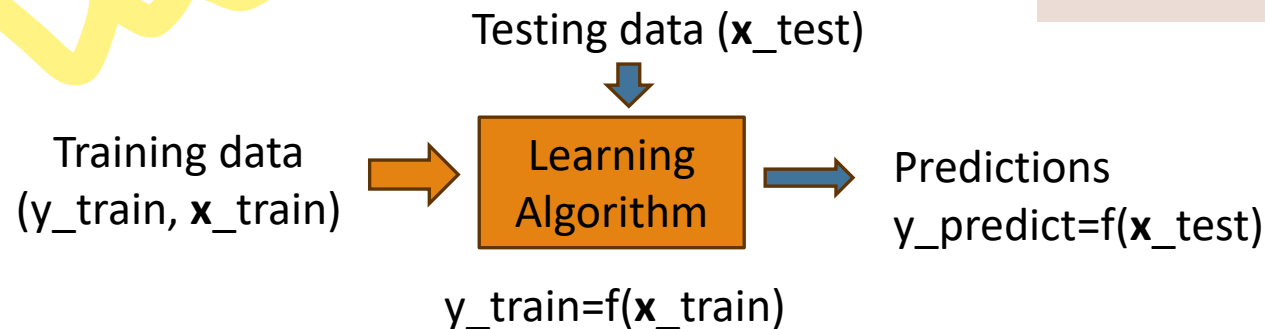# EN3150 Pattern Recognition
Linear Models for Regression

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Semester 5 – Batch 20.

What is regression ?

Predict the value of **dependent variable** based on the values of one or more **independent variables**

➢ Regression is a supervised learning technique

Dependent variable is often a quantitative or continuous variable

Testing data (**x**_test)

Training data
(y_train, **x**_train) → Learning Algorithm → Predictions
y_predict=f(**x**_test)

y_train=f(**x**_train)

➢ Applications
  ➢ Trend forecasting (e.g., forecast future sales)
  ➢ Forecasting an effect (e.g., predicting the effect of advertising spending on sales)
  ➢ To determine the strength of predictors (regression coefficients can indicate the magnitude and direction of influence each predictor)
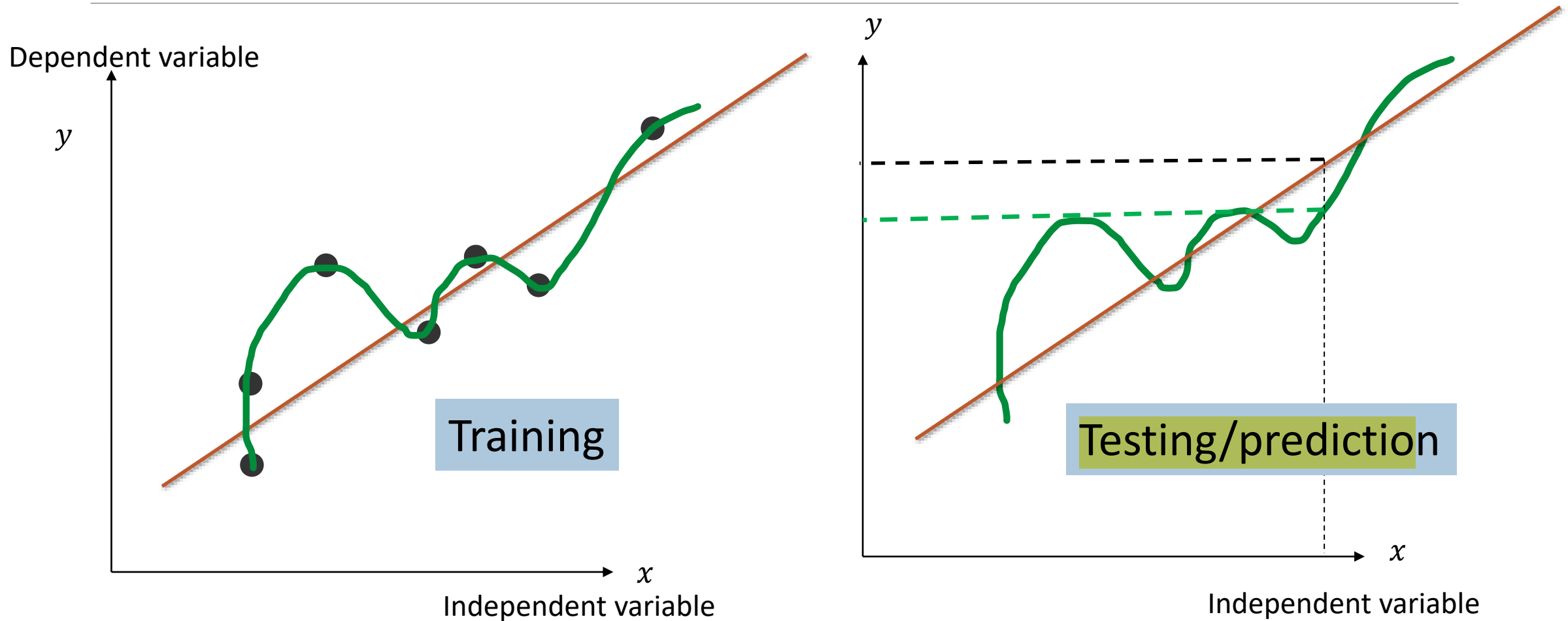
Key questions

➤ Is there a <mark>relationship between dependent variable a</mark>nd independent variable(s)?

➤ How <mark>strong i</mark>s the relationship ? and is it positive or negative relationship ? Linear or non-linear?

➤ How <mark>each feature/ independent variable contribute</mark>s to the dependent variable, which are strong?

➤ How a<mark>ccurate our predictions?</mark>

➤ Is there synergy among features/ independent variables

Diabetes dataset: independent variable(s) **Diabetes Data (ncsu.edu)**	
age	tc total serum cholesterol
sex	ldl, low-density lipoproteins
body mass index	hdl, high-density lipoproteins
average blood pressure	ltg, possibly log of serum triglycerides level
tch, total cholesterol / HDL	glu, blood sugar level

Dependent variable: quantitative measure of disease progression one year after baseline

Gareth James, Daniela Witten, Trevor Hastie and Robert Tibshirani, An Introduction to Statistical Learning with Applications in R, 2013.

What is regression ?

Dependent variable

y

Training

x

Independent variable

y

Testing/prediction

x

Independent variable

Linear Regression

➤ Most basic form of regression

➤ Relationship between the dependent and independent variables is assumed to be linear.

$$y(\mathbf{x}) \approx w_0 + w_1 x_1 + \cdots, + w_D x_D$$
$$y(\mathbf{x}) = w_0 + w_1 x_1 + \cdots, + w_D x_D + \epsilon = \mathbf{w}^T \mathbf{x} + \epsilon$$

$$\mathbf{X} = \begin{bmatrix} 1 \\ x_1 \\ . \\ . \\ . \\ x_D \end{bmatrix} \qquad \mathbf{W} = \begin{bmatrix} w_0 \\ w_1 \\ . \\ . \\ . \\ w_D \end{bmatrix}$$

➤ w_0 - Intercept or bias term

➤ What bias represents?

➤ ϵ – Error term, Why this term?

➤ $\mathbf{w}_{(1:D)}$ – Weights or regression coefficients **(parameters)** of independent variables

Linear Regression

$$y(\mathbf{x}) = w_0 + w_1\, x_1 + \cdots, + w_D\, x_D + \epsilon = \mathbf{w}^T\mathbf{x} + \epsilon$$

$$\mathbf{y} = \begin{bmatrix} y_1 \\ . \\ y_i \\ . \\ y_N \end{bmatrix} \quad \mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \\ . \\ . \\ . \\ w_D \end{bmatrix} \quad \mathbf{x}_i = \begin{bmatrix} 1 \\ x_{1,i} \\ . \\ . \\ . \\ x_{D,i} \end{bmatrix}$$

➢ $\mathbf{w}^T\mathbf{x}$ = inner or scalar product between the input vector $\mathbf{x}$ and the weight vector $\mathbf{w}$
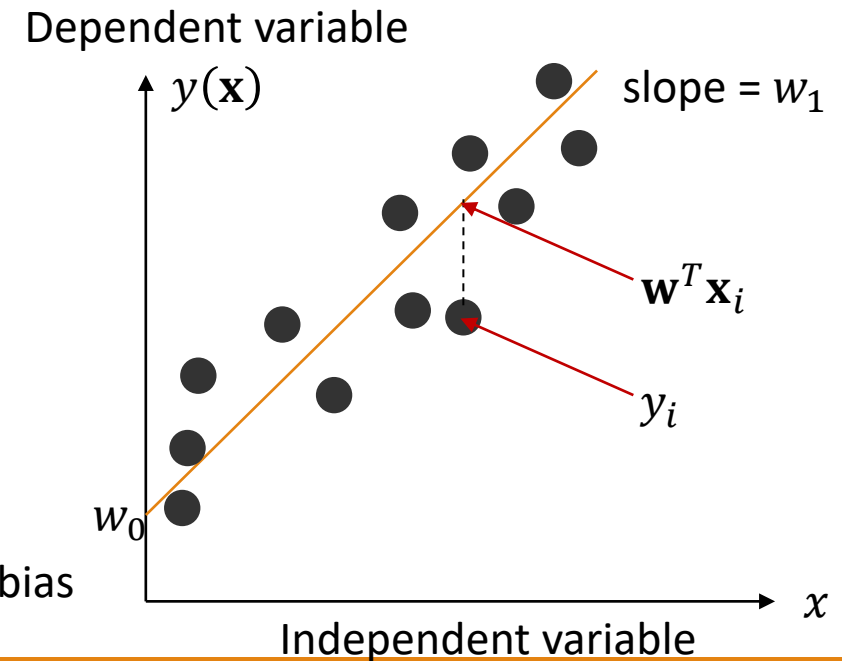
➢ $y(\mathbf{x})$ is dependent variable (continuous)

➢ $\mathbf{w}$ To be learned from data. How?

➢ Cost function

$$J(\mathbf{w}) = \sum_{i=1}^{N} (y_i - \mathbf{w}^T\mathbf{x}_i)^2$$

➢ Objective: Find $\mathbf{w}$ which has the minimum J($\mathbf{w}$) for our training samples (N number of samples)

➢ How?

Dependent variable

$y(\mathbf{x})$ slope = w_1

$\mathbf{w}^T\mathbf{x}_i$

y_i

w_0

intercept or bias

x

Independent variable

Linear Regression

➢ $y(\mathbf{x}) = w_0 + w_1 x_1 + \cdots, + w_D x_D + \epsilon = \mathbf{w}^T \mathbf{x} + \epsilon$

➢ Hypothesis: $y(\mathbf{x}) = w_0 + w_1 x_1 + \cdots, + w_D x_D$

➢ Parameters : $w_0, w_1, \ldots, w_D$

➢ Cost function : J($\mathbf{w}$)= $\sum_{i=1}^{N}(y_i - \mathbf{w}^T \mathbf{x}_i)^2$

➢ Objective: Find $\mathbf{w}$ which has the minimum J($\mathbf{w}$)

$\widehat{\mathbf{w}}$ = arg min J($\mathbf{w}$)
$\mathbf{w}$

Linear Regression

➤ Cost function

$$J(\mathbf{w}) = \frac{1}{2} \sum_{i=1}^{N} (y_i - \mathbf{w}^T \mathbf{x}_i)^2$$

➤ Objective: Find which has the minimum J($\mathbf{w}$) for our training samples (N number of samples)

➤ $\widehat{\mathbf{w}}$ = arg min J($\mathbf{w}$)
$\qquad$ $\mathbf{w}$

Gradient descent

Update for w_j $\qquad$ learning rate

$$w_j \leftarrow w_j - \alpha \frac{\partial J(\boldsymbol{w})}{\partial w_j}$$

For one training sample

$$\frac{\partial J(\boldsymbol{w})}{\partial w_j} = \frac{1}{2} \frac{\partial (y_i - \mathbf{w}^T \mathbf{x}_i)^2}{\partial w_j} = \frac{2(y_i - \mathbf{w}^T \mathbf{x}_i)}{2} \frac{\partial (y_i - \mathbf{w}^T \mathbf{x}_i)}{\partial w_j} = (y_i - \mathbf{w}^T \mathbf{x}_i)(-\mathbf{x}_i)$$
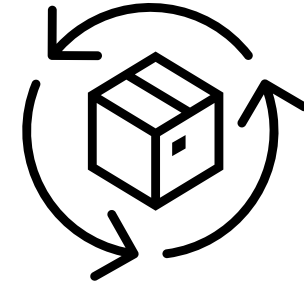
If model output and true value are close, we need little update on parameter

Update rule

$$w_j \leftarrow w_j + \alpha \cdot \sum_{i=1}^{N} (y_i - \mathbf{w}^T \mathbf{x}_i) \mathbf{x}_i$$

Batch gradient descent

Linear Regression

Initialize $\mathbf{w}$

Repeat until convergence {

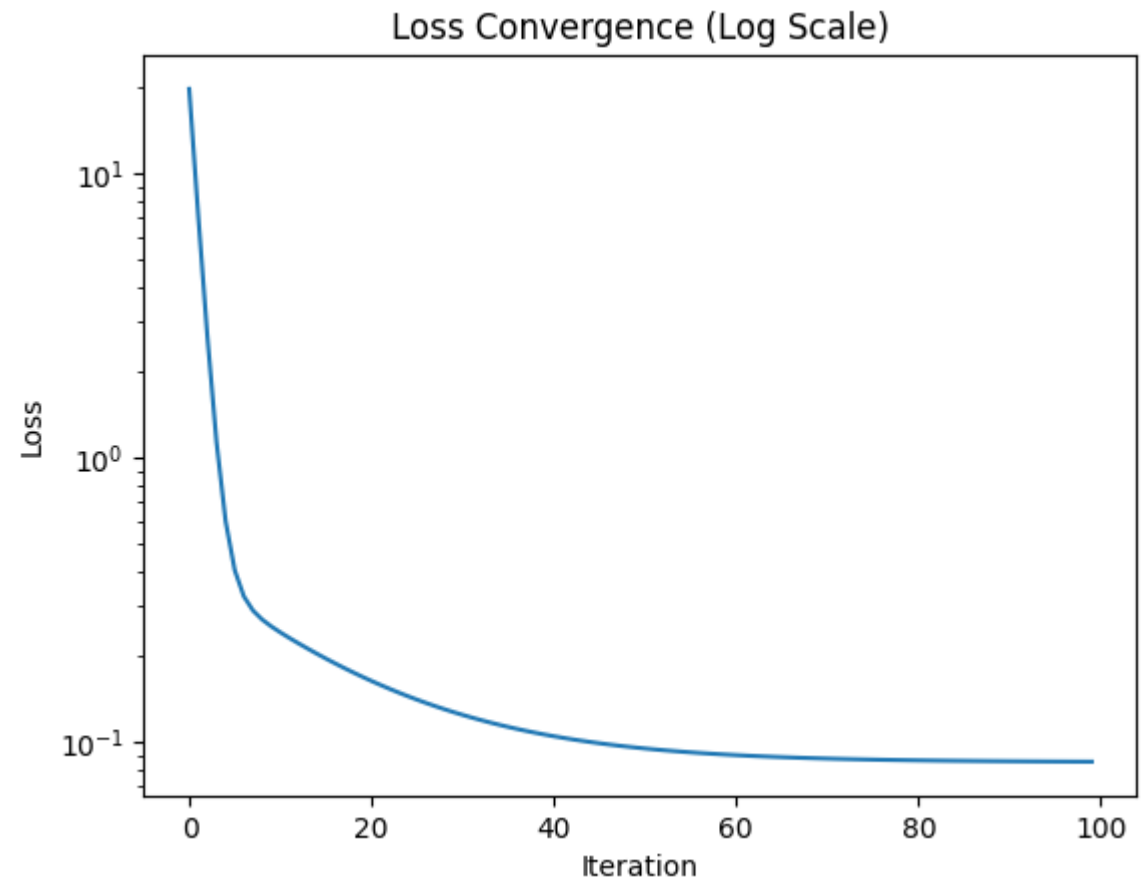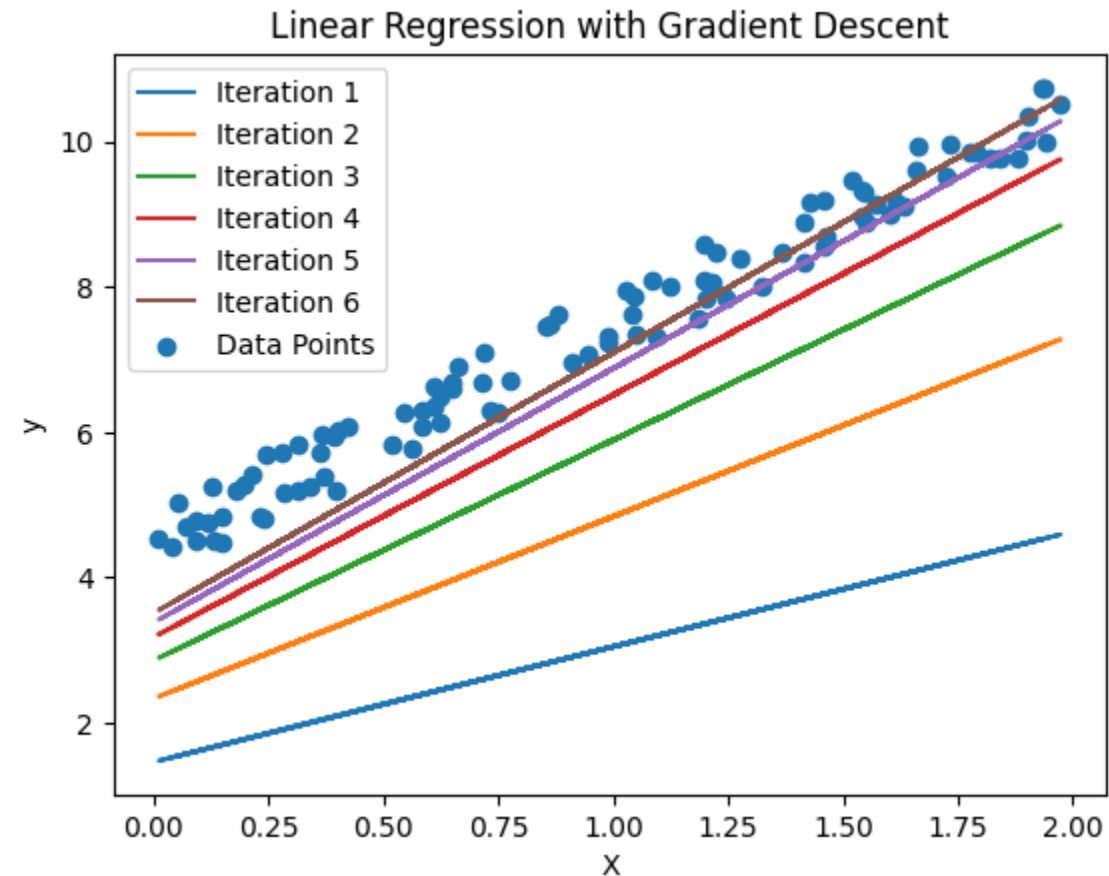$$w_j \leftarrow w_j + \alpha \sum_{i=1}^{N} (y_i - \mathbf{w}^T \mathbf{x}_i) \mathbf{x}_i \qquad \text{for every j}$$

}

iterative algorithm

Linear Regression

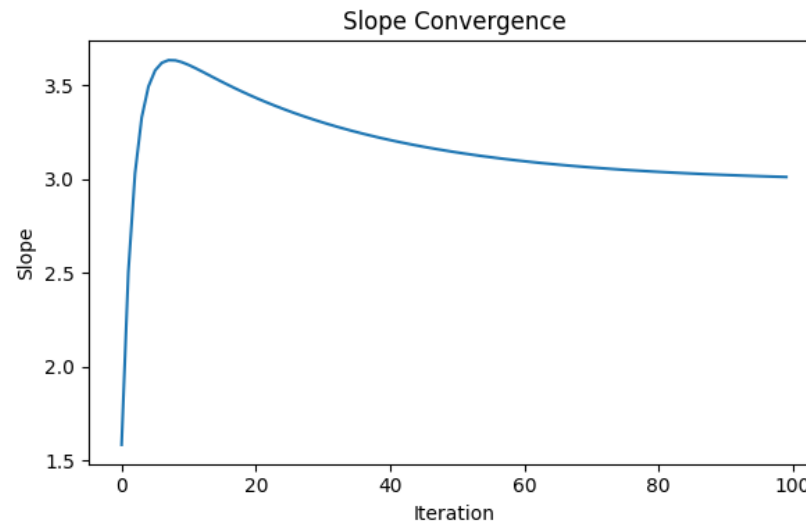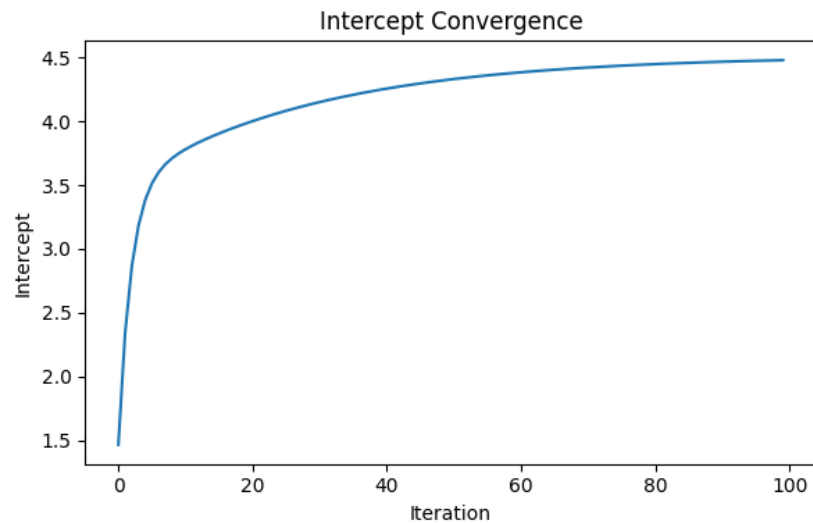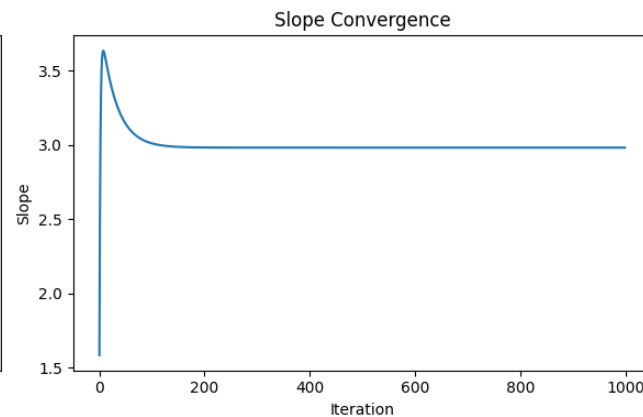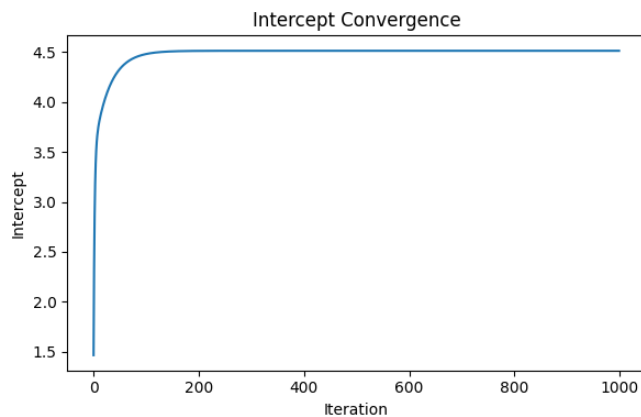y= 4 + 3x, Initialization w_0, w_1=[0,0], learning rate =0.001

Linear Regression

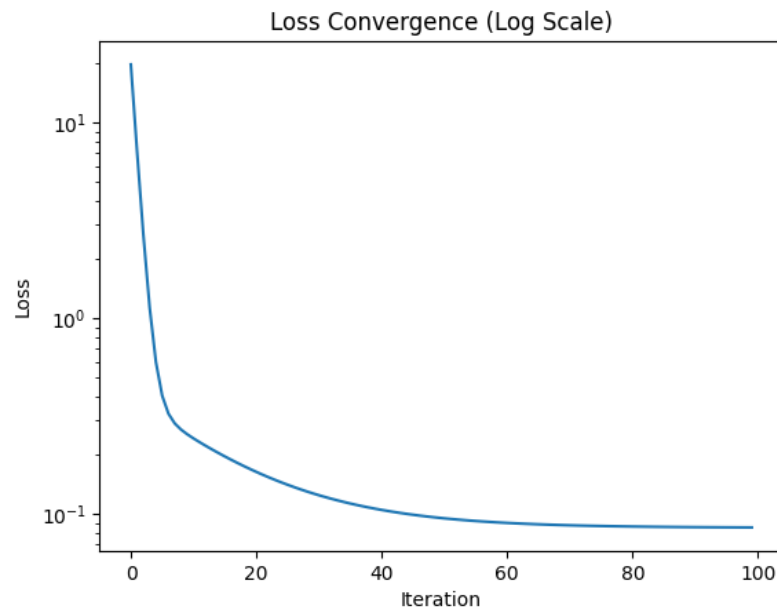y= 4 + 3x, Initialization w_0, w_1=[0,0], learning rate =0.001

After 100 iterations
Intercept: 4.48
Slope: 3.01

Linear Regression

`y= 4 + 3x, learning rate =0.001`
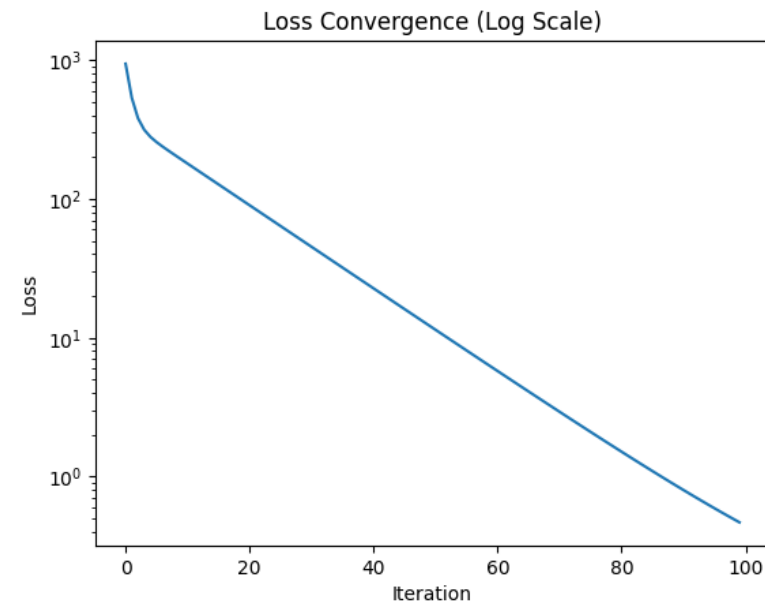
Initialization $w_0, w_1 = [0,0]$,

After 100 iterations
Intercept: 4.48
Slope: 3.01

Initialization $w_0, w_1 = [-50,13]$,

After 100 iterations
Intercept: 3.38
Slope: 3.97

Linear Regression

Y= 4 + 3x, Initialization w_0, w_1=[0,0],

learning rate =0.01
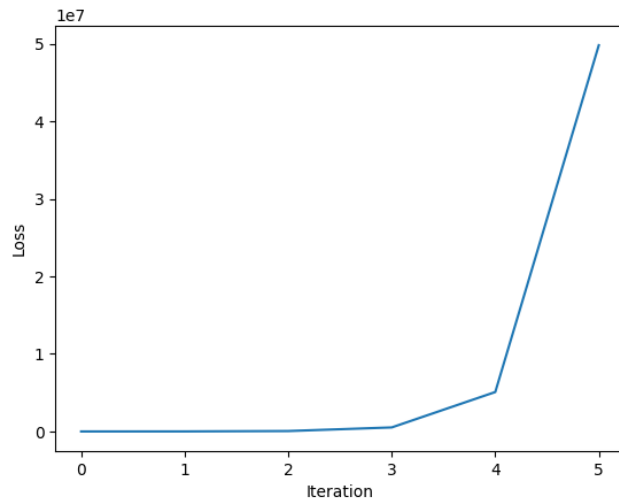
learning rate =0.005
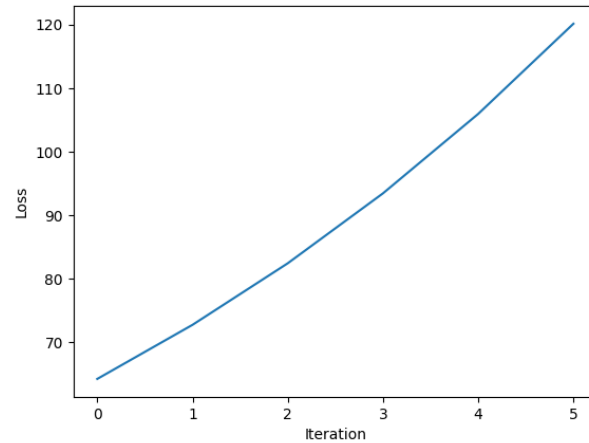
learning rate =0.001
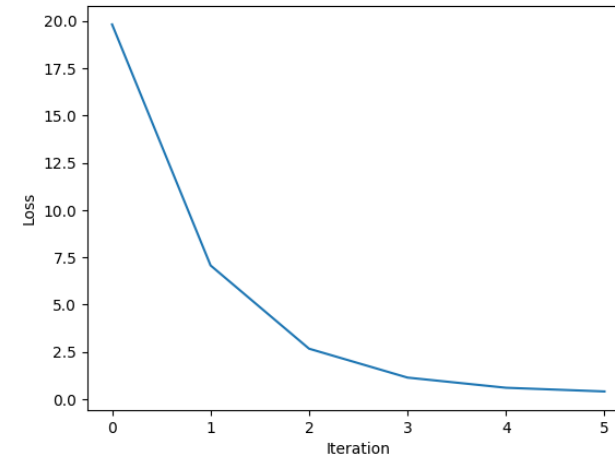
learning rate =0.0005
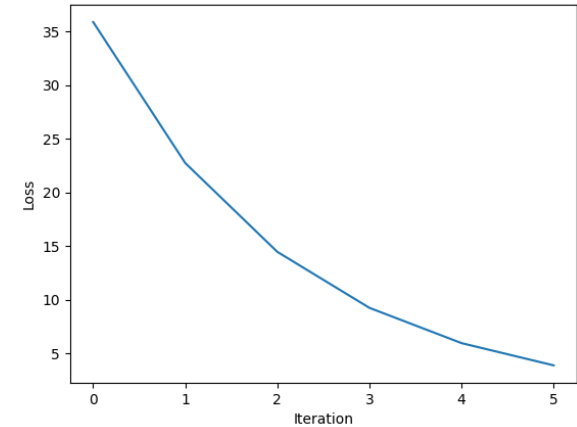
Linear Regression
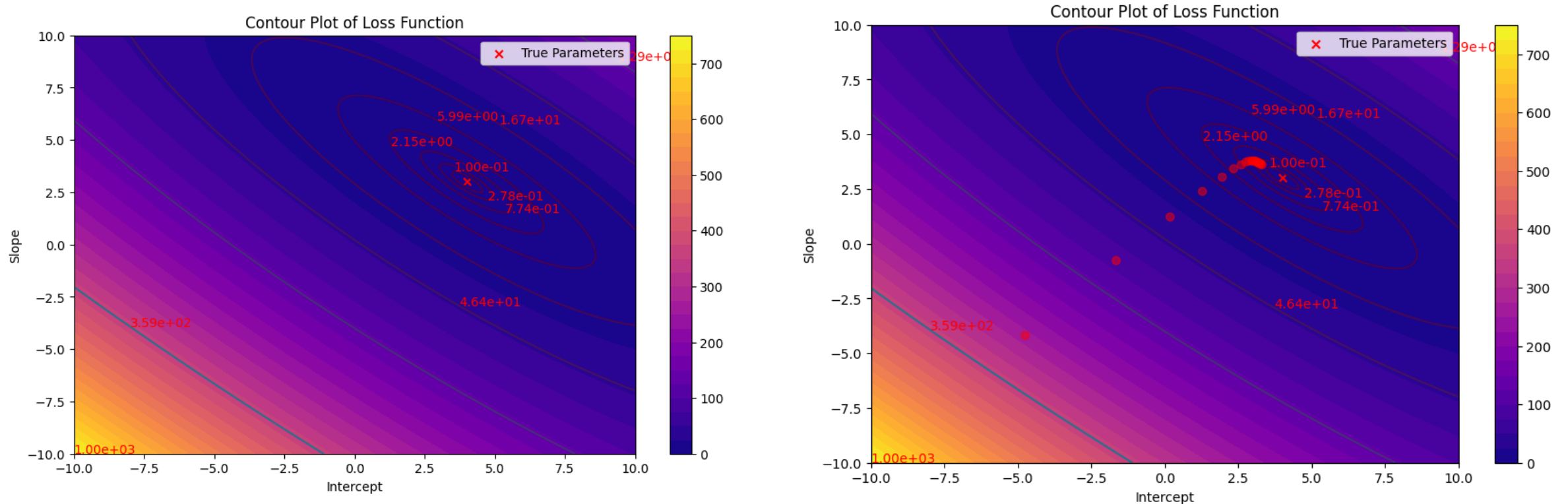
A contour plot is a graphical representation used to visualize a function F(x,y) of two variables. In this type of plot, distinct colors are assigned to different values of F. You'll observe a set of curves on the graph. These curves are called contours and are drawn in such a way that they follow paths along which the values of F(x,y) remain constant. Each contour line corresponds to a specific value of F.

Gradient descent variants

Batch Gradient Descent

➢Calculate the gradient (derivative) of the objective function with respect to all the training data points

➢Slow but more accurate

Stochastic Gradient Descent (SGD)

➢SGD uses only one randomly selected data point at a time

➢Faster convergence

➢Can be noisy and might converge to a suboptimal solution

Mini-batch Gradient Descent:

➢Computes the gradient using a small randomly selected subset (mini-batch) of the dataset

Gradient Descent Explained (ibm.com)

Linear Regression:

➢ For one independent variable (one dimensional, D=1)

$$y(\mathbf{x}) = w_0 + w_1 x_1 + \cdots, + w_D x_D = \mathbf{w}^T \mathbf{x}$$

$$y(\mathbf{x}) = w_0 + w_1 x_1$$

Residual Sum of Squares (RSS) or
Sum of Squared Error (SSE)

$$\text{RSS}(\mathbf{w}) \triangleq \sum_{i=1}^{N} (y_i - \mathbf{w}^T \mathbf{x}_i)^2$$

Mean Squared Error (MSE) = SSE/N or RSS/N

Dependent variable
$y(\mathbf{x})$
slope = w_1

$\mathbf{w}^T \mathbf{x}_i$

y_i

w_0
intercept or bias

x

Independent variable
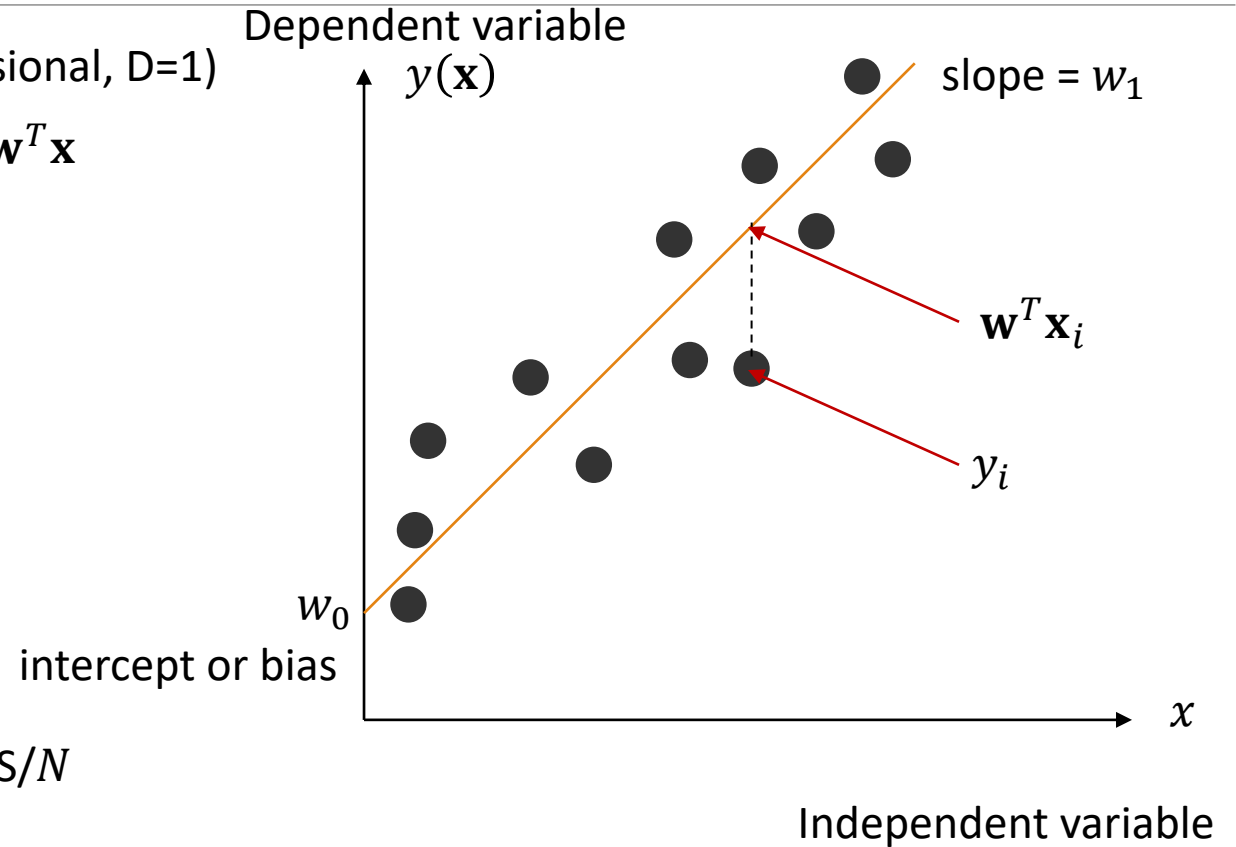
Linear Regression: Normal equations

$$\text{RSS}(\mathbf{w}) \triangleq \sum_{i=1}^{N} (y_i - \mathbf{w}^T \mathbf{x}_i)^2 \quad = \mathbf{y} - [w_0 \; w_1 \ldots w_D]\begin{bmatrix} 1 \\ x_{1,1} \\ \cdot \\ \cdot \\ \cdot \\ x_{D,1} \end{bmatrix} - [w_0 \; w_1 \ldots w_D]\begin{bmatrix} 1 \\ x_{1,2} \\ \cdot \\ \cdot \\ \cdot \\ x_{D-1,2} \end{bmatrix} - \ldots - [w_0 \; w_1 \ldots w_D]\begin{bmatrix} 1 \\ x_{1,N} \\ \cdot \\ \cdot \\ \cdot \\ x_{D,N} \end{bmatrix}$$

$$= ||\mathbf{y} - \boldsymbol{X}\boldsymbol{w}||_2^2$$

$$= (\mathbf{y} - \mathbf{Xw})^T (\mathbf{y} - \mathbf{Xw})$$

$$\boldsymbol{X} = \begin{bmatrix} 1 & x_{1,1} & x_{D,1} \\ 1 & x_{1,2} & x_{D,2} \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ 1 & x_{1,N} & x_{D,N} \end{bmatrix}$$

- $\boldsymbol{w}$ are estimated by minimizing the MSE.
- How ? Setting the gradient to zero
- Gradient $\mathbf{g}(\mathbf{w}) = (\mathbf{X}^T\mathbf{X})\mathbf{w} - \mathbf{X}^T\mathbf{y}$
- $\mathbf{g}(\mathbf{w}) = 0 \Rightarrow (\mathbf{X}^T\mathbf{X})\mathbf{w} = \mathbf{X}^T\mathbf{y}$

  normal equations

- $\widehat{\mathbf{w}}_{\text{OLS}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$

  Known as ordinary least squares

Linear Regression

Example:

X (independent variable)	y
1	2.5
2	4
3	7.3
4	9
5	11
6	14

$$\mathbf{y} = \begin{bmatrix} y_1 \\ . \\ . \\ . \\ y_N \end{bmatrix} \quad \mathbf{X} = \begin{bmatrix} 1 & x_{1,1} & x_{D,1} \\ 1 & x_{1,2} & x_{D,2} \\ . & . & . \\ . & . & . \\ . & . & . \\ 1 & x_{1,N} & x_{D,N} \end{bmatrix}$$

$$\widehat{\mathbf{w}}_{\text{OLS}} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

1. Write down $\mathbf{X}$ and $\mathbf{y}$

2. What is $\widehat{\mathbf{w}}_{\text{OLS}}$?

3. Predict value of y for x=8.

Linear Regression
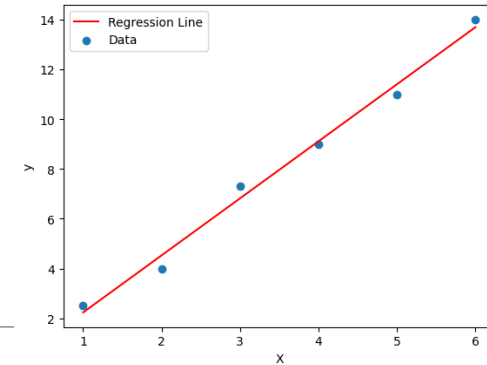
X	y
1	2.5
2	4
3	7.3
4	9
5	11
6	14

$$X = \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \\ 1 & 4 \\ 1 & 5 \\ 1 & 6 \end{bmatrix}$$

$$\mathbf{y} = [2.5 \ 4 \ 7.3 \ 9 \ 11 \ 14]$$

$$\mathbf{X}^T\mathbf{y} = \begin{bmatrix} 47.8 \\ 207.4 \end{bmatrix}$$

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix}^{-1} = \frac{1}{ad - bc}\begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$$

$$(\mathbf{X}^T\mathbf{X}) = \begin{bmatrix} 6 & 21 \\ 21 & 91 \end{bmatrix}$$

$$(\mathbf{X}^T\mathbf{X})^{-1} = \begin{bmatrix} 0.86 & -0.2 \\ -0.2 & 0.057 \end{bmatrix}$$

1. Write down $\mathbf{X}$ and $\mathbf{y}$
2. What is $\widehat{\mathbf{w}}_{\text{OLS}}$?
3. Predict value of y for x=8.

$$\widehat{\mathbf{w}}_{\text{OLS}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$
$$= \begin{bmatrix} 0.86 & -0.2 \\ -0.2 & 0.057 \end{bmatrix}\begin{bmatrix} 47.8 \\ 207.4 \end{bmatrix} = \begin{bmatrix} -0.053 \\ 2.29 \end{bmatrix}$$

$\hat{y} = -0.053 + 2.29 \times 8 = 18.267$

Linear Regression

➢ $y(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + \epsilon$ ➜ $\epsilon = y(\mathbf{x}) - \mathbf{w}^T\mathbf{x}$

➢ Gaussian noise model: assume that error term ϵ follows a Gaussian distribution (zero mean and variance σ^2) $p(\epsilon) = \mathcal{N}(0|\sigma^2)$

➢ $p(y|\mathbf{x}, \mathbf{w}) = \mathcal{N}(y|\mathbf{w}^T\mathbf{x}, \sigma^2)$

Mean $\mathbf{w}^T\mathbf{x}$ and variance σ^2

conditional probability of the output variable y given the input variable $\mathbf{x}$ and model parameters $\mathbf{w}$

Linear Regression: Likelihood

Linear Regression: Likelihood

$$\mathcal{N}(z_1|\mu,\sigma^2) \longrightarrow \frac{1}{\sqrt{2\pi\sigma^2}}\, e^{-\frac{(z_1-\mu)^2}{2\sigma^2}}$$

$$\mathcal{N}(z_2|\mu,\sigma^2) \longrightarrow \frac{1}{\sqrt{2\pi\sigma^2}}\, e^{-\frac{(z_2-\mu)^2}{2\sigma^2}}$$

$$L(z_1,z_2|\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}}\, e^{-\frac{(z_1-\mu)^2}{2\sigma^2}} \quad X \quad \frac{1}{\sqrt{2\pi\sigma^2}}\, e^{-\frac{(z_2-\mu)^2}{2\sigma^2}}$$

z_1 z_2

$$L(z_1,z_{2,\ldots}z_N|\mu,\sigma^2) = \prod_{i=1}^{N}\mathcal{N}(z_i|\mu,\sigma^2) = \prod_{i=1}^{N}\frac{1}{\sqrt{2\pi\sigma^2}}\, e^{-\frac{(z_i-\mu)^2}{2\sigma^2}}$$
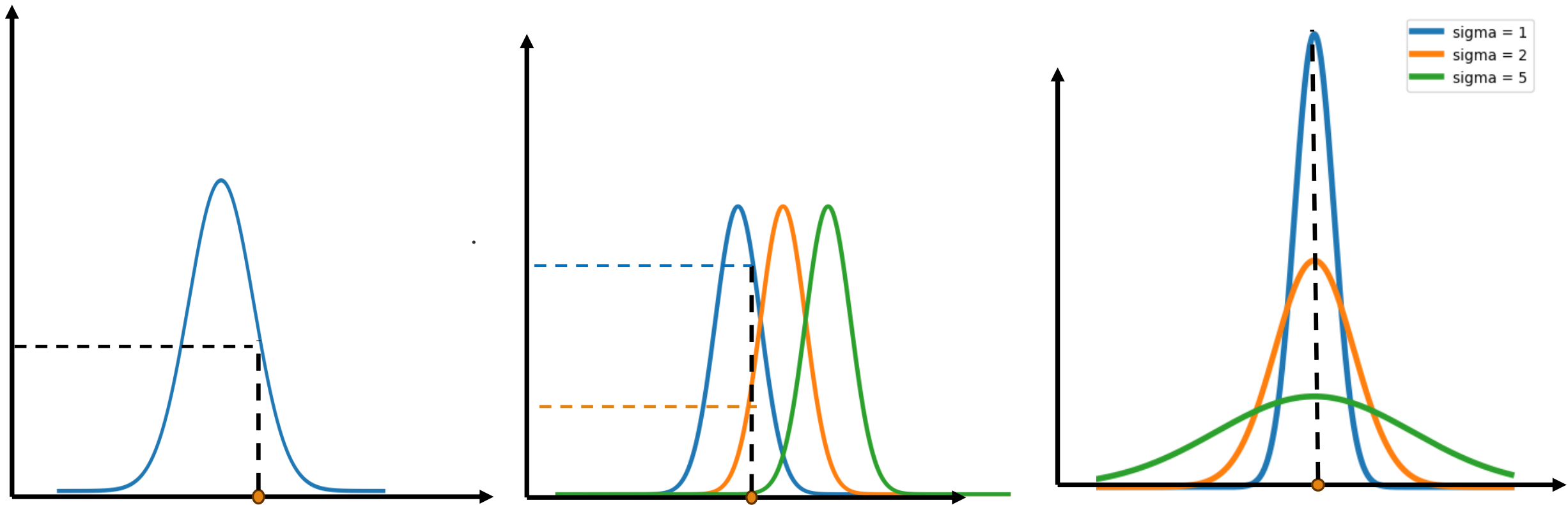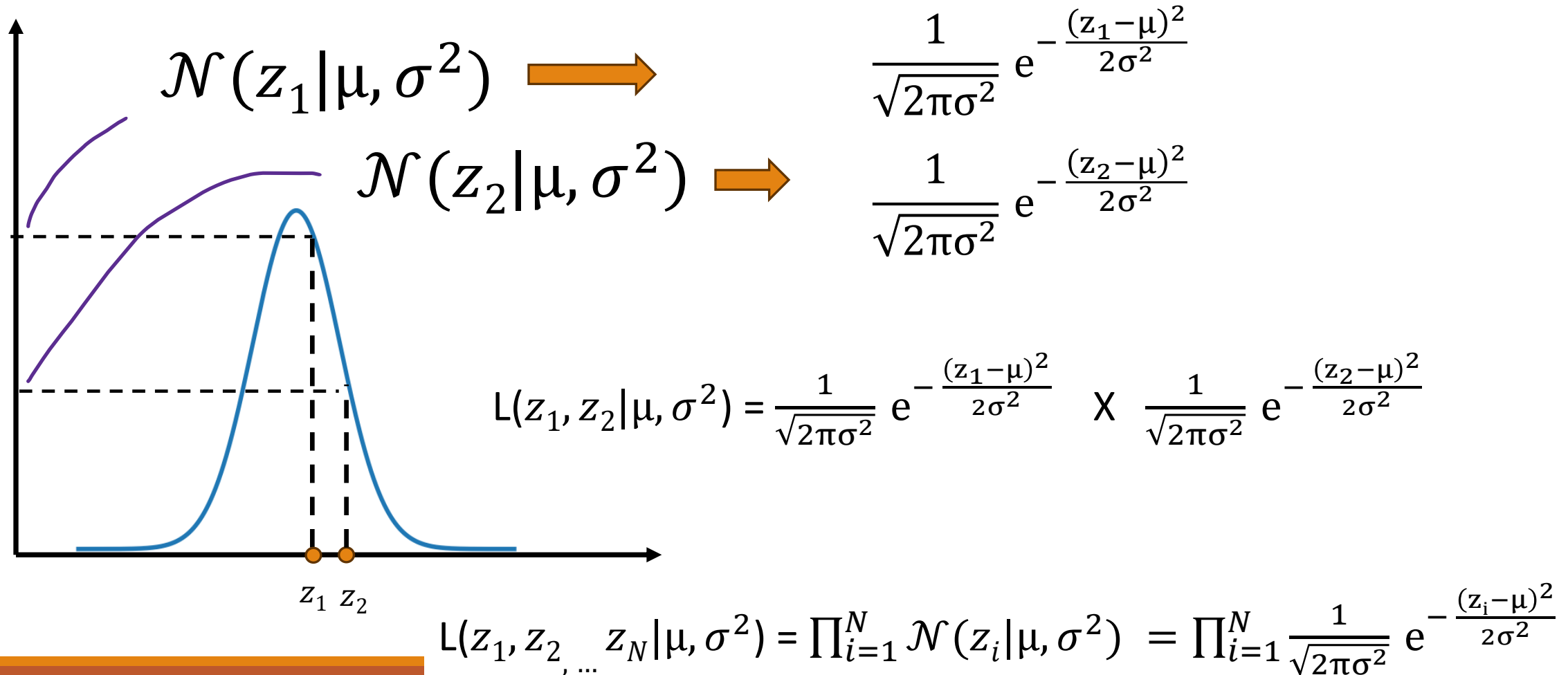
Linear Regression: Likelihood

$L(y_1, y_{2, \dots} y_N | \mathbf{w}^T \mathbf{x}, \sigma^2) = \prod_{i=1}^{N} \mathcal{N}(y_i | \mathbf{w}^T \mathbf{x}_i, \sigma^2)$

Log likelihood = $\ln\left(\prod_{i=1}^{N} \mathcal{N}(y_i | \mathbf{w}^T \mathbf{x}_i, \sigma^2)\right) = \ln\left(\prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y_i-\mu)^2}{2\sigma^2}}\right)$

$$= N \ln\left(\frac{1}{\sqrt{2\pi\sigma^2}}\right) - \sum_{i=1}^{N} \frac{(y_i-\mu)^2}{2\sigma^2}$$

$$= -\frac{N}{2}\ln(\sqrt{2\pi}) - \frac{N}{2}\ln(\sigma) - \sum_{i=1}^{N} \frac{(y_i-\mu)^2}{2\sigma^2}$$

Linear Regression: Likelihood

$$L(y_1, y_{2, \ldots} y_N | \mathbf{w}^T \mathbf{x}, \sigma^2) = -\frac{N}{2}\ln(\sqrt{2\pi}) - \frac{N}{2}\ln(\sigma) - \sum_{i=1}^{N} \frac{(y_i - \mu)^2}{2\sigma^2}$$

$\mu = (\mathbf{w}^T \mathbf{x})$ and $\mathbf{x}$ is given too.

In vector-matrix form (with a ½, NLL – Negative Log Likelihood)

$$\text{NLL}(\mathbf{w}) = \frac{1}{2}(\mathbf{y} - \mathbf{Xw})^T(\mathbf{y} - \mathbf{Xw})$$

- In this case, NLL $(\mathbf{w})$ is equivalent to **residual sum of squares (RSS)***
- How to find $\mathbf{w}$ (assuming σ is fixed),Setting the gradient to zero
- Gradient $\mathbf{g}(\mathbf{w}) = (\mathbf{X}^T\mathbf{X})\mathbf{w} - \mathbf{X}^T\mathbf{y}$
- $\mathbf{g}(\mathbf{w}) = 0 \Rightarrow (\mathbf{X}^T\mathbf{X})\mathbf{w} = \mathbf{X}^T\mathbf{y}$
- $\widehat{\mathbf{w}}_{\text{OLS}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$

Maximum likelihood estimator (MLE)**

*with certain constant factors in the expression are disregarded
**Minimizing the negative log-likelihood is equivalent to maximizing the likelihood

Linear Regression

$$\hat{\mathbf{w}}_{\text{OLS}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} = \mathbf{X}^\dagger\,\mathbf{y}$$

pseudo inverse of the (non-square) matrix $\mathbf{X}$

$$X = \begin{bmatrix} 1 & x_{1,1} & x_{D,1} \\ 1 & x_{1,2} & x_{D,2} \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ 1 & x_{1,N} & x_{D,N} \end{bmatrix}$$

➢ Condition for unique solution

  ➢ $\mathbf{X}$ is a full rank matrix* (columns of $\mathbf{X}$ are linearly independent)

  ➢ Full rank matrix ➡ No row or column can be expressed as a linear combination of the other rows or columns, respectively

full rank matrix, where rank is equal to the minimum of the number of its rows and columns

Linear Regression: Likelihood

➤ Deriving the MLE for σ^2

$$L(y_1, y_{2,\dots} y_N | \widehat{\mathbf{w}}^T \mathbf{x}, \sigma^2) = -\frac{N}{2}\ln(\sqrt{2\pi}) - \frac{N}{2}\ln(\sigma) - \sum_{i=1}^{N} \frac{(y_i - \widehat{\mathbf{w}}^T \mathbf{x}_i)^2}{2\sigma^2}$$

$$\sigma^2 = \arg\min_{\sigma^2} \text{NLL}(\widehat{\mathbf{w}}, \sigma^2) = \frac{1}{N}\sum_{i=1}^{N}(y_i - \widehat{\mathbf{w}}^T \mathbf{x}_i)^2$$

Linear Regression: Solving w_0 separately

➤ $\mathcal{N}(y|w_0 + w_1\, x_1 + \cdots, + w_D\, x_D,\, \sigma^2)$

➤ $L(y_1, y_{2,\ldots} y_N | \mathbf{w}^T\mathbf{x}, \sigma^2) = -\dfrac{N}{2}\ln(\sqrt{2\pi}) - \dfrac{N}{2}\ln(\sigma) - \sum_{i=1}^{N}\dfrac{(y_i - \mathbf{w}^T\mathbf{x}_i)^2}{2\sigma^2}$

$$= -\dfrac{N}{2}\ln(\sqrt{2\pi}) - \dfrac{N}{2}\ln(\sigma) - \sum_{i=1}^{N}\dfrac{(y_i - (w_0 + w_1 x_{1i} + \cdots, + w_D x_{Di}))^2}{2\sigma^2}$$

$$= -\dfrac{N}{2}\ln(\sqrt{2\pi}) - \dfrac{N}{2}\ln(\sigma) - \sum_{i=1}^{N}\dfrac{(y_i - (w_0 + \widetilde{\mathbf{w}}^T\widetilde{\boldsymbol{x}}_i))^2}{2\sigma^2}$$

➤ Solving w_0 (Intercept or bias) and feature coefficients are separately

$$\dfrac{\partial L}{\partial w_0} = 0 \qquad w_0 = \dfrac{1}{N}\sum_{i=1}^{N}(y_i - \widetilde{\mathbf{w}}^T\widetilde{\boldsymbol{x}}_i) = \bar{y} - \dfrac{1}{N}\sum_{i=1}^{N}(\widetilde{\mathbf{w}}^T\widetilde{\boldsymbol{x}}_i) = \bar{y} - \widetilde{\mathbf{w}}^T\bar{x}$$

Average of the model outcome

Average of the target values

Linear Regression

➢ $\widetilde{\mathbf{w}}^T = [w_1, \ldots, w_D]$

➢ Solving feature coefficients are separately

➢ $\widehat{\widetilde{\mathbf{w}}} = \left[\sum_{i=1}^{N}(\widetilde{\boldsymbol{x}}_i - \bar{x})(\widetilde{\boldsymbol{x}}_i - \bar{x})^{\mathsf{T}}\right]^{-1}\left[\sum_{i=1}^{N}(y_i - \bar{y})(\widetilde{\boldsymbol{x}}_i - \bar{x})\right] = (\mathbf{X_C}^T\mathbf{X_C})^{-1}\mathbf{X_C}^T\mathbf{y_C}$

Centered input matrix

Centered output vector

➢ For 1D $y = w_0 + w_1 x$

$\widehat{w_1} = \sum_{i=1}^{N}(yi - \bar{y})(x - \bar{x}) / \sum_{i=1}^{N}(x - \bar{x})^2$ = Cov [X; Y] / Cov [X; X] $= C_{xy} / C_{xx}$

$\widehat{w_0} = \bar{y} - \widehat{w_1}\bar{x}$

Procedure: Estimating $\widetilde{\mathbf{w}}$ by centered data then estimating the w_0 by $\bar{y} - \widetilde{\mathbf{w}}^T\bar{x}$

Linear Regression: Geometric interpretation

$$X = \begin{bmatrix} 1 & x_{1,1} & x_{D,1} \\ 1 & x_{1,2} & x_{D,2} \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ 1 & x_{1,N} & x_{D,N} \end{bmatrix}$$

sample
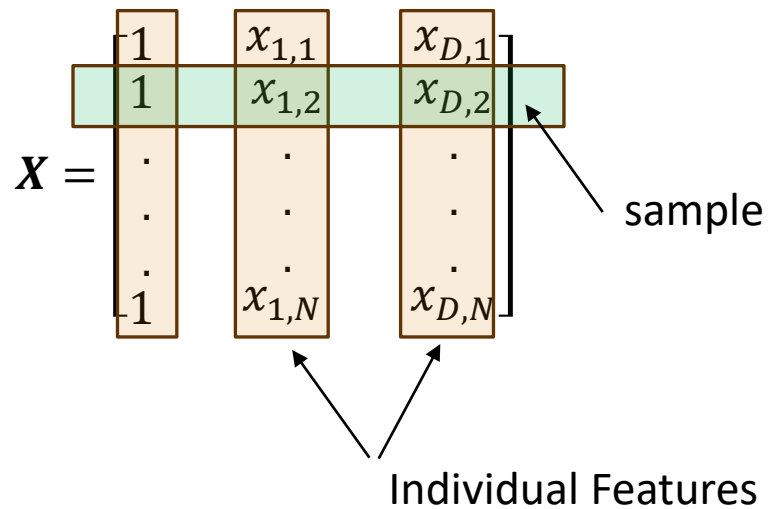
$$X = \begin{bmatrix} 1 & x_{1,1} & x_{D,1} \\ 1 & x_{1,2} & x_{D,2} \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ 1 & x_{1,N} & x_{D,N} \end{bmatrix} \qquad \mathbf{y} = \begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_N \end{bmatrix} \qquad \mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \\ \cdot \\ \cdot \\ \cdot \\ w_D \end{bmatrix}$$

Individual Features

$$\mathbf{x}_i = \begin{bmatrix} 1 \\ x_{1,i} \\ \cdot \\ \cdot \\ \cdot \\ x_{D,i} \end{bmatrix}$$

$$\mathbf{Proj}\,(\mathbf{X}) = \mathbf{X}\,(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$$

$$\hat{\mathbf{y}} = \mathbf{Proj}\,(\mathbf{X})\,\mathbf{y}$$

$$\widehat{\mathbf{w}}_{\mathrm{OLS}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

$$\hat{\mathbf{y}} = \mathbf{X}\,\widehat{\mathbf{w}}_{\mathrm{OLS}} = \mathbf{X}\,(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

The orthogonal projection of vector $\mathbf{y}$ onto the column space of matrix $\mathbf{X}$
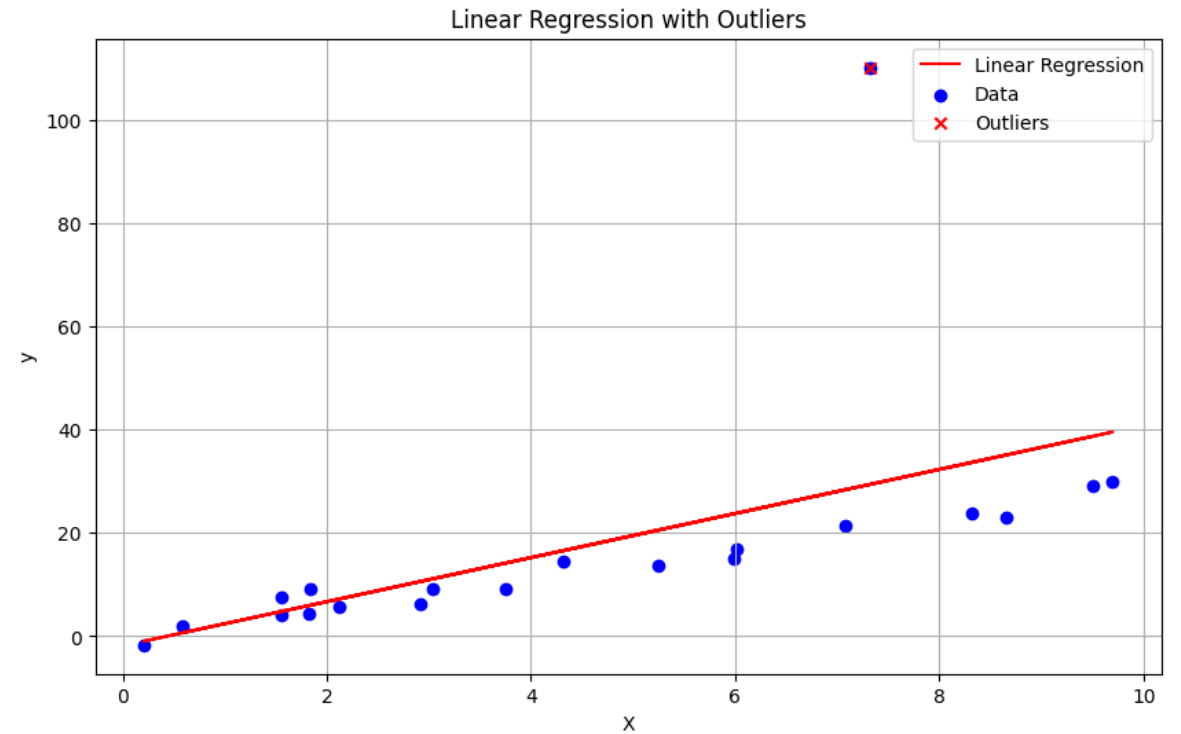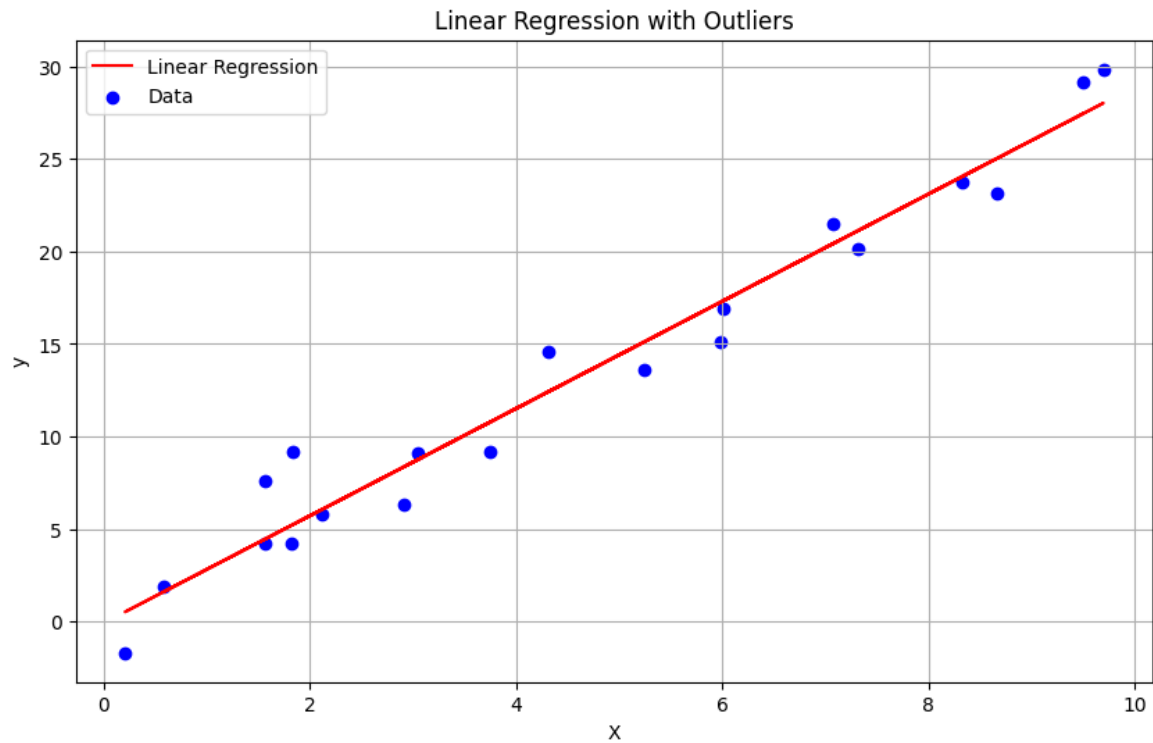
Linear Regression: Implementation

$$\widehat{\mathbf{w}}_{\text{OLS}} = \boxed{(\mathbf{X}^T\mathbf{X})}^{-1}\mathbf{X}^T\mathbf{y}$$

may be ill conditioned or singular ➔ cause issues in numerical computations

➤ SVD based pseudo inverse calculation (see sklearn implementation)

Linear Regression: Example

R^2 Statistic

"Amount of variability that is **left unexplained** after performing the regression (amount of unexplained)"

$$R^2 = 1 - \frac{\sum_{i=1}^{N}(y_i - \mathbf{w}^T\mathbf{x})^2}{\sum_{i=1}^{N}(y_i - \bar{y})^2} = 1 - \frac{RSS}{\sum_{i=1}^{N}(y_i - \bar{y})^2} = 1 - \frac{RSS}{TSS} \in (0,1)$$
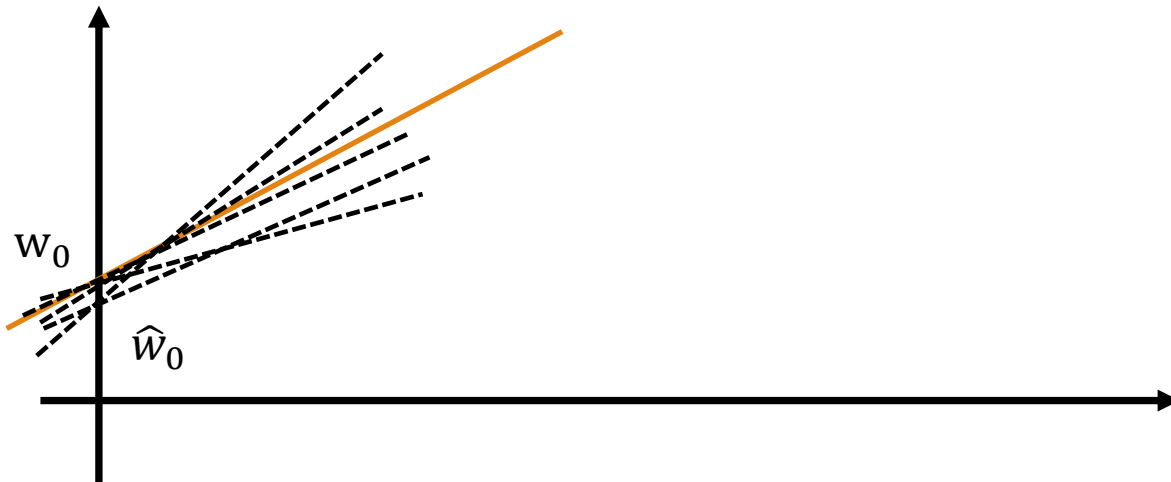
"Total variance in the y"

TSS – RSS "measures the amount of variability in the response that is explained (or removed) by performing the regression" [1].

"R^2 measures proportion of variability in Y that can be explained using X" ("R^2 is close to 1 mean that the large proportion of the variability in the response has been explained by the regression"[1].

[1] Gareth James, Daniela Witten, Trevor Hastie and Robert Tibshirani, An Introduction to Statistical Learning with Applications in R, 2013.

Standard errors

➤ True relationship $y = w_0 + w_1 x$

➤ How close our estimate (w_0, w_1) to true values $(\hat{w}_0, \hat{w}_1)$

➤ Standard errors

$$\text{SE}^2(\hat{w}_0) = \sigma^2 \left[\frac{1}{N} + \frac{\bar{x}^2}{\sum_{i=1}^{N}(x_i - \bar{x})^2} \right]$$

$$\text{SE}^2(\hat{w}_1) = \frac{\sigma^2}{\sum_{i=1}^{N}(x_i - \bar{x})^2}$$

Gareth James, Daniela Witten, Trevor Hastie and Robert Tibshirani, An Introduction to Statistical Learning with Applications in R, 2013.

t-statistic

➤Standard errors

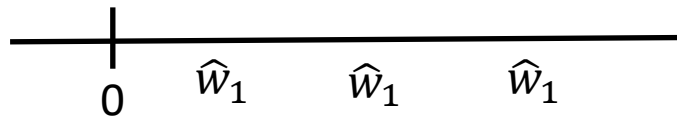$$\text{SE}^2(\widehat{w}_0) = \sigma^2 \left[\frac{1}{N} + \frac{\bar{x}^2}{\sum_{i=1}^{N}(x_i - \bar{x})^2} \right] \qquad \text{SE}^2(\widehat{w}_1) = \frac{\sigma^2}{\sum_{i=1}^{N}(x_i - \bar{x})^2}$$

➤Is there a true relationship?

➤Hypothesis testing

  ➤H_0: No relationship between y and w_1 ➜$w_1 = 0$

  ➤H_1: There is a relationship between y and w_1 ➜$w_1 \neq 0$

0	$\widehat{w}_1$	$\widehat{w}_1$	$\widehat{w}_1$

t-statistic
$$t = \frac{\widehat{w}_1 - 0}{\text{SE}^2(\widehat{w}_1)}$$

number of standard deviations that $\widehat{w}_1$ is away from 0

Need to determine $\widehat{w}_1$
1. Sufficiently far from zero ➜ $\widehat{w}_1 \neq 0 \ or$
2. Sufficiently *close to zero* $\widehat{w}_1$ =0

$\widehat{w}_1$ =0.1 Sufficiently close to zero? Far away from zero?
Depends on $\text{SE}^2(\widehat{w}_1)$

True $w_1 = 5, \text{SE}^2(\widehat{w}_1) = 10 \ is \ significant$
True =1000, $\text{SE}^2(\widehat{w}_1)$ =10 is not significant

Gareth James, Daniela Witten, Trevor Hastie and Robert Tibshirani,
An Introduction to Statistical Learning with Applications in R, 2013.

Confidence intervals

➢ Standard errors can be used to calculate confidence level.

➢ 95% Confidence Interval: Range of values containing true parameter value with 95% probability

➢ The range is calculated from training data.

➢ For linear regression

For w_0: $\widehat{w}_0 \pm 2\,\text{SE}^2(\widehat{w}_0)$

For w_1: $\widehat{w}_1 \pm 2\,\text{SE}^2(\widehat{w}_1)$

# p -value

t–statistic

$$t = \frac{\widehat{w}_1 - 0}{\text{SE}^2(\widehat{w}_1)}$$

number of standard deviations that $\widehat{w}_1$ is away from 0

t-distribution with N - 2 degrees of freedom if there is no relationship between x and y

p-value "the probability of observing any values equal to $|t|$ or larger, assuming true $w_1 = 0$. (no association between the predictor and the response variable)"

small p -value reject null hypothesis H$_0$: No relationship between y and $w_1(w_1 = 0)$
Typical values 1% or 5%.
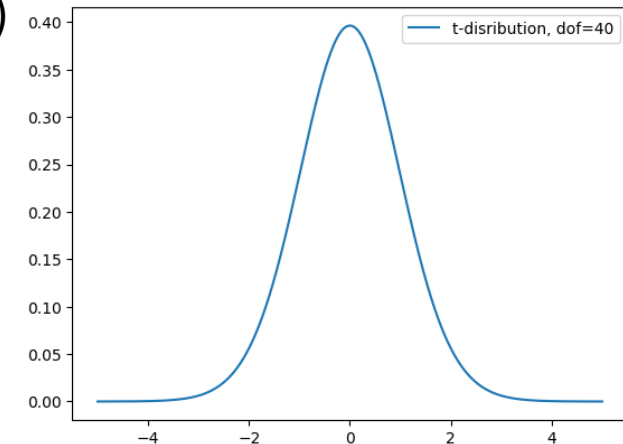
Linear Regression: Example

California housing dataset

#Attribute Information: (independent variables)

\#   - MedInc   median income in block group

\#   - HouseAge   median house age in block group

\#   - AveRooms   average number of rooms per household

\#   - AveBedrms   average number of bedrooms per household

\#   - Population   block group population

\#   - AveOccup   average number of household members

\#   - Latitude   block group latitude

\#   - Longitude   block group longitude

Dependent variable is median house value (y)

	MedInc	HouseAge	AveRooms	AveBedrms	Population	AveOccup	Latitude	Longitude
0	8.3252	41.0	6.984127	1.023810	322.0	2.555556	37.88	-122.23
1	8.3014	21.0	6.238137	0.971880	2401.0	2.109842	37.86	-122.22
2	7.2574	52.0	8.288136	1.073446	496.0	2.802260	37.85	-122.24
3	5.6431	52.0	5.817352	1.073059	558.0	2.547945	37.85	-122.25
4	3.8462	52.0	6.281853	1.081081	565.0	2.181467	37.85	-122.25

x_1	x_2	x_3	x_4	x_5	x_6	x_7	x_8
8.3252	41.0	6.984127	1.023810	322.0	2.555556	37.88	-122.23
8.3014	21.0	6.238137	0.971880	2401.0	2.109842	37.86	-122.22
7.2574	52.0	8.288136	1.073446	496.0	2.802260	37.85	-122.24
5.6431	52.0	5.817352	1.073059	558.0	2.547945	37.85	-122.25
3.8462	52.0	6.281853	1.081081	565.0	2.181467	37.85	-122.25

y
4.526
3.585
3.521
3.413

$$X = \begin{bmatrix} 1 & x_{1,1} & x_{D,1} \\ 1 & x_{1,2} & x_{D,2} \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot 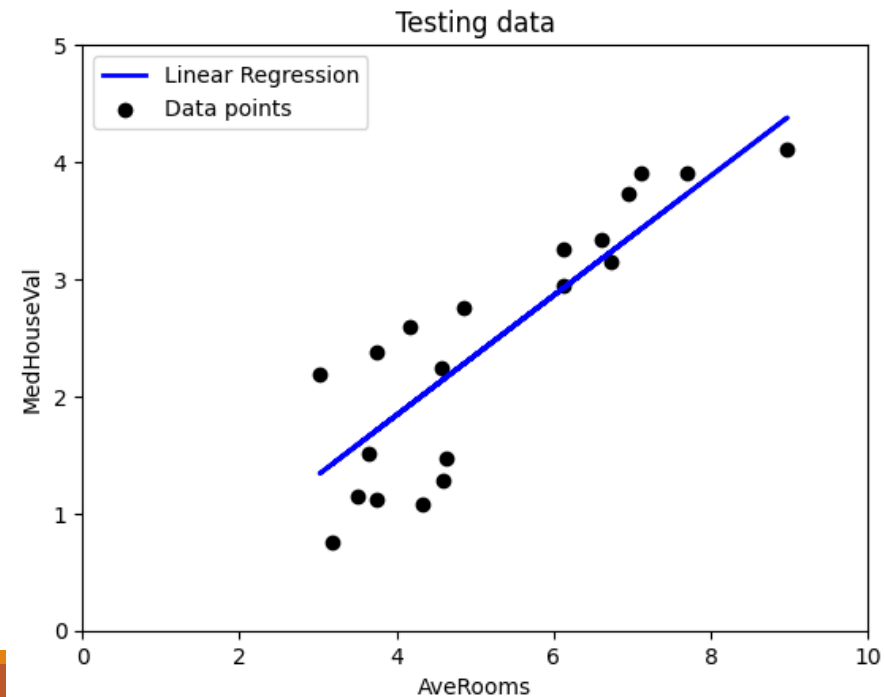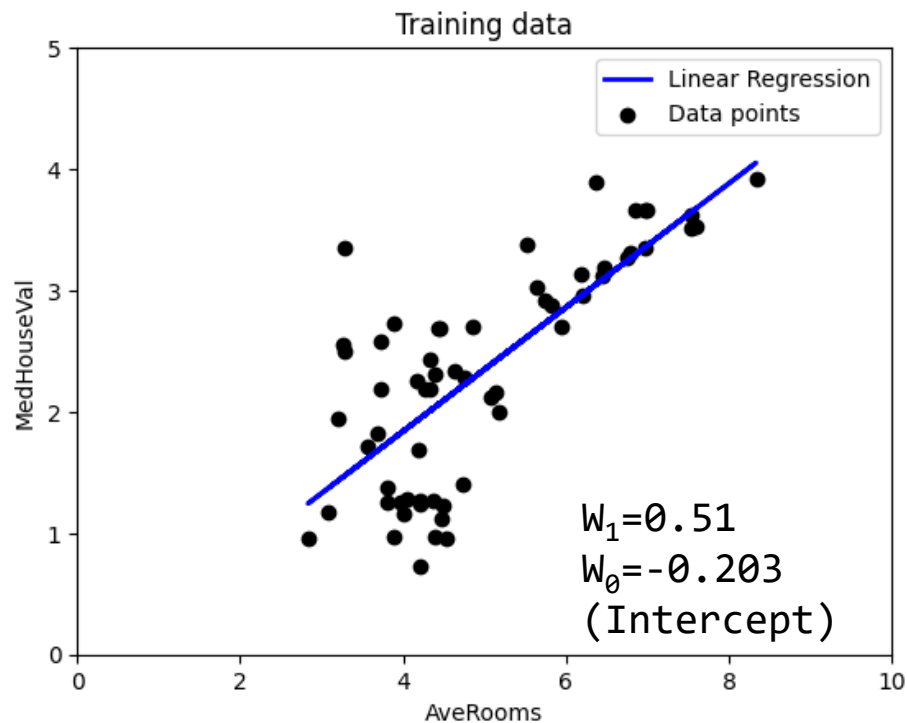& \cdot & \cdot \\ 1 & x_{1,N} & x_{D,N} \end{bmatrix} \qquad X = \begin{bmatrix} 1 & 8.3252 & -122.23 \\ 1 & 8.3014 & -122.22 \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ 1 & 3.8462 & -122.25 \end{bmatrix}$$

Linear Regression: Example

California housing dataset (100 data samples were taken)

Independent variables- AveRooms

Dependent variable is median house value

W_1=0.51
W_0=-0.203
(Intercept)

Linear Regression: Example

Independent variables- AveRooms, Dependent variable is median house value

➢ RSS 21.89 RSE 0.61 TSS 49.85 R^2 = 0.56
➢ standard errors for intercept and w_1: 0.089 0.0034
➢ t-statistic for intercept and w_1: -0.68 8.75
➢ pvale for intercept and w_1 : 0.25 1.69e^{-12}

P-value for intercept = 0.25
not statistically significant at conventional significance levels
(such as 0.05 or 0.01)
There's no strong evidence to suggest that the constant term in
the model significantly affects the response variable. This could
imply that the relationship between the predictor and the
response starts from or passes through the origin (0,0)

P-value for w_1 = 1.69e-12
coefficient w_1 is likely to be statistically
significant and suggests that there is a
meaningful linear relationship between
the predictor variable (w_1) and the
response variable

Linear Regression: Example

Independent variables- AveRooms, Dependent variable is median house value

Impact of outliers
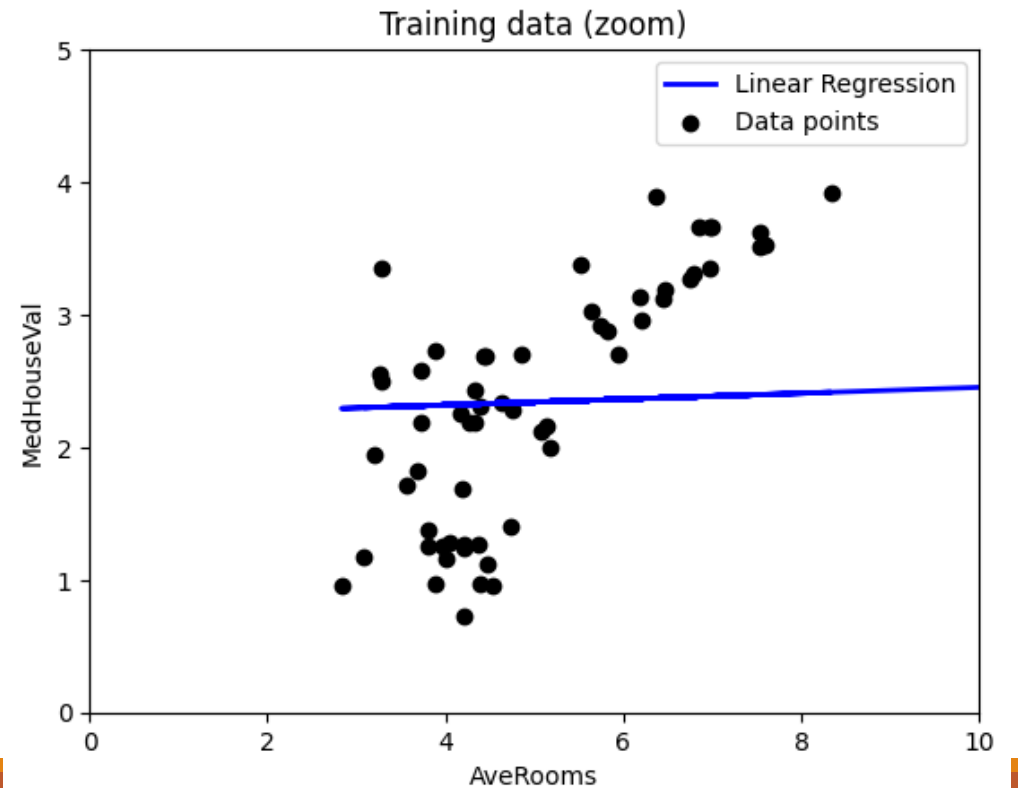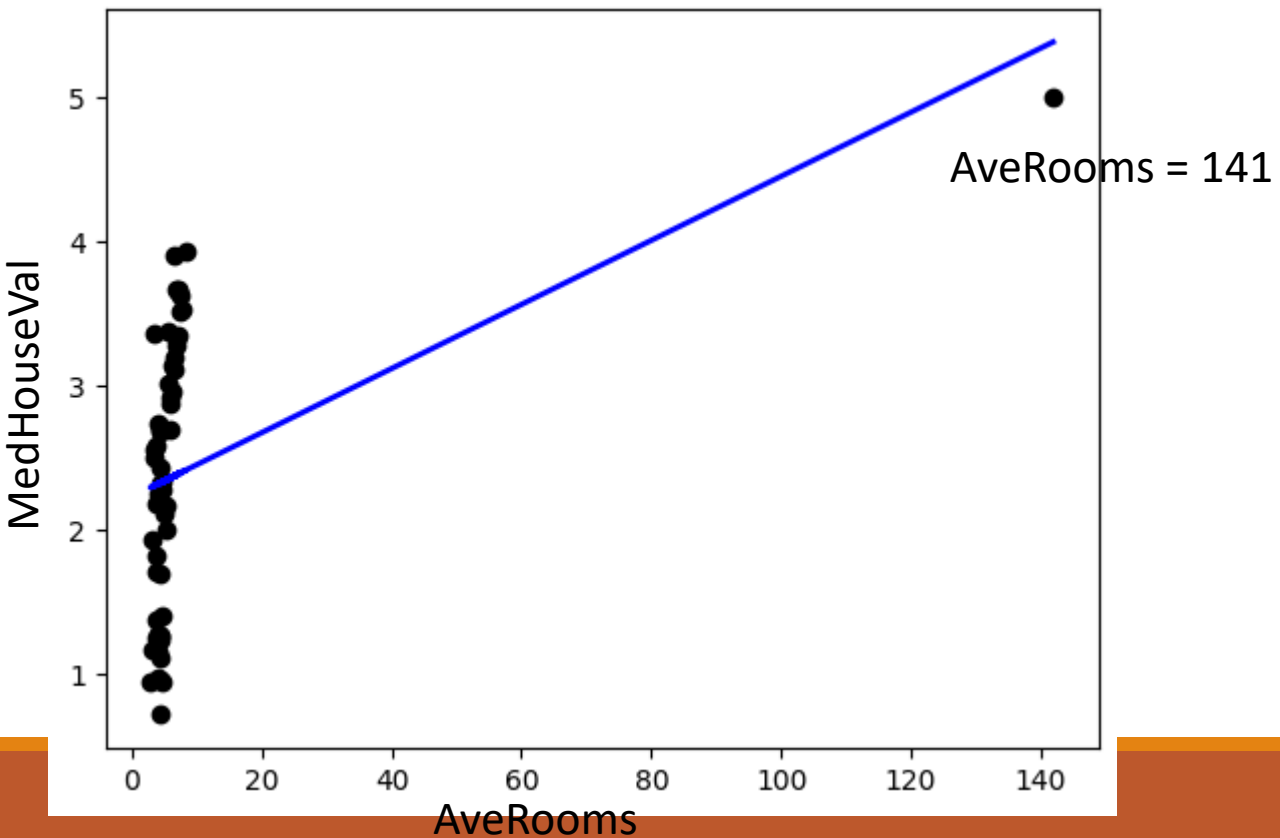
Linear Regression: Example

Independent variables	MedInc	HouseAge	AveRooms	AveBedrms	Population	AveOccup	Latitude	Longitude

Dependent variable   MedHouseVal

	MedInc	HouseAge	AveRooms	AveBedrms	Population	AveOccup	Latitude	Longitude
Coefficients:	$4.52e^{-1}$	$9.44e^{-3}$	$-1.30e^{-1}$	$8.24e^{-1}$	$-5.84e^{-6}$	$-7.62e^{-3}$	$-4.06e^{-1}$	$-4.187e^{-1}$

```
==================================================================
               coef      std err           t      P>|t|       [0.025      0.975]
------------------------------------------------------------------
const      -35.6684        0.849     -42.006      0.000      -37.333     -34.004
x1           0.4527        0.006      81.204      0.000        0.442       0.464
x2           0.0094        0.001      16.493      0.000        0.008       0.011
x3          -0.1302        0.008     -16.185      0.000       -0.146      -0.114
x4           0.8249        0.041      20.252      0.000        0.745       0.905
x5       -5.847e-06     6.15e-06      -0.951      0.341    -1.79e-05      6.2e-06
x6          -0.0076        0.001      -6.442      0.000       -0.010      -0.005
x7          -0.4063        0.009     -43.858      0.000       -0.424      -0.388
x8          -0.4184        0.010     -43.176      0.000       -0.437      -0.399
```

R-squared: 0.614

Mean squared error: 0.53

A small p-value (usually < 0.05) suggests that the feature is likely to have a significant impact on the target variable. A large p-value suggests that the feature might not have a statistically significant impact on the target variable.

Ridge Regression

$$J(\mathbf{w}) = \frac{1}{N}\sum_{i=1}^{N}(y_i - \mathbf{w}^T\mathbf{x}_i)^2 + \lambda \boxed{\|\mathbf{w}\|_2^2}$$

L2 regularization penalty (shrinkage penalty)

➤ $\|\mathbf{w}\|_2^2 = \sum_j w_j^2 = \mathbf{w}^T\mathbf{w}$ = the squared two-norm.

➤ $\lambda \geq 0$, is a complexity penalty (hyper parameter, need to tune).

➤ Ridge regression also known as Tikhonov regularization, penalized least squares L_2 regularization, or weight decay.

➤ Address multicollinearity (high correlation between predictor (independent) variables)

➤ Avoid overfitting

➤ Regularization discourages the model from assigning overly large coefficients to predictor variables

$$\widehat{\mathbf{w}}_{\text{ridge}} = (\lambda\mathbf{I}_D + \mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

Ridge Regression: Impact of λ

➤ $J(\mathbf{w}) = \frac{1}{N}\sum_{i=1}^{N}(y_i - \mathbf{w}^T\mathbf{x}_i)^2 + \lambda\|\mathbf{w}\|_2^2$

➤ When λ is very large (coefficinets $\mathbf{w} \rightarrow 0$).

➤ When λ tends toward zero, Ordinary least square ➜ coefficients exhibit big oscillations.

➤ Need to tune λ to balance

Ridge Coefficients as a Function of Regularization
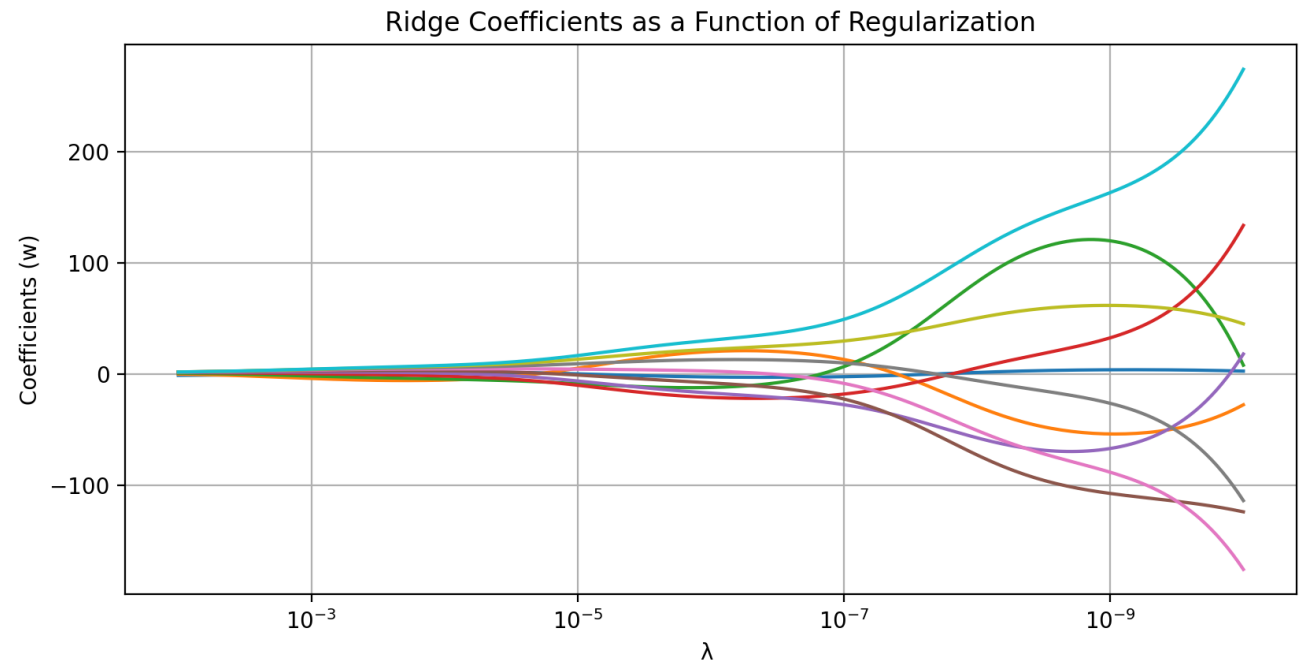
Polynomial Regression

➤ Model: Relationship between the independent variable(s) and the dependent variable is modeled as an nth-degree polynomial*.

➤ $y = \mathbf{w}^T \phi(\mathbf{x})$ and for single variable $\phi(\mathbf{x}) = [1, x, x^2, \ldots, x^d]$

➤ For two feature $d = 2$, $\phi(\mathbf{x}) = [1, x_1, x_2, x_1^2, x_1 x_2, x_2{}^2]$

➤ Example $y = w_0 + w_1 x_1 + w_2 x_2 + w_3 x_1^2 + w_4 x_1 x_2 + w_5 x_2^2$
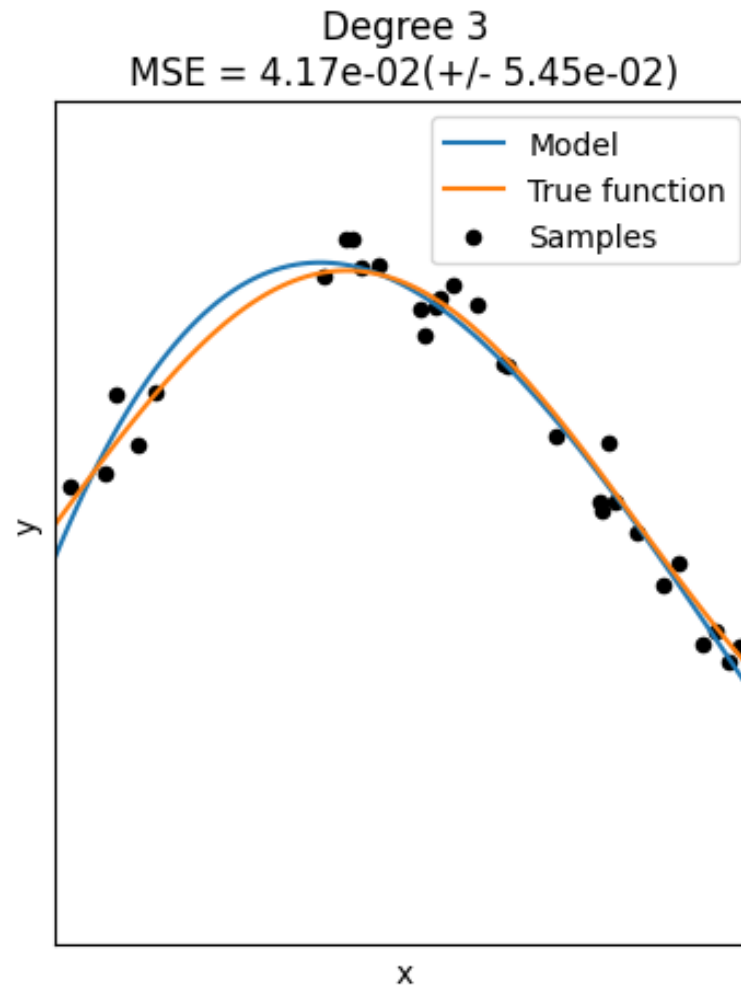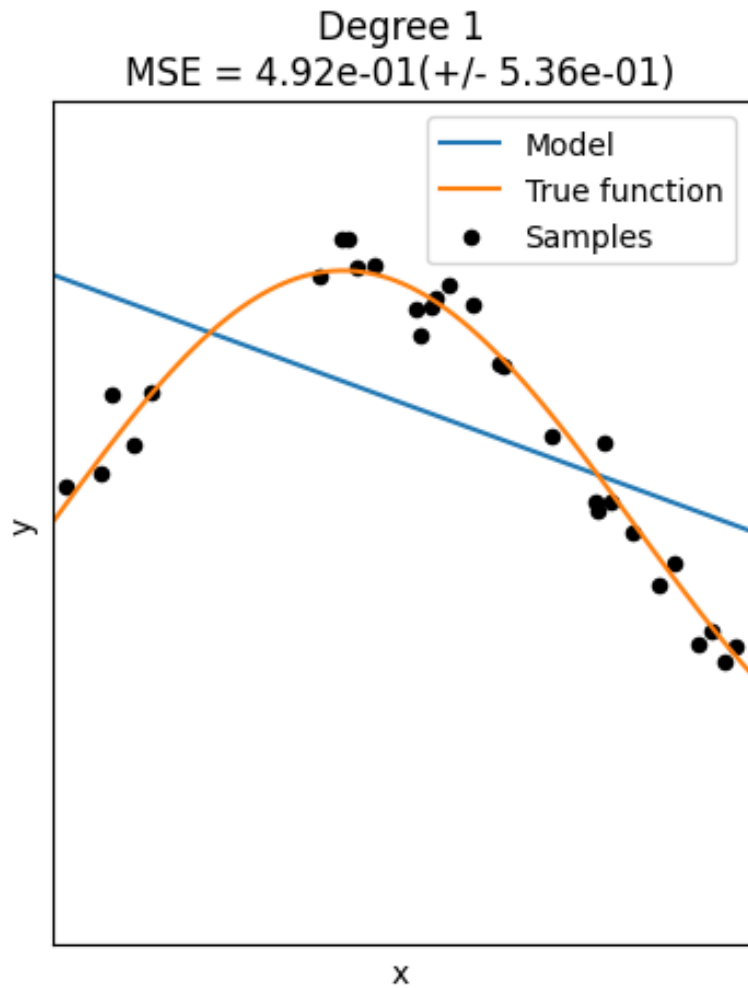
$y = w_0 + w_1 z_1 + w_2 z_2 + w_3 z_3 + w_4 z_4 + w_5 z_5$

➤ Cost function

$$J(\mathbf{w}) = \frac{1}{N} \sum_{i=1}^{N} (y_i - \mathbf{w}^T \phi(\mathbf{x}))^2$$
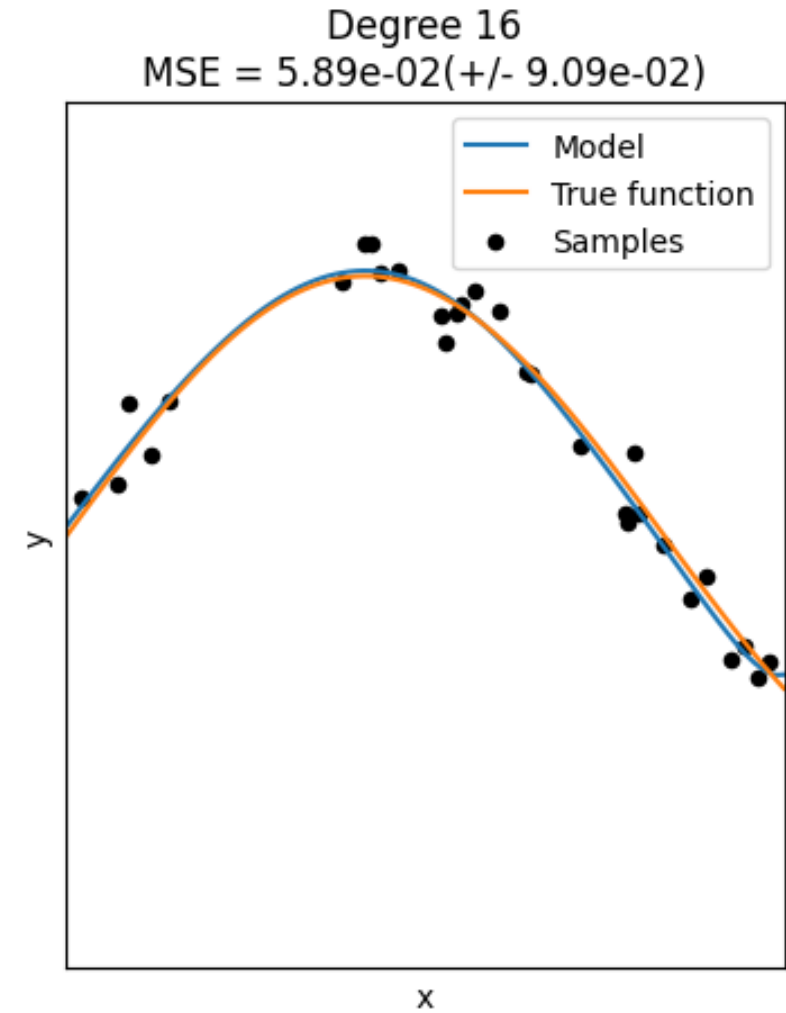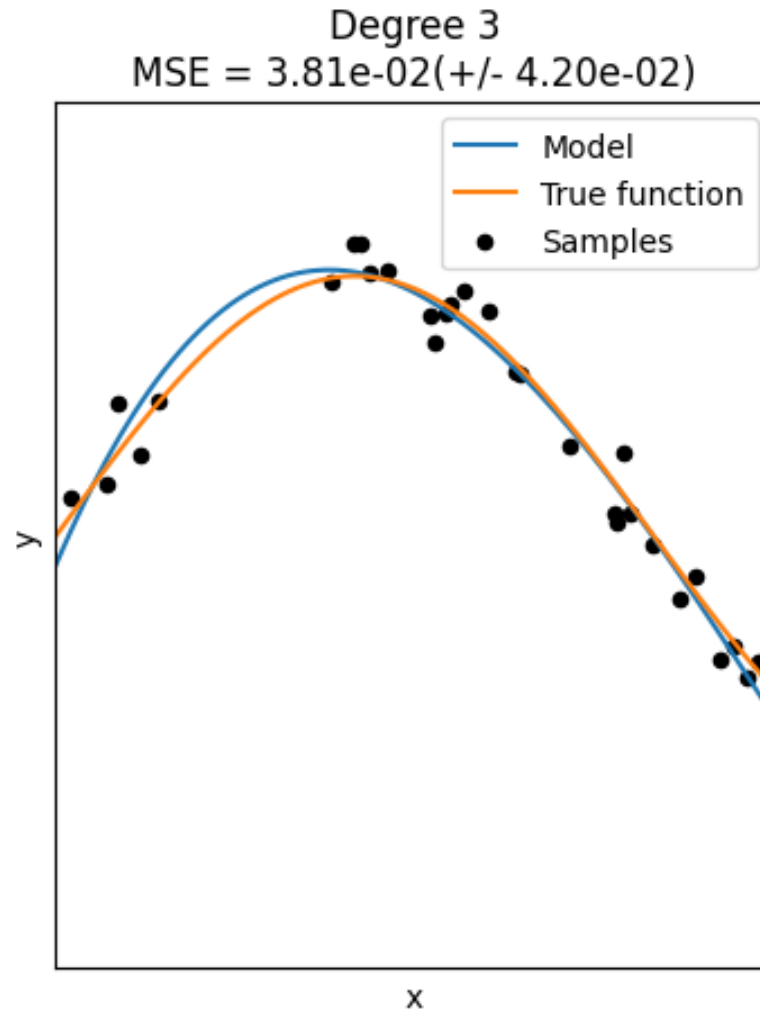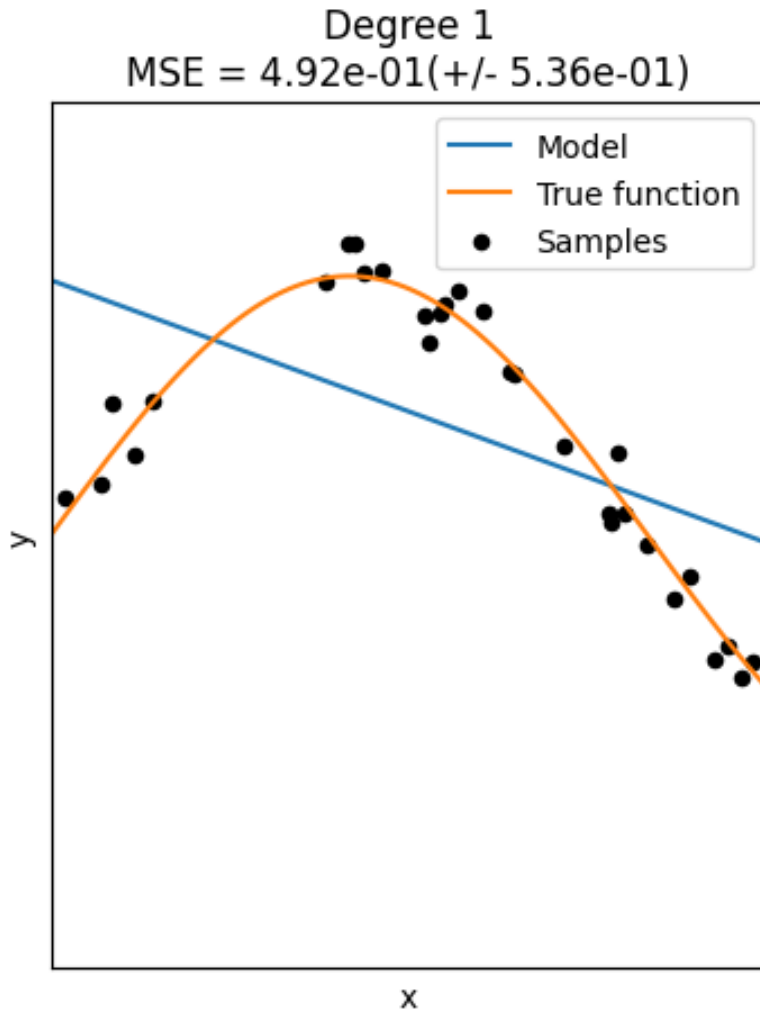
➤ Polynomial **Ridge** Regression

$$J(\mathbf{w}) = \frac{1}{N} \sum_{i=1}^{N} (y_i - \mathbf{w}^T \phi(\mathbf{x}))^2 + \lambda \|\mathbf{w}\|_2^2$$

* Still a linear model with respect to weights. Nonlinear model when $x_1 \wedge w_1$

Polynomial Regression

Polynomial Ridge Regression

Degree 1
MSE = 4.92e-01(+/- 5.36e-01)

Degree 3
MSE = 3.81e-02(+/- 4.20e-02)

Degree 16
MSE = 5.89e-02(+/- 9.09e-02)
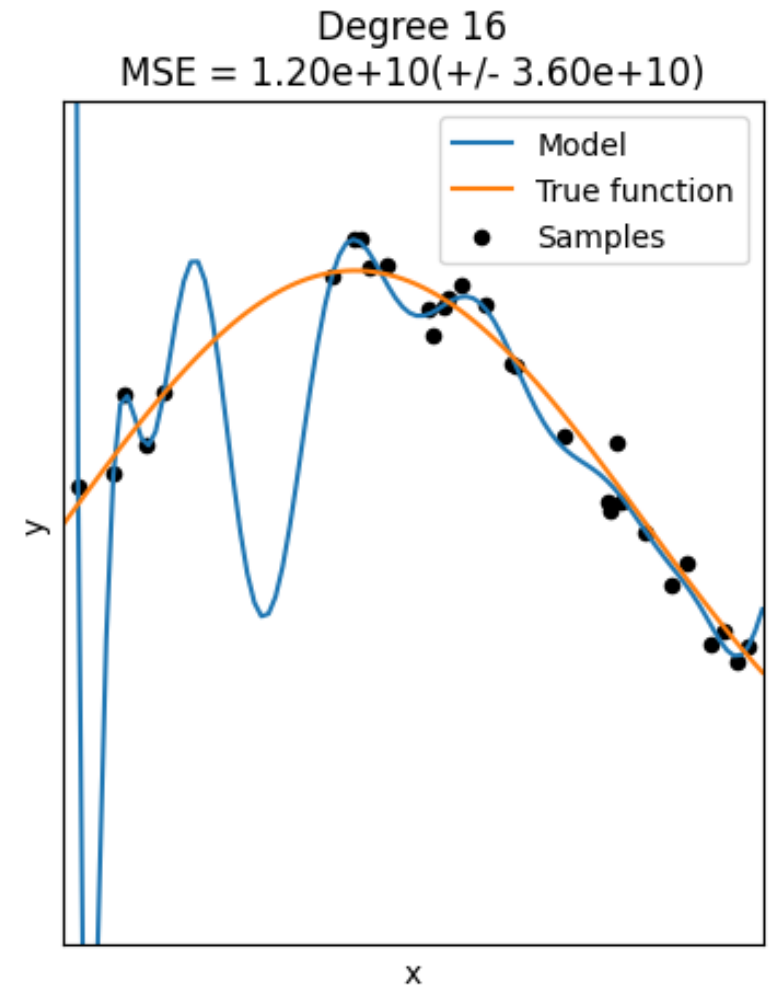
Lasso

➤ Least Absolute Shrinkage and Selection Operator

➤ Cost function

$$J(\mathbf{w}) = \frac{1}{N} \sum_{i=1}^{N} (y_i - \mathbf{w}^T \mathbf{x})^2 + \lambda \|\mathbf{w}\|_1$$

L1 regularization penalty

➤ Select a subset of important features while reducing the coefficients of less important features to nearly zero (Encourages sparsity)
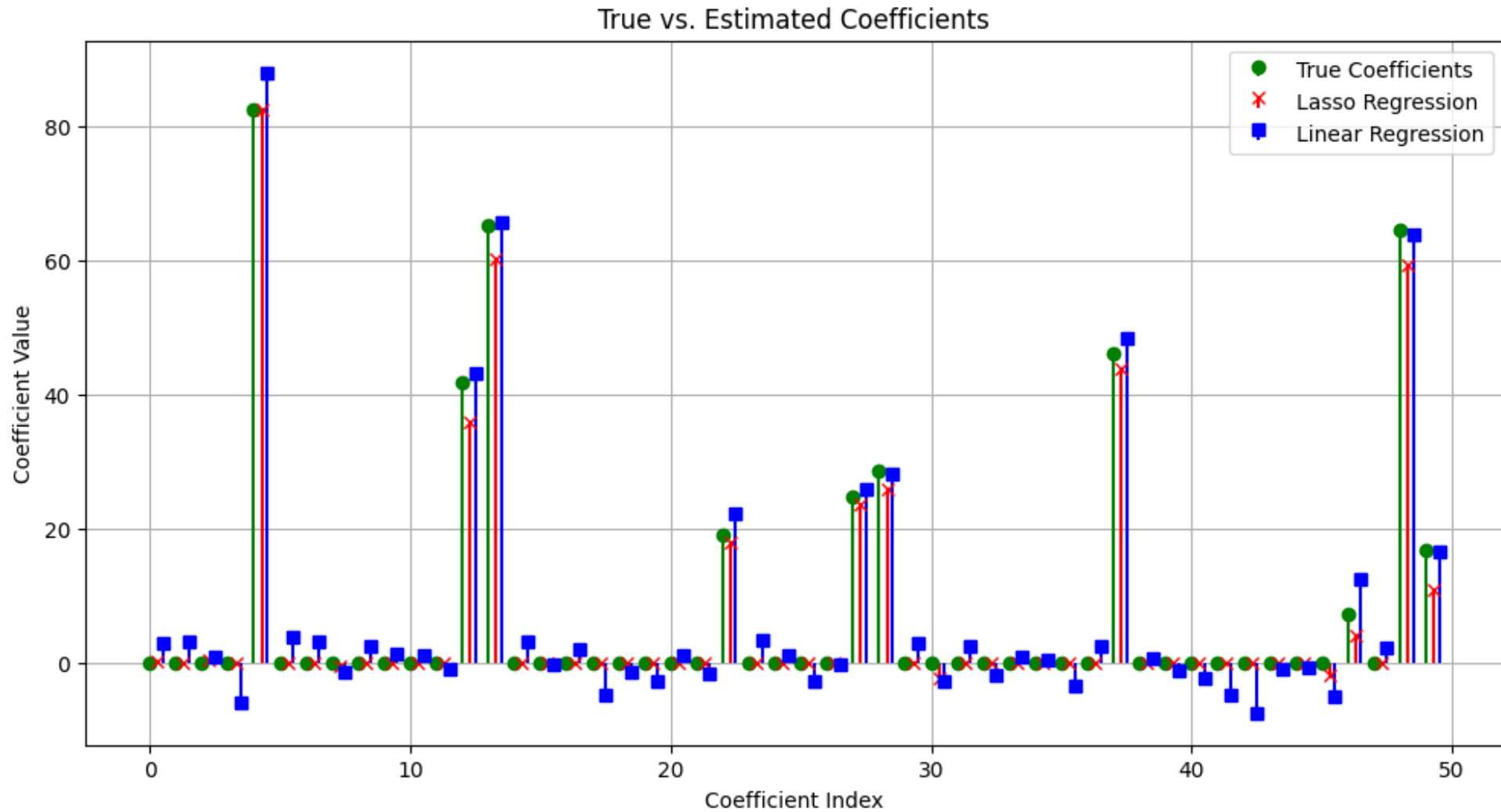
➤ Useful for feature selection or dimensionality reduction

➤ Lasso plays important role in compressed sensing
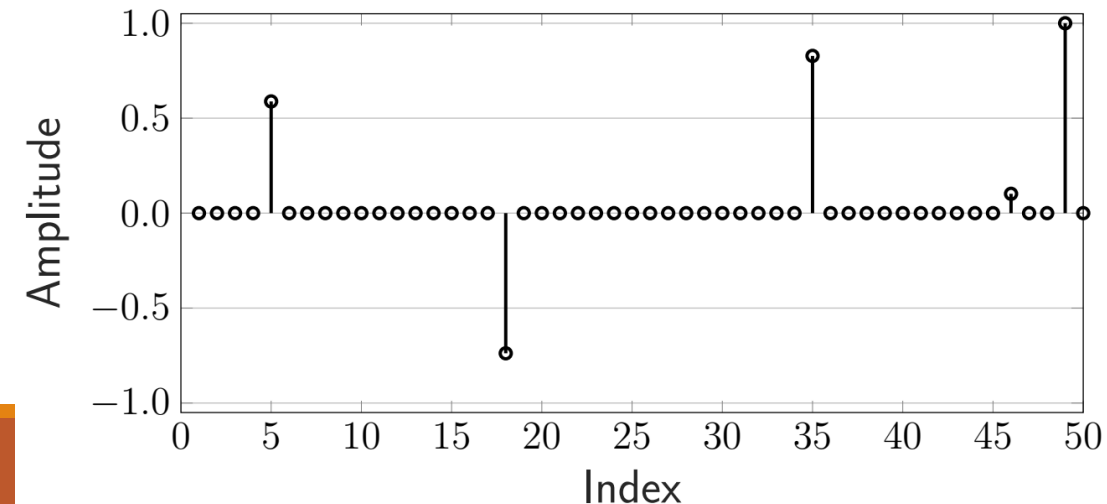
Introduction to Sparsity in Signal Processing (nyu.edu)

Lasso

True vs. Estimated Coefficients

Number of non-zero coefficients (Linear Regression): 50
Number of non-zero coefficients (Lasso Regression): 16
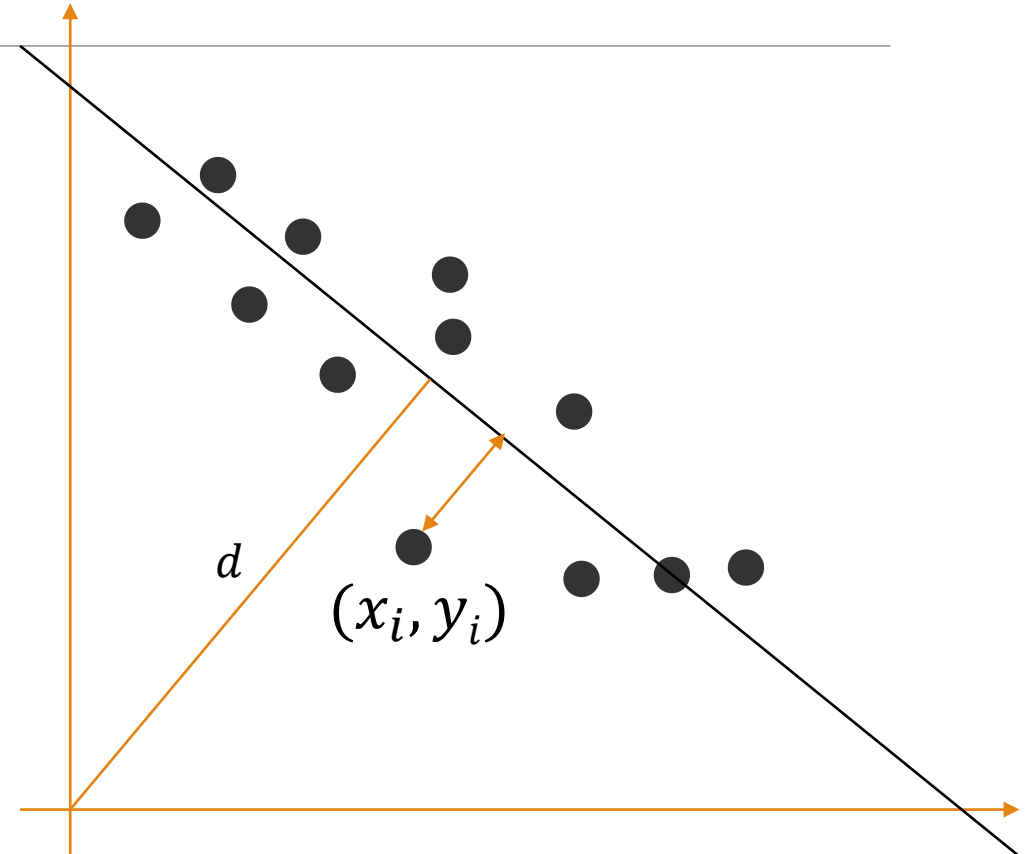True number of non-zero coefficients =10 and total number of coefficients =50

Total least squares (TLS)

➢ Equation of a line can be written as $ax + by = d$

➢ $a^2 + b^2 = 1$, where (a, b) is the unit normal to the line

➢ Distance between line and the origin is given as d

➢ Extension to 3d, $ax + by + cz = d$ and $a^2 + b^2 + c^2 = 1$

➢ Distance (perpendicular) from point to line is $\frac{|ax+by-d\,|}{\sqrt{a^2+b^2}}$

➢ Loss function:

$E = \sum_{i=1}^{n}(ax_i + by_i - d)^2$

$\widehat{a}, \widehat{b}, \widehat{d}, = \underset{a,b,d}{\text{arg min E}}$ ✖

$\widehat{a}, \widehat{b}, \widehat{d}, = \underset{a,b,d}{\text{arg min E}}$

such that $a^2 + b^2 = 1$

d

(x_i, y_i)

Total least squares (TLS)

➤Solve for d ➡ $\dfrac{\partial E}{\partial d} = 0$

$$E = \sum_{i=1}^{n}(ax_i + by_i - d)^2$$

$$\sum_{i=1}^{n} 2\,(ax_i + by_i - d)\ (-1) = 0$$

$$\sum_{i=1}^{n}(-ax_i - by_i + d) = 0$$

$$n\,d = \sum_{i=1}^{n}(ax_i + by_i)$$

$$d = \frac{a}{n}\sum_{i=1}^{n} x_i + \frac{b}{n}\sum_{i=1}^{n} y_i = a\bar{x} + b\bar{y}$$

$$E = \sum_{i=1}^{n}(a(x_i - \bar{x}) + b(y_i - \bar{y}))^2 = \left\| \begin{bmatrix} x_1 - \bar{x} & y_1 - \bar{y} \\ \vdots & \vdots \\ x_n - \bar{x} & y_n - \bar{y} \end{bmatrix} \begin{pmatrix} a \\ b \end{pmatrix} \right\|^2 = \|\boldsymbol{Xu}\|^2$$

Total least squares (TLS)

➢Optimization problem minimizes $\|Xu\|^2$ subject to $\|u\|^2 = 1$

➢Lagrangian function E(u, λ)= $\|Xu\|^2$ +λ ($\|u\|^2$-1) and λ is Lagrange multiplier

➢$\frac{\partial E}{\partial u} = 0, \Rightarrow 2\ X^\mathsf{T}(X\ u) + \lambda\ u$ =0 ➜($X^\mathsf{T}X$) u = - $\lambda\ u$

➢($X^\mathsf{T}X$) u = - $\lambda\ u$ Some thing familiar?

➢ u is the eigenvector of ($X^\mathsf{T}X$), if ($X^\mathsf{T}X$) is p by p vector and there can be p number of eigen vectors and eigen values (λ)

➢Which one should I pick?

➢$\frac{\partial E}{\partial \lambda} = 0$ ➜ $\|u\|^2$-1 => $\|u\|^2$ =1 already known.

➢($X^\mathsf{T}X$) u = - $\lambda\ u$ multiply both sides by u^T

➢u^T ($X^\mathsf{T}X$) u = - $\lambda\ u^\mathsf{T}u$

➢ ($u^\mathsf{T} X^\mathsf{T}$) ($X\ u$) = - λ any insight for picking value to value for λ ?

Total least squares (TLS)

➢ $(\boldsymbol{u}^\top \boldsymbol{X}^\top)\ (\boldsymbol{X}\ \boldsymbol{u})$ = - λ any insight for picking value to value for λ ?

➢ $\|\boldsymbol{X}\boldsymbol{u}\|^2$ = - λ, we need to minimize the $\|\mathbf{X}\mathbf{u}\|^2$.

➢ Pick a smallest eigen value.

➢ Solution: eigenvector of $(\boldsymbol{X}^\top\boldsymbol{X})$ associated with the smallest eigenvalue.

e.g., $\begin{bmatrix} 0.4 & 0.68 \\ 0.05 & 0.39 \end{bmatrix}$ for this matrix eigenvalues and eigenvectors are $[0.58\ \boxed{0.22}]$ and $\begin{bmatrix} 0.96 & \boxed{-0.96} \\ 0.25 & \boxed{0.26} \end{bmatrix}$

➢ LS assume that measurement errors primarily affect the dependent variable (the y-values).

➢ TLS consider both dependent and independent variables have measurement errors.

➢ TLS is less sensitive to outliers compared to traditional least squares.

TLS and LS
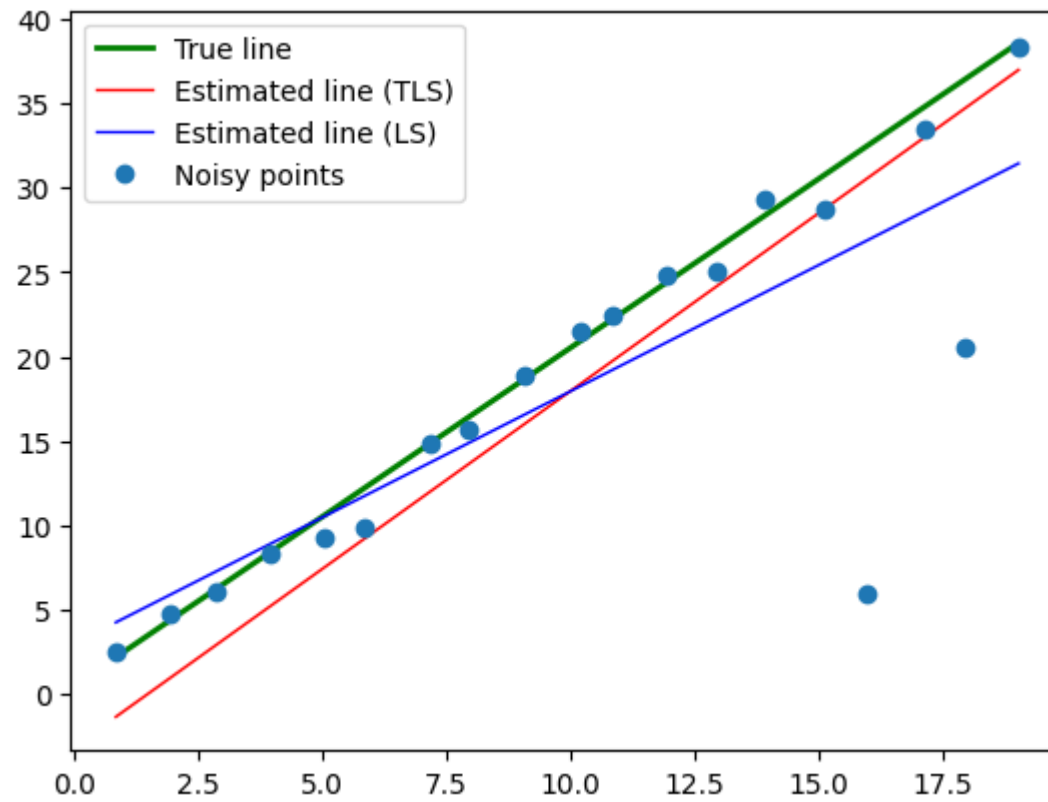
Self Study

➤ **RANSAC** (RANdom SAmple Consensus)

➤ Fischler, Martin A., and Robert C. Bolles. "Random sample consensus: a paradigm for model fitting with applications to image analysis and automated cartography." *Communications of the ACM* 24.6 (1981): 381-395.

➤ https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.RANSACRegressor.html

➤ Robust linear model estimation using RANSAC — scikit-learn 1.3.0 documentation

Thank You
Q & A