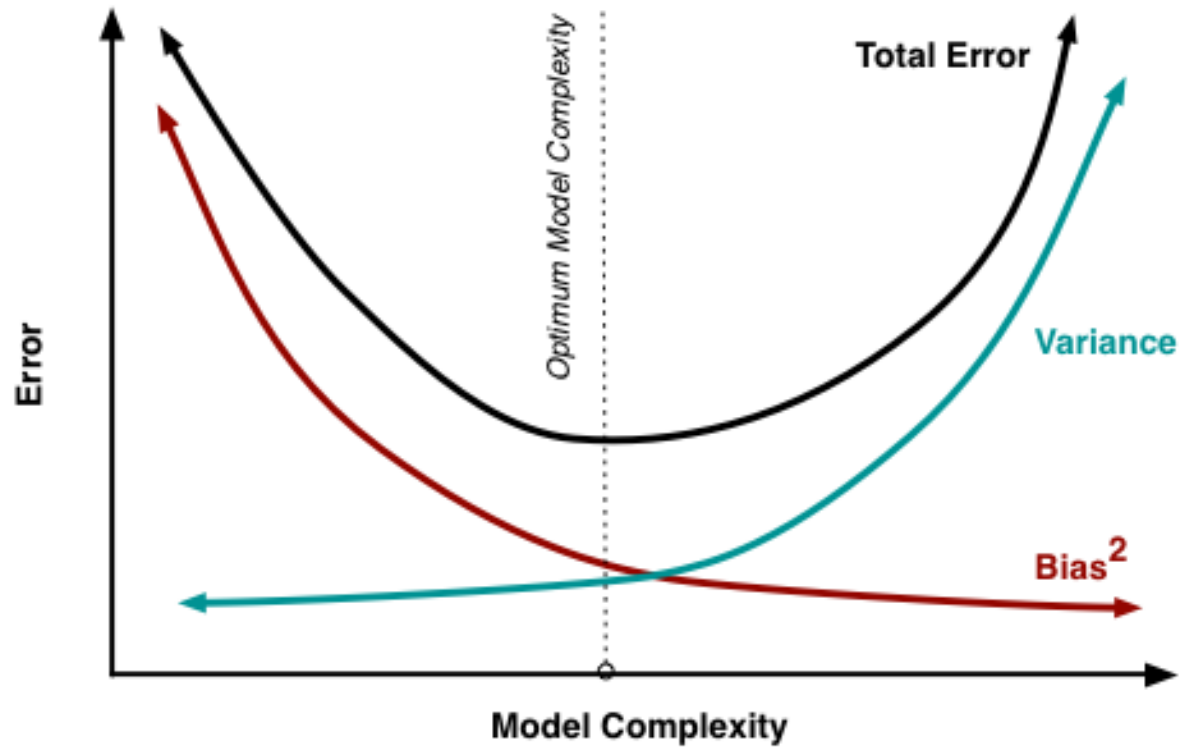
# Bias-Variance tradeoff

- If model is too simple
  - High bias
- If model is too complex
  - High Variance
- Goal
  - To have low bias and low variance in model simultaneously
  - Bull's eye represents target function
  - Closer we are to red circle, better the model is





# Bias-Variance tradeoff

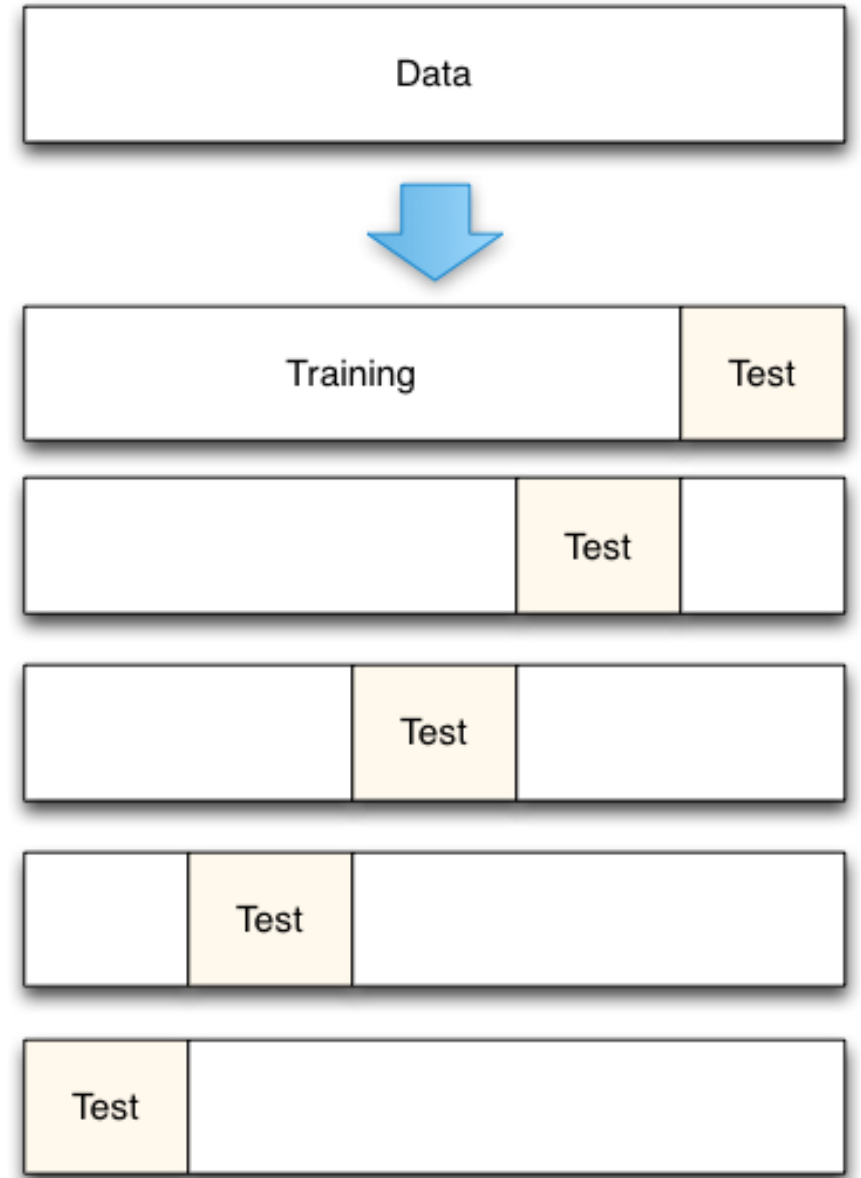


# Bias-Variance tradeoff in practice

- In real life, we don't have infinite amount of training sample populations
- How to compute bias and variance
  - Split the available data
  - Make multiple training and testing datasets
    - For each train-test data prepared: compute  $\hat{y}$
  - Using these values, calculate bias and variance
- A common procedure normally used:
  - K-cross validation

# K-cross validation

- A widely used validation technique
- Figure shows 5-cross validation
- Value of K affects the results
  - High Value of K: Low Bias, High Variance
  - Low value of K: High Bias, Low Variance



# K-cross validation

- If 5-cross validation is to be performed on this dataset
  - Total data points 10
  - Then total no. of instances per fold will be 2.
- 1<sup>st</sup> fold contents:
  - Train: [0.2,0.3,0.4,0.5,0.6,0.7,0.8,0.9]
  - Test: [0,0.1]
- 2<sup>nd</sup> fold contents:
  - Train: [0,0.1,0.4,0.5,0.6,0.7,0.8,0.9]
  - Test: [0.2,0.3]
- ....

[illegible]

# Data Splitting

- Cross validation is amongst a widely used method for data split
- Another widely used method of data splitting involves formation of two mutually exclusive datasets
  - One for training
  - Other for testing
- Other techniques
  - Bootstrapping
  - Subsampling
    - With replacement
    - Without replacement (etc.)
- If we are to train our model on training and evaluate on testing, then how to model hyper-parameters?

# Hyperparameters

- Recall the regularized Error-gradient function

$$\frac{\partial E}{\partial \hat{w}_i} = -2 \sum_{i=1}^n e_i * x_i + \lambda w_i$$

- Here  $\lambda$  is not a parameter of our predicted function, but it greatly affects the overall error
- Such parameters are known as hyperparameters
- Hyperparameters are set before the training begins
  - Their values are require while model training

# Hyperparameters

- How to model hyperparameters:
  - Instead of having two splits, make three:
    - Training ( to learn the model parameters)
    - Validation (to figure out the value of hyper-parameter)
    - Testing ( to assess the model performance i.e. generalization)
- Usually train-test split of (80%, 20%) is used
  - For Validation: 10-20% records of training set are used

# Hyperparameters

- Firstly:
  - Data will be divided in train and test splits
  - 80% records will be used for training
    - Train set: [0,0.1,0.2,0.3,0.4,0.5,0.6,0.7]
  - Remaining records will be used for testing
    - Test set: [0.8, 0.9]
- Then, training set split will be performed:
  - Train set: [0,0.1,0.2,0.3,0.4,0.5,0.6]
  - Validation set: [0.7]

[illegible]



# Hyperparameters

- Consider that the value of  $\lambda$  can reside between [0-1] with 0.25 interval
  - Then for  $\lambda = 0.0$ , model will be trained
    - When training is done; trained model will be validated using validation set
    - Model error will be logged
  - for  $\lambda = 0.25$ , model will be trained
  - for  $\lambda = 0.50$ , model will be trained
  - for  $\lambda = 0.75$ , model will be trained
  - for  $\lambda = 1.0$ , model will be trained
- As errors are logged against all  $\lambda$  values:
  - Value of  $\lambda$  that resulted in least error on Validation set will be selected

# Hyperparameters

- Generalization Testing
  - Now, the dataset we reserved earlier for Testing will be used
  - Using best model against validation set
    - Testing error will be calculated
- Widely used Hyperparameters
  - Learning step size
  - Value of regularization Term ( $\lambda$ )
  - Number of layers in deep networks
  - Number of hidden layer neurons

# Data Splitting and Hyperparameters (Summary)

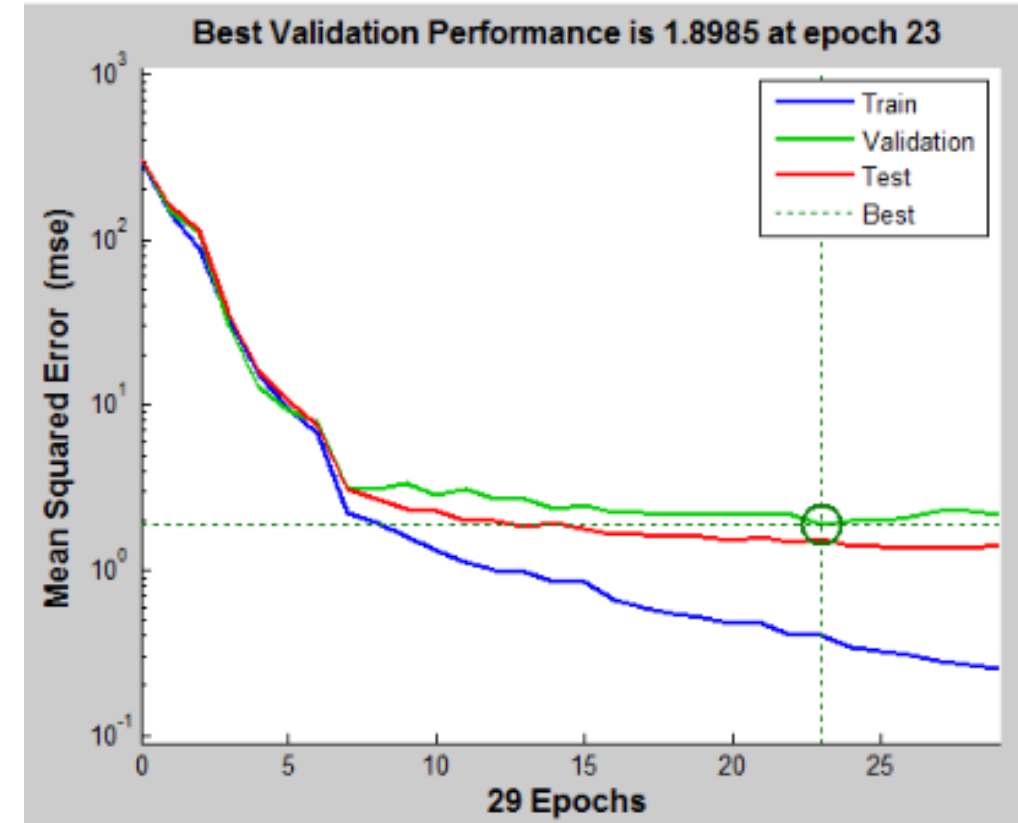
- For each distinct value of a hyperparameter:
  - Model training is carried out
  - Trained model is evaluated on validation set
- The model's parameter setting as well as respective hyperparameter setting that results in least error are selected
- Using the optimal parameters and hyperparameter values, testing is performed

# Error Graphs

- A widely used approach to see the model performance is to plot various errors
- It plots graph using training, testing and/or validation errors
- Training error is computed using trained model and training records.
  - These training records are already seen by the trained model during training
- Testing error is calculated using trained model and unseen data
- Validation error is calculated using trained model and validation dataset.
  - During model training, this dataset is not used, hence, it is also unseen data

# Error Graphs

- Figure presents a sample plot using various errors
- Best refers to the point, where model's performance is relatively high
- Here Epoch refers to total number of times, complete dataset is exhausted.
- There are multiple ways to stop the training
  - One is to graphically view the error plots
  - Second is to use difference thresholds
  - Third is to hard-code the iterations manually



# Coefficient of Determination $R^2$

- In regression, the  $R^2$  coefficient of determination is a statistical measure
- It measure how well the regression predictions approximate the real data points.
- An  $R^2$  of 1 indicates that the regression predictions perfectly fit the data.
- It ranges from [0-1]
- Its formulation is:

$$R^2 = 1 - \frac{SSR}{SSTotal}$$

# Coefficient of Determination $R^2$

- Consider example from last lecture
- For linear regression:
  - $SST = \sum_{i=1}^n (y_i - \bar{y})^2 = \sum_{i=1}^n (TErr)^2$  where  $\bar{y}$  is mean of population
  - $SSR = \sum_{i=1}^n (y_i - \hat{y}_i)^2 = \sum_{i=1}^n (RErr)^2$

$x$	$y$	$\hat{y}$	$TErr$	$RErr$	$TErr^2$	$RErr^2$
60	3.1	3.302	-0.62	-0.202	0.3844	0.040804
61	3.6	3.492	-0.12	0.108	0.0144	0.011664
62	3.8	3.682	0.08	0.118	0.0064	0.013924
63	4	3.872	0.28	0.128	0.0784	0.016384
65	4.1	4.252	0.38	-0.152	0.1444	0.023104
Mean(y) = 3.72			SST = 0.628		SSR = 0.10588	

Hence  $R^2$  would become:

$$R^2 = 1 - \frac{0.10588}{0.628} = 0.831$$