EE2211 Lecture 5: Least Squares and Linear Regression

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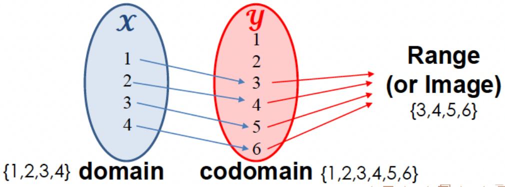
Some Basic Mathematical Notions : Sets

- A set S is an unordered collection of objects.
- $S = \{1, 2, 3, 4, 5, 6\}$ is the possible outcomes of the toss of a die.
- $S = [a, b] = \{x \in \mathbb{R} : a \leq x \leq b\}$ is the set of all numbers from a to b inclusive.
- $S = (a, b] = \{x \in \mathbb{R} : a < x \leq b\}$ is the set of all numbers from a to b, excluding a including b.
- $\mathbb{R}$ is the set of all real numbers.
- $\mathbb{R}^d$ is the set of all real vectors of length d

- A function f is a map from a set X to another set Y. We write this as
$$f : X \to Y.$$
- For example, the function $f : \mathbb{R} \to [0, \infty)$ could be given by the recipe $f(x) = x^2$.
- The set of inputs is called the domain; the set of possible outputs is called the codomain; the set $\{f(x) : x \in X\}$ is called the range (or image).
- For example $f : \{1, 2, 3, 4\} \to \{1, 2, 3, 4, 5, 6\}$ given by the recipe $f(x) = x + 2$ has codomain $\{1, 2, 3, 4, 5, 6\}$ and range $\{3, 4, 5, 6\}$.



Linear Functions

A function $f : \mathbb{R}^d \to \mathbb{R}$ is linear if it satisfies

- (Homogeneity) For any vector $\mathbf{x} \in \mathbb{R}^d$ and scalar $a \in \mathbb{R}$,

$$f(a\,\mathbf{x}) = a\,f(\mathbf{x})$$

- (Additivity) For any two vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$,

$$f(\mathbf{x}+\mathbf{y}) = f(\mathbf{x}) + f(\mathbf{y})$$

Note that a linear function $f : \mathbb{R}^d \to \mathbb{R}$ must pass through the origin, i.e., $f(\mathbf{0}) = 0$ where $\mathbf{0} \in \mathbb{R}^d$ is the zero vector in d dimensions. Why?

Linear Functions : Exercises I

Exercise: Show that if a function $f : \mathbb{R}^d \to \mathbb{R}$ is linear, then for any two vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$ and two scalars $a, b \in \mathbb{R}$, then

$$f(a\,\mathbf{x} + b\,\mathbf{y}) = a\,f(\mathbf{x}) + b\,f(\mathbf{y}).$$

Show also that if we have n vectors $\mathbf{x}_i \in \mathbb{R}^d, i = 1, \ldots, n$ and n scalars $a_i \in \mathbb{R}, i = 1, \ldots, n$, a linear function satisfies

$$f\left(\sum_{i=1}^{n} a_i\,\mathbf{x}_i\right) = \sum_{i=1}^{n} a_i\,f(\mathbf{x}_i).$$

Exercise: Let $f : \mathbb{R} \to \mathbb{R}$ be the absolute value function

$$f(x) = |x|.$$

Is f linear?

Linear Functions : Exercises II

Exercise: Fix a vector $\mathbf{a} \in \mathbb{R}^d$ and define the function $f : \mathbb{R}^d \to \mathbb{R}$ as

$$f(\mathbf{x}) = \mathbf{a}^\top \mathbf{x} = \sum_{i=1}^{d} a_i x_i.$$

This is called the inner product function. Show that f is linear.

Exercise: Fix a matrix $\mathbf{A} \in \mathbb{R}^{m \times d}$ and define the function $f : \mathbb{R}^d \to \mathbb{R}^m$ as

$$f(\mathbf{x}) = \mathbf{A}\mathbf{x}.$$

This is the regular matrix multiplication. Show that f is linear.

Affine Functions

- An affine function f is a linear function plus possibly a constant.
- More precisely, a function $f : \mathbb{R}^d \to \mathbb{R}$ is affine if it can be expressed as

$$f(\mathbf{x}) = \mathbf{a}^\top \mathbf{x} + b$$

for some vector $\mathbf{a} \in \mathbb{R}^d$ and some scalar $b \in \mathbb{R}$.
- The scalar b is called the bias or offset.

Example: The following function $f : \mathbb{R}^2 \to \mathbb{R}$ is affine. Why?

$$f(\mathbf{x}) = f(x_1, x_2) = -x_1 + 3x_2 + 7.$$

Exercise: Is a linear function affine? Is an affine function linear?

Linear and Affine Functions

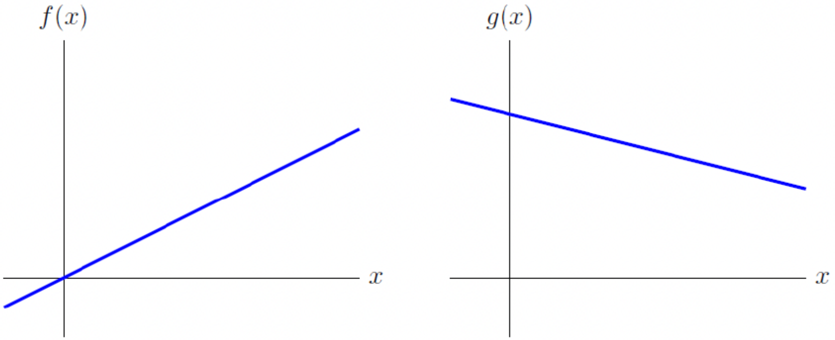


Figure 2.1 *Left.* The function f is linear. *Right.* The function g is affine, but not linear.

Local and Global Extrema

- Consider a function $f : [a,b] \to \mathbb{R}$.
- The function f has a local minimum at $c \in \mathbb{R}$ if

$$f(x) \geq f(c)$$

  for all x in an open neighborhood of c.
- The function f has a global minimum at $c \in \mathbb{R}$ if

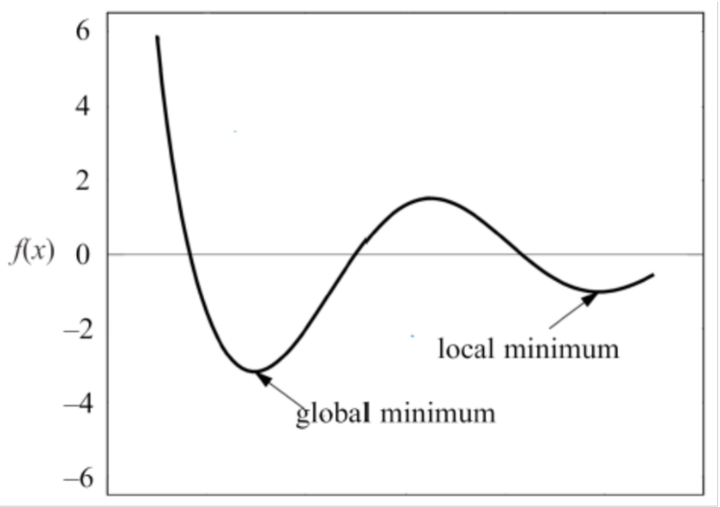
$$f(x) \geq f(c)$$

  for all $x \in [a,b]$.

Exercise: If c is a local minimum of f, is it a global minimum? If c is a global minimum of f, is it a local minimum?

Exercise: How would you define local maximum and global maximum?

Local and Global Extrema



$\min$ and $\arg\min$

- For a function $f : X \to Y$, the minimum $\min_{x\in X} f(x)$ returns the smallest value among all elements in the set $\{f(x) : x \in X\}$.
- For a function $f : X \to Y$, the argmin $x^* = \arg\min_{x\in X} f(x)$ returns the value of $x \in X$ that minimizes $f(x)$, i.e.,

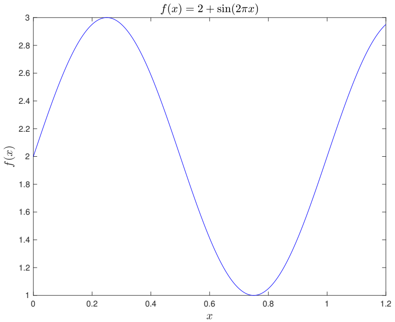
$$f(x^*) = \min_{x\in X} f(x)$$

- $\arg\min$ returns a value from the domain of the function X and $\min$ returns from the range (codomain) Y of the function.
- Let $X = \{0, 1\}$ and $f(0) = \pi$ and $f(1) = e$. Then

$$\arg\min_{x\in X} f(x) = 1 \qquad \min_{x\in X} f(x) = e,$$

and

$$\arg\max_{x\in X} f(x) = 0 \qquad \max_{x\in X} f(x) = \pi.$$



- Let $f : X = [0, 1.2] \to \mathbb{R}$ be defined as $f(x) = 2 + \sin(2\pi x)$ (see plot above). Then

$$\arg\min_{x \in X} f(x) = 3/4 \qquad \min_{x \in X} f(x) = +1$$

- Note that $f(3/4) = +1$.

Derivatives

- For a multivariable function $f : \mathbb{R}^d \to \mathbb{R}$, its gradient vector or derivative at $\mathbf{x} \in \mathbb{R}^d$ is the column vector

$$\nabla_{\mathbf{x}} f(\mathbf{x}) = \frac{\mathrm{d}f}{\mathrm{d}\mathbf{x}} = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} & \cdots & \frac{\partial f}{\partial x_d} \end{bmatrix}^\top$$

- Recall that $\frac{\partial f}{\partial x_i}$ is the partial derivative of f with respect to the scalar variable x_i.
- For example, if $f(x_1, x_2) = 2x_1^2 + 5x_1x_2 + 3x_2^3$, then

$$\frac{\partial f}{\partial x_1} = 4x_1 + 5x_2 \quad \text{and} \quad \frac{\partial f}{\partial x_2} = 5x_1 + 9x_2^2.$$

Important Derivatives

- There are only two derivatives for functions $f : \mathbb{R}^d \to \mathbb{R}$ that take vectors to scalars you need to know for now.
- For a fixed vector $\mathbf{a} \in \mathbb{R}^d$, consider $f(\mathbf{x}) = \mathbf{a}^\top \mathbf{x}$ (known as the inner or dot product). Then
$$\nabla_{\mathbf{x}} f(\mathbf{x}) = \mathbf{a}.$$
- For a fixed matrix $\mathbf{A} \in \mathbb{R}^{d\times d}$, consider $f(\mathbf{x}) = \mathbf{x}^\top \mathbf{A}\mathbf{x}$ (known as the quadratic form). Then
$$\nabla_{\mathbf{x}} f(\mathbf{x}) = (\mathbf{A} + \mathbf{A}^\top)\mathbf{x}.$$
- In most applications, $\mathbf{A}$ is a symmetric matrix (i.e., $\mathbf{A} = \mathbf{A}^\top$) so
$$\nabla_{\mathbf{x}} f(\mathbf{x}) = 2\mathbf{A}\mathbf{x}.$$
- This generalizes the basic fact that if $f(x) = ax^2$, then $\frac{\mathrm{d}f}{\mathrm{d}x} = 2ax$.

Important Derivatives

Exercise: Show from the definition of $f(\mathbf{x}) = \mathbf{a}^\top \mathbf{x}$ that

$$\nabla_{\mathbf{x}} f(\mathbf{x}) = \mathbf{a}.$$

Exercise: Show from the definition of $f(\mathbf{x}) = \mathbf{x}^\top \mathbf{A}\mathbf{x}$ that

$$\nabla_{\mathbf{x}} f(\mathbf{x}) = (\mathbf{A} + \mathbf{A}^\top)\mathbf{x}.$$

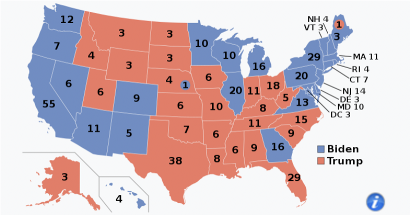
You'll be forgiven for having to exhibit a substantial amount of meticulous bookkeeping here.

Advice: It is difficult to remember a lot of derivative formulae of complicated multivariate functions. Usually, one consults the Matrix Cookbook

https://www2.imm.dtu.dk/pubdb/edoc/imm3274.pdf

Motivation for Linear Regression

- When I first taught this module in the Fall of 2020, we were in the midst of Covid sans vaccines, but there was another important global event.
- It was the 2020 United States presidential election, pitting the incumbent Republican Donald J. Trump against Democrat challenger Joseph R. Biden.



- Could we have used historical trends to predict who will win and by how much?

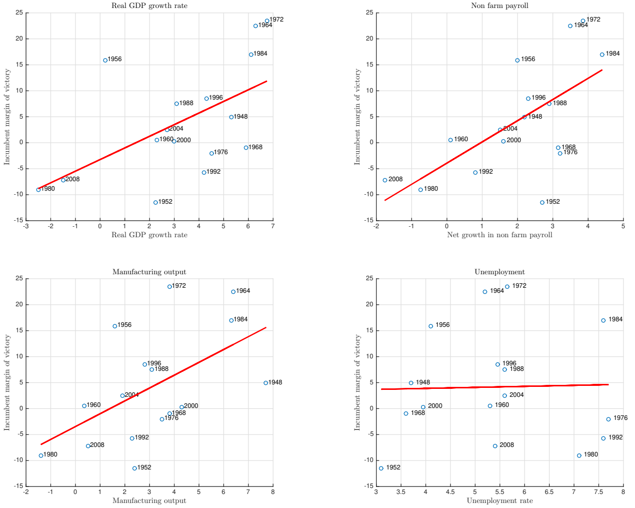
Motivation for Linear Regression

- Consider four economic indicators:
  (a) Real GDP growth rate x_1;
  (b) Change in non-farm payrolls x_2;
  (c) ISM (Institute of Supply Management) manufacturing index x_3;
  (d) Unemployment rate x_4.
- Which factor is the most important for determining the incumbent's winning margin?
- Data obtained from Nate Silver's blog at the New York Times.
- Data is of the form

$$\mathbf{x}_i = \begin{bmatrix} x_{i,1} \\ x_{i,2} \\ x_{i,3} \\ x_{i,4} \end{bmatrix} \quad \text{and} \quad y_t \quad \text{for} \quad i \in \{1948, 1952, \ldots, 2008\}$$

where $x_{i,1}$ is the real GDP growth rate in election in year i (etc.) and y_i is the incumbent's winning margin.

Motivation for Linear Regression



Scatter plots of incumbent's victory margin against various economic factors

Linear Regression

- Linear regression is a linear approach for modelling the relationship between a scalar response y and one or more explanatory variables (or attributes, or features) $\mathbf{x}$.
- We have a dataset $\{(\mathbf{x}_i, y_i) : i = 1, \ldots, m\}$ where $\mathbf{x}_i \in \mathbb{R}^d$ and $y_i \in \mathbb{R}$ are the feature vector and target of the i-th sample respectively.
- Without the offset, we can form the design matrix and the target vector

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^\top \\ \mathbf{x}_2^\top \\ \vdots \\ \mathbf{x}_m^\top \end{bmatrix} = \begin{bmatrix} x_{1,1} & x_{1,2} & \ldots & x_{1,d} \\ x_{2,1} & x_{2,2} & \ldots & x_{2,d} \\ \vdots & \vdots & \ddots & \vdots \\ x_{m,1} & x_{m,2} & \ldots & x_{m,d} \end{bmatrix} \in \mathbb{R}^{m \times d} \qquad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} \in \mathbb{R}^m$$

- We wish to find $\mathbf{w} \in \mathbb{R}^d$ satisfying (or approximately satisfying) the linear system

$$\mathbf{X}\mathbf{w} = \mathbf{y}.$$

Linear Regression (With Offset)

- m: size of the dataset
- d: dimension/length of each feature vector (input)
- y_i: scalar or real-valued target/output (e.g., height, exam marks)

Goal:

- Design a function/model/regressor $f_{\mathbf{w},b}$ as a linear combination of the features in $\mathbf{x}$, i.e.,

$$f_{\mathbf{w},b}(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b,$$

  where $\mathbf{w} \in \mathbb{R}^d$, the unknown, is the d-dimensional weight vector and b is the bias or offset.
- The notation $f_{\mathbf{w},b}$ means that the model is parametrized by two quantities $\mathbf{w}$ and b.
- Note that the model can also be more compactly written as

$$f_{\mathbf{w},b}(\mathbf{x}) = \begin{bmatrix} b \\ \mathbf{w} \end{bmatrix}^\top \begin{bmatrix} 1 \\ \mathbf{x} \end{bmatrix}.$$

Objective (Loss) Function in Linear Regression

- We wish to minimize the error e_i between the prediction $f_{\mathbf{w},b}(\mathbf{x}_i)$ and the target, where

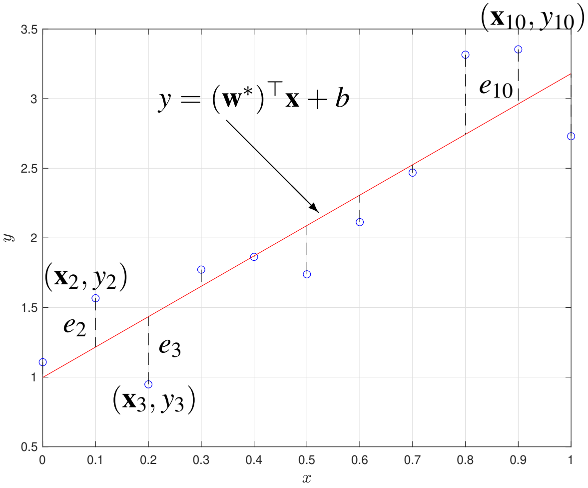
$$e_i = f_{\mathbf{w},b}(\mathbf{x}_i) - y_i$$

- We average the square of the errors over all training samples. This defines the objective or loss function

$$\mathrm{Loss}(\mathbf{w}, b) = \frac{1}{m} \sum_{i=1}^{m} (f_{\mathbf{w},b}(\mathbf{x}_i) - y_i)^2$$

- $\mathrm{Loss}(\mathbf{w}, b)$ is known as the (squared or ℓ_2) loss or objective function
- $(f_{\mathbf{w},b}(\mathbf{x}_i) - y_i)^2$ is also called the per-sample loss or objective function and is a measure of the difference or penalty between the prediction $f_{\mathbf{w},b}(\mathbf{x}_i)$ and the target y_i

Objective (Loss) Function in Linear Regression



Linear Regression: Minimize the sum of squares of the errors e_i, i.e. $\sum_{i=1}^{11} e_i^2$.
Note that here $\mathbf{x}$ is a scalar, but in general $\mathbf{x}$ can be a vector

Objective (Loss) Function in Linear Regression

- Define $\overline{\mathbf{w}} \in \mathbb{R}^{d+1}$ as the $(d+1)$-dimensional vector that concatenates b and $\mathbf{w}$, i.e.,

$$\overline{\mathbf{w}} = \begin{bmatrix} b \\ \mathbf{w} \end{bmatrix} = \begin{bmatrix} b \\ w_1 \\ w_2 \\ \vdots \\ w_d \end{bmatrix}.$$

- Similarly, define $\bar{\mathbf{x}}_i \in \mathbb{R}^{d+1}$ as the $(d+1)$-dimensional vector that concatenates 1 and $\mathbf{x}_i$

$$\overline{\mathbf{x}}_i = \begin{bmatrix} 1 \\ \mathbf{x}_i \end{bmatrix} = \begin{bmatrix} 1 \\ x_{i,1} \\ x_{i,2} \\ \vdots \\ x_{i,d} \end{bmatrix}.$$

Objective (Loss) Function in Linear Regression

- We wish to find $\overline{\mathbf{w}}^* = [b^*, \mathbf{w}^*]^\top \in \mathbb{R}^{d+1}$ that minimizes

$$\overline{\mathbf{w}}^* = \operatorname*{arg\,min}_{\overline{\mathbf{w}}=[b,\mathbf{w}]^\top} \mathrm{Loss}(\mathbf{w}, b)$$

  where the ℓ_2 or squared loss is

$$\mathrm{Loss}(\mathbf{w}, b) = \frac{1}{m} \sum_{i=1}^{m} \left(f_{\mathbf{w},b}(\mathbf{x}_i) - y_i\right)^2$$

- The $1/m$ does not affect the solution so we can choose to include or exclude it.

Objective (Loss) Function in Linear Regression

- Note that
$$f_{\mathbf{w},b}(\mathbf{x}_i) - y_i = \begin{bmatrix} 1 \\ \mathbf{x}_i \end{bmatrix}^\top \begin{bmatrix} b \\ \mathbf{w} \end{bmatrix} - y_i = \overline{\mathbf{x}}_i^\top \overline{\mathbf{w}} - y_i,$$
so that
$$\sum_{i=1}^m (f_{\mathbf{w},b}(\mathbf{x}_i) - y_i)^2 = \sum_{i=1}^m \left(\overline{\mathbf{x}}_i^\top \overline{\mathbf{w}} - y_i\right)^2.$$
In other words,
$$\sum_{i=1}^m (f_{\mathbf{w},b}(\mathbf{x}_i) - y_i)^2 = (\mathbf{X}\overline{\mathbf{w}} - \mathbf{y})^\top (\mathbf{X}\overline{\mathbf{w}} - \mathbf{y})$$
- The design matrix is now the $m \times (d+1)$ matrix
$$\mathbf{X} = \begin{bmatrix} \overline{\mathbf{x}}_1^\top \\ \overline{\mathbf{x}}_2^\top \\ \vdots \\ \overline{\mathbf{x}}_m^\top \end{bmatrix} = \begin{bmatrix} 1 & \mathbf{x}_1^\top \\ 1 & \mathbf{x}_2^\top \\ \vdots & \vdots \\ 1 & \mathbf{x}_m^\top \end{bmatrix} = \begin{bmatrix} 1 & x_{1,1} & x_{1,2} & \dots & x_{1,d} \\ 1 & x_{2,1} & x_{2,2} & \dots & x_{2,d} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{m,1} & x_{m,2} & \dots & x_{m,d} \end{bmatrix} \in \mathbb{R}^{m\times(d+1)}$$

Optimizing the Loss Function in Linear Regression

- The objective function is now simplified to

$$\begin{aligned} J(\overline{\mathbf{w}}) &= (\mathbf{X}\overline{\mathbf{w}} - \mathbf{y})^\top (\mathbf{X}\overline{\mathbf{w}} - \mathbf{y}) \\ &= \overline{\mathbf{w}}^\top \mathbf{X}^\top \mathbf{X}\overline{\mathbf{w}} - \overline{\mathbf{w}}^\top \mathbf{X}^\top \mathbf{y} - \mathbf{y}^\top \mathbf{X}\overline{\mathbf{w}} + \mathbf{y}^\top \mathbf{y} \\ &= \overline{\mathbf{w}}^\top \mathbf{X}^\top \mathbf{X}\overline{\mathbf{w}} - 2\overline{\mathbf{w}}^\top (\mathbf{X}^\top \mathbf{y}) + \mathbf{y}^\top \mathbf{y} \end{aligned}$$

  The terms in blue are the same. Why?
- Differentiating this w.r.t. $\overline{\mathbf{w}}$ (see the rules on slide 14),

$$\nabla_{\overline{\mathbf{w}}} J(\overline{\mathbf{w}}) = 2\mathbf{X}^\top \mathbf{X}\overline{\mathbf{w}} - 2\mathbf{X}^\top \mathbf{y}.$$

- Setting this to zero yields

$$2\mathbf{X}^\top \mathbf{X}\overline{\mathbf{w}}^* = 2\mathbf{X}^\top \mathbf{y}.$$

- If $\mathbf{X}$ has full column rank, $\mathbf{X}^\top \mathbf{X}$ is invertible and

$$\overline{\mathbf{w}}^* = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}.$$

  This is the least squares solution. Is it a global or local minimum?

Least Squares : Training and Prediction

- In summary, given a dataset $(\mathbf{x}_i, y_i)$ for $i = 1, 2, \ldots, m$, form the design matrix and target vector

$$\mathbf{X} = \begin{bmatrix} \overline{\mathbf{x}}_1^\top \\ \overline{\mathbf{x}}_2^\top \\ \vdots \\ \overline{\mathbf{x}}_m^\top \end{bmatrix} = \begin{bmatrix} 1 & \mathbf{x}_1^\top \\ 1 & \mathbf{x}_2^\top \\ \vdots & \vdots \\ 1 & \mathbf{x}_m^\top \end{bmatrix} \in \mathbb{R}^{m\times(d+1)} \quad \text{and} \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} \in \mathbb{R}^m$$

- Training/Learning:

$$\overline{\mathbf{w}}^* = \begin{bmatrix} b^* \\ \mathbf{w}^* \end{bmatrix} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}.$$

- Prediction/Testing: Given a new training sample $\mathbf{x}_{\text{new}}$,

$$\hat{y}_{\text{new}} = \begin{bmatrix} 1 \\ \mathbf{x}_{\text{new}} \end{bmatrix}^\top \overline{\mathbf{w}}^* = b^* + \mathbf{x}_{\text{new}}^\top \mathbf{w}^*.$$

Linear Regression: Example 1

- Dataset $(\mathbf{x}_i, y_i), i = 1, 2, 3, 4$ includes the samples

$$\mathbf{x}_1 = -7, \quad \mathbf{x}_2 = -5, \quad \mathbf{x}_3 = 1, \quad \mathbf{x}_4 = 5$$
$$y_1 = -6, \quad y_2 = -4, \quad y_3 = -1, \quad y_4 = 4$$

- Here, $m = 4$ and $d = 1$.
- Design matrix and target vector are

$$\mathbf{X} = \begin{bmatrix} 1 & -7 \\ 1 & -5 \\ 1 & 1 \\ 1 & 5 \end{bmatrix} \quad \text{and} \quad \mathbf{y} = \begin{bmatrix} -6 \\ -4 \\ -1 \\ 4 \end{bmatrix}$$

- The linear system $\mathbf{X}\overline{\mathbf{w}} = \mathbf{y}$ is overdetermined and there is no solution for $\overline{\mathbf{w}}$ because

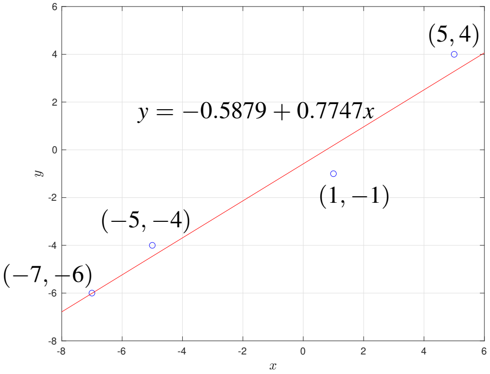
$$\operatorname{rank}(\mathbf{X}) < \operatorname{rank}(\tilde{\mathbf{X}}).$$

Linear Regression: Example 1 (Training)

- Using some numerical software, we can find

$$\overline{\mathbf{w}}^* = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y} = \begin{bmatrix} -0.5879 \\ 0.7747 \end{bmatrix}$$

- We can plot the points and the least squares line.

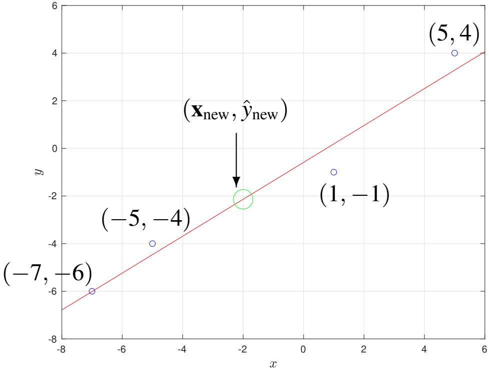


Linear Regression: Example 1 (Prediction)

- Suppose we want to predict the value of y_{new} when $\mathbf{x}_{\text{new}} = -2$. Then we plug $\mathbf{x}_{\text{new}} = -2$ into model to get

$$\hat{y}_{\text{new}} = \begin{bmatrix} 1 \\ \mathbf{x}_{\text{new}} \end{bmatrix}^{\top} \overline{\mathbf{w}}^* = 1 \times (-0.5879) + (-2) \times (0.7747) = -2.1374$$

- Pictorially,



Linear Regression: Example 2

- Now our feature vectors are

$$\mathbf{x}_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \quad \mathbf{x}_2 = \begin{bmatrix} -1 \\ 1 \end{bmatrix} \quad \mathbf{x}_3 = \begin{bmatrix} 1 \\ 3 \end{bmatrix} \quad \mathbf{x}_4 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

and targets are

$$y_1 = 1 \quad y_2 = 0 \quad y_3 = 2 \quad y_4 = -1.$$

- The design matrix and target vector are

$$\mathbf{X} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & 3 \\ 1 & 1 & 0 \end{bmatrix} \quad \text{and} \quad \mathbf{y} = \begin{bmatrix} 1 \\ 0 \\ 2 \\ -1 \end{bmatrix}.$$

- Note that $3 = \mathrm{rank}(\mathbf{X}) < \mathrm{rank}(\tilde{\mathbf{X}}) = 4$ so the overdetermined system does not have a solution.

Linear Regression: Example 2 (Training & Prediction)

- But we can check that $\mathbf{X}$ has full column rank and so the least squares solution exists and is given by

$$\overline{\mathbf{w}}^* = \begin{bmatrix} b^* \\ \mathbf{w}^* \end{bmatrix} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y} = \begin{bmatrix} -0.7500 \\ 0.1786 \\ 0.9286 \end{bmatrix}$$

  This is the training or learning step.

- If we want to make predictions for $\mathbf{x}_{\text{new}} = [0, -1]^\top$, we use the model

$$\hat{y}_{\text{new}} = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}^\top \overline{\mathbf{w}}^* = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}^\top \begin{bmatrix} -0.7500 \\ 0.1786 \\ 0.9286 \end{bmatrix} = -1.6786.$$

  This is the prediction step. [Python Demo]

Learning Vector-Valued Linear Functions

- Suppose we want to predict:
  1. Donald Trump's winning margin;
  2. The number of number of house seats won by Republicans;
  3. The number of incumbent governors that retain their governorships.
- Suppose there are h outputs we want to predict (above $h = 3$).
- Given a dataset $\{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^m$ where $\mathbf{x}_i \in \mathbb{R}^d$ (column vector) and $\mathbf{y}_i \in \mathbb{R}^{1\times h}$ (row vector), the model to be used is

$$\underbrace{\begin{bmatrix} y_{1,1} & \dots & y_{1,h} \\ y_{2,1} & \dots & y_{2,h} \\ \vdots & \ddots & \vdots \\ y_{m,1} & \dots & y_{m,h} \end{bmatrix}}_{\mathbf{Y}\in\mathbb{R}^{m\times h}} = \underbrace{\begin{bmatrix} 1 & x_{1,1} & \dots & x_{1,d} \\ 1 & x_{2,1} & \dots & x_{2,d} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{m,1} & \dots & x_{m,d} \end{bmatrix}}_{\mathbf{X}\in\mathbb{R}^{m\times(d+1)}} \underbrace{\begin{bmatrix} b_1 & b_2 & \dots & b_h \\ w_{1,1} & w_{1,2} & \dots & w_{1,h} \\ \vdots & \vdots & \ddots & \vdots \\ w_{d,1} & w_{d,2} & \dots & w_{d,h} \end{bmatrix}}_{\overline{\mathbf{W}}\in\mathbb{R}^{(d+1)\times h}}$$

- When $h = 1$, this particularizes to standard linear regression.
- This is exactly h separate linear regression problems.

Learning Vector-Valued Linear Functions: Objective

- Our loss function is a generalization of the previous study

$$\mathrm{Loss}(\overline{\mathbf{W}}) = \mathrm{Loss}(\mathbf{W}, \mathbf{b}) = \sum_{k=1}^{h} (\mathbf{X}\overline{\mathbf{w}}_k - \mathbf{y}^{(k)})^\top (\mathbf{X}\overline{\mathbf{w}}_k - \mathbf{y}^{(k)})$$

  where for each $1 \le k \le h$,

$$\overline{\mathbf{w}}_k = \begin{bmatrix} b_k \\ w_{1,k} \\ \vdots \\ w_{d,k} \end{bmatrix} \in \mathbb{R}^{d+1} \quad \text{and} \quad \mathbf{y}^{(k)} = \begin{bmatrix} y_{1,k} \\ y_{2,k} \\ \vdots \\ y_{m,k} \end{bmatrix} \in \mathbb{R}^{m}$$

  are the k-th columns of $\mathbf{W}$ and $\mathbf{Y}$ respectively.

- We are aggregating or summing the contributions of the errors from each of the h prediction tasks.
- Our goal is to find

$$\overline{\mathbf{W}}^* = \arg\min_{\mathbf{W},\mathbf{b}} \mathrm{Loss}(\overline{\mathbf{W}}) \quad \text{where} \quad \overline{\mathbf{W}} = \begin{bmatrix} \mathbf{b}^\top \\ \mathbf{W} \end{bmatrix}.$$

Learning Vector-Valued Linear Functions: Training

- Objective:

$$\overline{\mathbf{W}}^* = \arg\min_{\mathbf{W},\mathbf{b}} \mathrm{Loss}(\overline{\mathbf{W}}) \quad \text{where} \quad \overline{\mathbf{W}} = \begin{bmatrix} \mathbf{b}^\top \\ \mathbf{W} \end{bmatrix}.$$

- By differentiating with respect to each column $\overline{\mathbf{w}}_k$ and setting the result to zero, we find that the least squares solution is

$$\overline{\mathbf{W}}^* = \begin{bmatrix} \overline{\mathbf{w}}_1^* & \overline{\mathbf{w}}_2^* & \ldots & \overline{\mathbf{w}}_h^* \end{bmatrix} = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{Y} \in \mathbb{R}^{(d+1)\times h}.$$

  This will be an exercise in a tutorial.
- In this new setting, what condition does $\mathbf{X}$ have to satisfy for $\overline{\mathbf{W}}^*$ to exist?
- We need $(\mathbf{X}^\top\mathbf{X})^{-1}$ to exist, which means that $\mathbf{X}$ has to have full column rank.

Learning Vector-Valued Linear Functions: Prediction

- Given a dataset $\{(\mathbf{x}_i, \mathbf{y}_i)\}$ where $\mathbf{x}_i \in \mathbb{R}^d$ and $\mathbf{y}_i \in \mathbb{R}^{1\times h}$ and $1 \le i \le m$, we can use the above procedure to learn the least squares solution

$$\overline{\mathbf{W}}^* = \begin{bmatrix} \overline{\mathbf{w}}_1^* & \overline{\mathbf{w}}_2^* & \dots & \overline{\mathbf{w}}_h^* \end{bmatrix} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{Y} \in \mathbb{R}^{(d+1)\times h}.$$

- Given a new sample $\mathbf{x}_{\text{new}} \in \mathbb{R}^d$, the predictions are contained in the row vector

$$\hat{\mathbf{y}}_{\text{new}} = \begin{bmatrix} 1 \\ \mathbf{x}_{\text{new}} \end{bmatrix}^\top \overline{\mathbf{W}}^* \in \mathbb{R}^{1\times h}$$

Linear Regression: Example 3

- Now our feature vectors are

$$\mathbf{x}_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \quad \mathbf{x}_2 = \begin{bmatrix} -1 \\ 1 \end{bmatrix} \quad \mathbf{x}_3 = \begin{bmatrix} 1 \\ 3 \end{bmatrix} \quad \mathbf{x}_4 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

  and targets are

$$\mathbf{y}_1 = \begin{bmatrix} 1 & 0 \end{bmatrix} \quad \mathbf{y}_2 = \begin{bmatrix} 0 & 1 \end{bmatrix} \quad \mathbf{y}_3 = \begin{bmatrix} 2 & -1 \end{bmatrix} \quad \mathbf{y}_4 = \begin{bmatrix} -1 & 3 \end{bmatrix}$$

- Here, $m = 4$, $d = 2$, $h = 2$.
- The design matrix and target matrix are

$$\mathbf{X} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & 3 \\ 1 & 1 & 0 \end{bmatrix} \quad \text{and} \quad \mathbf{Y} = \begin{bmatrix} 1 & 1 \\ 0 & 1 \\ 2 & -1 \\ -1 & 3 \end{bmatrix}.$$

- Note that the first regression problem here (corresponding to the first components of each $\mathbf{y}_i$) is exactly the same as that in Linear Regression Example 2 on Slide 31.

Linear Regression: Example 4 (Training & Prediction)

- We have already checked that $\mathbf{X}$ has full column rank. Hence, the least squares solution is

$$\overline{\mathbf{W}}^* = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{Y} = \begin{bmatrix} -0.7500 & 2.2500 \\ 0.1786 & 0.0357 \\ 0.9286 & 1.2143 \end{bmatrix} \in \mathbb{R}^{(d+1)\times h}.$$

- Now, someone gave us a new sample $\mathbf{x}_{\text{new}} = [0, -1]^\top$. The predicted output is

$$\hat{\mathbf{y}}_{\text{new}} = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}^\top \overline{\mathbf{W}}^* = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}^\top \begin{bmatrix} -0.7500 & 2.2500 \\ 0.1786 & 0.0357 \\ 0.9286 & 1.2143 \end{bmatrix} = \begin{bmatrix} -1.6786 & 3.4643 \end{bmatrix}$$

  The first prediction -1.6786 corresponds to that in Linear Regression Example 2 on Slide 32.

- This is the **prediction** step. [Python Demo]

Summary

- (Learning/Training) Given a dataset $\{(\mathbf{x}_i, y_i)\}_{i=1}^m$ where $\mathbf{x}_i \in \mathbb{R}^d$ and $y_i \in \mathbb{R}$, the least squares solution (with offset) is

$$\overline{\mathbf{w}}^* = \begin{bmatrix} b^* \\ \mathbf{w}^* \end{bmatrix} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y} \in \mathbb{R}^{d+1}$$

where

$$\mathbf{X} = \begin{bmatrix} \overline{\mathbf{x}}_1^\top \\ \overline{\mathbf{x}}_2^\top \\ \vdots \\ \overline{\mathbf{x}}_m^\top \end{bmatrix} = \begin{bmatrix} 1 & \mathbf{x}_1^\top \\ 1 & \mathbf{x}_2^\top \\ \vdots & \vdots \\ 1 & \mathbf{x}_m^\top \end{bmatrix} \in \mathbb{R}^{m \times (d+1)} \quad \text{and} \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} \in \mathbb{R}^m.$$

- (Prediction/Testing) Given a new feature vector (sample, example) $\mathbf{x}_{\text{new}}$, the prediction based on the least squares solution is

$$\hat{y}_{\text{new}} = \begin{bmatrix} 1 \\ \mathbf{x}_{\text{new}} \end{bmatrix}^\top \overline{\mathbf{w}}^* = b^* + \mathbf{x}_{\text{new}}^\top \mathbf{w}^*.$$