10-301/601: Introduction to Machine Learning Lecture 7 – Linear Regression

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5/30/23

Front Matter

- Announcements:
  - PA2 released 5/25, due 6/01 at 11:59 PM
- Recommended Readings:
  - Murphy, Chapters 7.1-7.3

Recall: Regression

- Learning to diagnose heart disease

  as a **(supervised)** **<u>regression</u> task**

features / targets

data points

x_1 Family History	x_2 Resting Blood Pressure	x_3 Cholesterol	y Heart Disease?
Yes	Low	Normal	\$0
No	Medium	Normal	\$20
No	Low	Abnormal	\$30
Yes	Medium	Normal	\$100
Yes	High	Abnormal	\$5000

Decision Tree Regression

- Learning to diagnose heart disease

  as a **(supervised)** **regression task**

features | targets

data points

x_1 Family History	x_2 Resting Blood Pressure	x_3 Cholesterol	y Heart Disease?
Yes	Low	Normal	\$0
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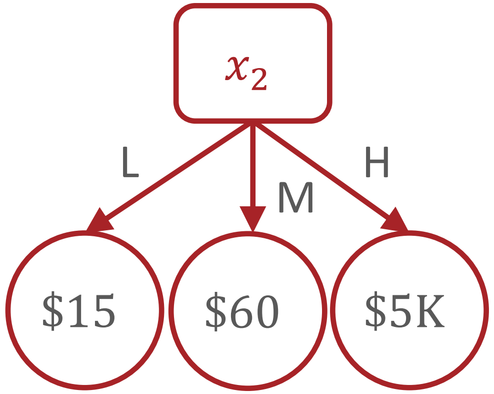
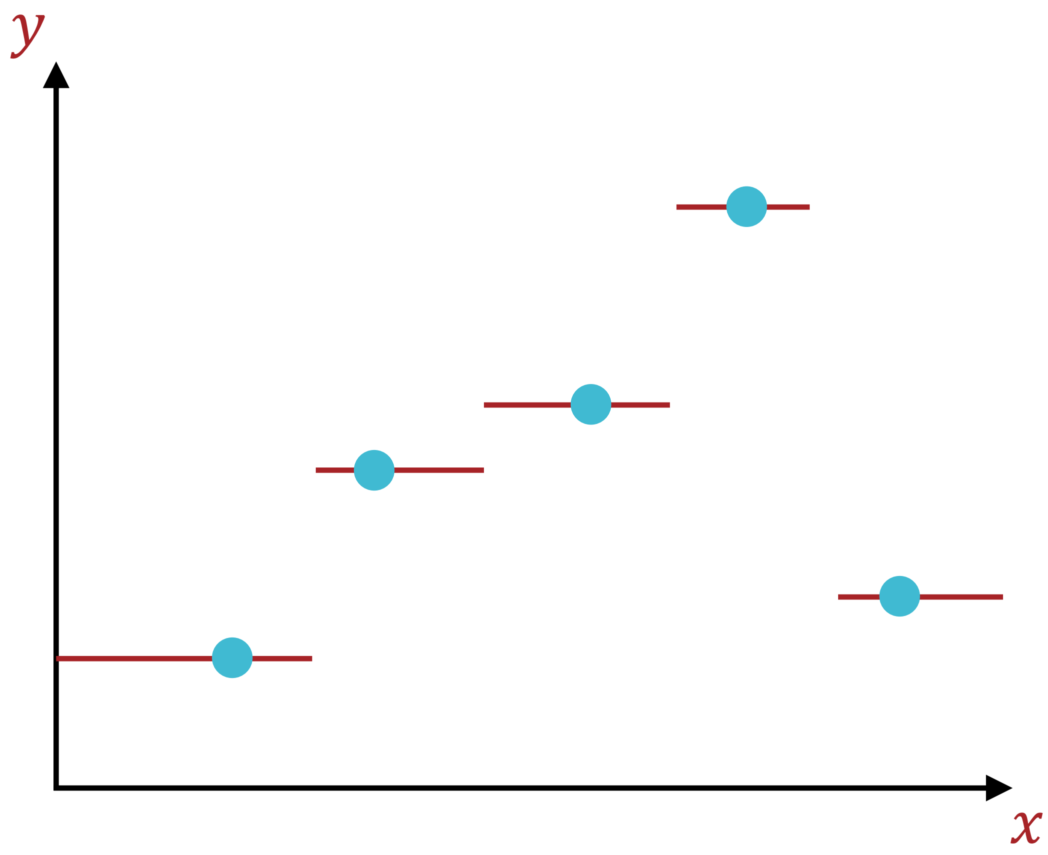
Yes	Medium	Normal	\$100
Yes	High	Abnormal	\$5000



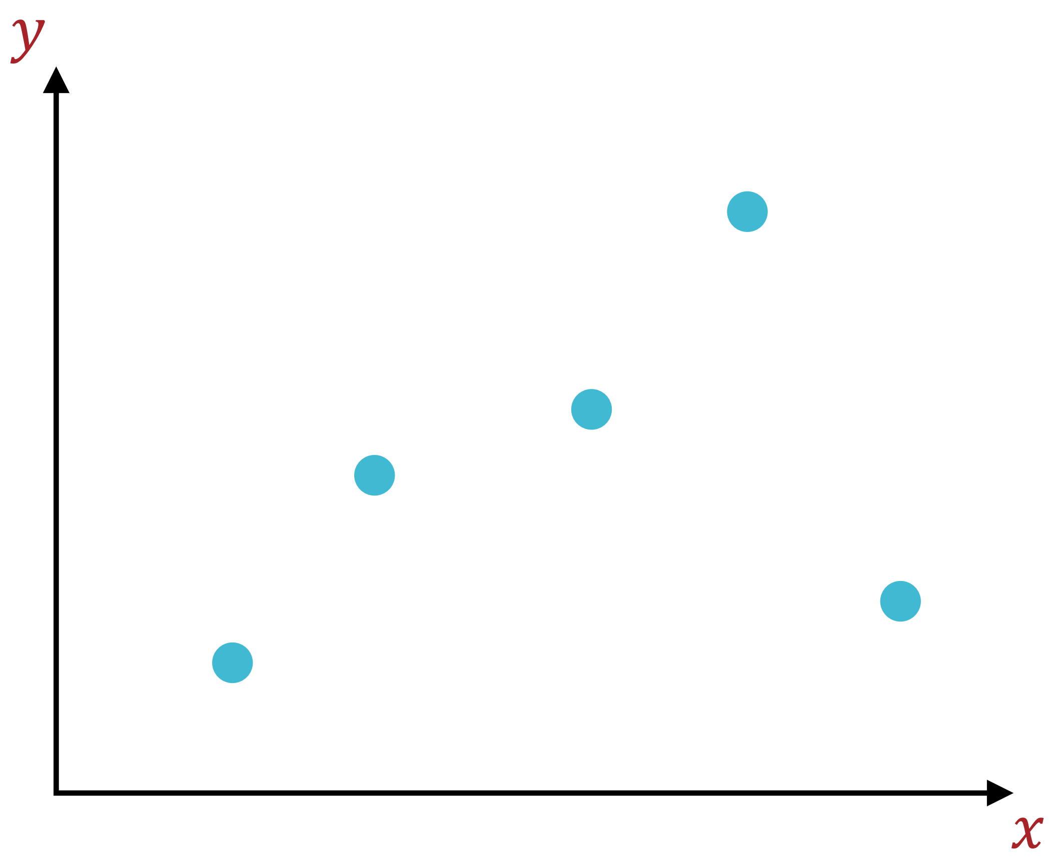
1-NN Regression

- Suppose we have real-valued targets $y \in \mathbb{R}$ and one-dimensional inputs $x \in \mathbb{R}$



2-NN Regression?

- Suppose we have real-valued targets $y \in \mathbb{R}$ and one-dimensional inputs $x \in \mathbb{R}$



Linear Regression

- Suppose we have real-valued targets $y \in \mathbb{R}$ and D-dimensional inputs $\boldsymbol{x} = [\quad x_1, \dots, x_D]^T \in \mathbb{R}^D$
- **Assume**

$$y = \boldsymbol{w}^T \boldsymbol{x} + w_0$$

Linear Regression

- Suppose we have real-valued targets $y \in \mathbb{R}$ and D-dimensional inputs $\boldsymbol{x} = [1, x_1, \ldots, x_D]^T \in \mathbb{R}^{D+1}$
- **Assume**

$$y = \boldsymbol{w}^T \boldsymbol{x}$$

General Recipe for Machine Learning

- Define a model and model parameters
- Write down an objective function
- Optimize the objective w.r.t. the model parameters

Recipe for Linear Regression

- Define a model and model parameters
  - Assume $y = \boldsymbol{w}^T \boldsymbol{x}$
  - Parameters: $\boldsymbol{w} = [w_0, w_1, \dots, w_D]$
- Write down an objective function
  - Minimize the squared error

$$\ell_{\mathcal{D}}(\boldsymbol{w}) = \sum_{n=1}^{N} \left(\boldsymbol{w}^T \boldsymbol{x}^{(n)} - y^{(n)}\right)^2$$

- Optimize the objective w.r.t. the model parameters
  - Solve in *closed form*: take partial derivatives, set to 0 and solve

Minimizing the Squared Error

$$\ell_{\mathcal{D}}(\boldsymbol{w}) = \sum_{n=1}^{N} \left(\boldsymbol{w}^T \boldsymbol{x}^{(n)} - y^{(n)}\right)^2$$

$$= \sum_{n=1}^{N} \left(\sum_{d=0}^{D} w_d x_d^{(n)} - y^{(n)}\right)^2$$

$$\frac{\partial \ell_{\mathcal{D}}(\boldsymbol{w})}{\partial w_d} = \sum_{n=1}^{N} 2 \left(\sum_{d=0}^{D} w_d x_d^{(n)} - y^{(n)}\right) \frac{\partial}{\partial w_d} \left(\sum_{d=0}^{D} w_d x_d^{(n)} - y^{(n)}\right)$$

$$= \sum_{n=1}^{N} 2 \left(\sum_{d=0}^{D} w_d x_d^{(n)} - y^{(n)}\right) x_d^{(n)}$$

Recipe for Linear Regression

- Define a model and model parameters
  - Assume $y = \boldsymbol{w}^T \boldsymbol{x}$
  - Parameters: $\boldsymbol{w} = [w_0, w_1, \dots, w_D]$
- Write down an objective function
  - Minimize the squared error

$$\ell_{\mathcal{D}}(\boldsymbol{w}) = \sum_{n=1}^{N} \left(\boldsymbol{w}^T \boldsymbol{x}^{(n)} - y^{(n)}\right)^2$$

- Optimize the objective w.r.t. the model parameters
  - Solve in *closed form*: take ~~partial derivatives~~ gradient, set to 0 and solve

Linear Regression

- Suppose we have real-valued targets $y \in \mathbb{R}$ and D-dimensional inputs $\boldsymbol{x} = [1, x_1, \dots, x_D]^T \in \mathbb{R}^{D+1}$
- **Assume**

$$y = \boldsymbol{w}^T \boldsymbol{x}$$

- Notation: given training data $\mathcal{D} = \left\{\left(\boldsymbol{x}^{(n)}, y^{(n)}\right)\right\}_{n=1}^{N}$
  - $X = \begin{bmatrix} 1 & \boldsymbol{x}^{(1)^T} \\ 1 & \boldsymbol{x}^{(2)^T} \\ \vdots & \vdots \\ 1 & \boldsymbol{x}^{(N)^T} \end{bmatrix} = \begin{bmatrix} 1 & x_1^{(1)} & \cdots & x_D^{(1)} \\ 1 & x_1^{(2)} & \cdots & x_D^{(2)} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(N)} & \cdots & x_D^{(N)} \end{bmatrix} \in \mathbb{R}^{N \times D+1}$

    is the *design matrix*
  - $\boldsymbol{y} = \left[y^{(1)}, \dots, y^{(N)}\right]^T \in \mathbb{R}^N$ is the *target vector*

Minimizing the Squared Error

$$\ell_{\mathcal{D}}(\boldsymbol{w}) = \sum_{n=1}^{N}\left(\boldsymbol{w}^T\boldsymbol{x}^{(n)} - y^{(n)}\right)^2 = \sum_{n=1}^{N}\left({\boldsymbol{x}^{(n)}}^T\boldsymbol{w} - y^{(n)}\right)^2$$

$$= \|X\boldsymbol{w} - \boldsymbol{y}\|_2^2 \text{ where } \|\boldsymbol{z}\|_2 = \sqrt{\sum_{d=1}^{D} z_d^2} = \sqrt{\boldsymbol{z}^T\boldsymbol{z}}$$

$$= (X\boldsymbol{w} - \boldsymbol{y})^T(X\boldsymbol{w} - \boldsymbol{y})$$

$$= (\boldsymbol{w}^T X^T X\boldsymbol{w} - 2\boldsymbol{w}^T X^T\boldsymbol{y} + \boldsymbol{y}^T\boldsymbol{y})$$

$$\nabla_{\boldsymbol{w}}\ell_{\mathcal{D}}(\boldsymbol{w}) = (2X^T X\boldsymbol{w} - 2X^T\boldsymbol{y})$$

Minimizing the Squared Error

$$\ell_{\mathcal{D}}(\boldsymbol{w}) = \sum_{n=1}^{N} \left(\boldsymbol{w}^T \boldsymbol{x}^{(n)} - y^{(n)}\right)^2 = \sum_{n=1}^{N} \left({\boldsymbol{x}^{(n)}}^T \boldsymbol{w} - y^{(n)}\right)^2$$

$$= \|X\boldsymbol{w} - \boldsymbol{y}\|_2^2 \text{ where } \|\boldsymbol{z}\|_2 = \sqrt{\sum_{d=1}^{D} z_d^2} = \sqrt{\boldsymbol{z}^T \boldsymbol{z}}$$

$$= (X\boldsymbol{w} - \boldsymbol{y})^T (X\boldsymbol{w} - \boldsymbol{y})$$

$$= (\boldsymbol{w}^T X^T X \boldsymbol{w} - 2\boldsymbol{w}^T X^T \boldsymbol{y} + \boldsymbol{y}^T \boldsymbol{y})$$

$$\nabla_{\boldsymbol{w}} \ell_{\mathcal{D}}(\widehat{\boldsymbol{w}}) = (2X^T X \widehat{\boldsymbol{w}} - 2X^T \boldsymbol{y}) = 0$$

$$\rightarrow X^T X \widehat{\boldsymbol{w}} = X^T \boldsymbol{y}$$

$$\rightarrow \widehat{\boldsymbol{w}} = (X^T X)^{-1} X^T \boldsymbol{y}$$

Minimizing the Squared Error

$$\ell_{\mathcal{D}}(\boldsymbol{w}) = \sum_{n=1}^{N} \left(\boldsymbol{w}^T \boldsymbol{x}^{(n)} - y^{(n)}\right)^2 = \sum_{n=1}^{N} \left(\boldsymbol{x}^{(n)^T} \boldsymbol{w} - y^{(n)}\right)^2$$

$$= \|X\boldsymbol{w} - \boldsymbol{y}\|_2^2 \text{ where } \|\boldsymbol{z}\|_2 = \sqrt{\sum_{d=1}^{D} z_d^2} = \sqrt{\boldsymbol{z}^T \boldsymbol{z}}$$

$$= (X\boldsymbol{w} - \boldsymbol{y})^T (X\boldsymbol{w} - \boldsymbol{y})$$

$$= (\boldsymbol{w}^T X^T X \boldsymbol{w} - 2\boldsymbol{w}^T X^T \boldsymbol{y} + \boldsymbol{y}^T \boldsymbol{y})$$

$$\nabla_{\boldsymbol{w}} \ell_{\mathcal{D}}(\boldsymbol{w}) = (2X^T X \boldsymbol{w} - 2X^T \boldsymbol{y})$$

$$H_{\boldsymbol{w}} \ell_{\mathcal{D}}(\boldsymbol{w}) = 2X^T X$$

$H_{\boldsymbol{w}} \ell_{\mathcal{D}}(\boldsymbol{w})$ is positive semi-definite

$$\hat{\boldsymbol{w}} = (X^T X)^{-1} X^T \boldsymbol{y}$$

Closed Form Solution

1. Is $X^T X$ invertible?
   - When $N \gg D + 1$, $X^T X$ is (almost always) full rank and therefore, invertible!
   - If $X^T X$ is not invertible (occurs when one of the features is a linear combination of the others), what does that imply about our problem?
2. If so, how computationally expensive is inverting $X^T X$?
   - $X^T X \in \mathbb{R}^{D+1 \times D+1}$ so inverting $X^T X$ takes $O(D^3)$ time…
     - Computing $X^T X$ takes $O(ND^2)$ time
   - What alternative optimization method(s) can we use to minimize the mean squared error?

Lecture 7 Polls

0 done

0 underway

Is [*loading eqn.*] always invertible?

- Yes
- No
- Unsure

If $X^T X$ is invertible, how computationally expensive is it to invert?

- $O(N^2)$
- $O(D^2)$
- $O(ND)$
- $O(N^3)$
- $O(D^3)$

$$\hat{\boldsymbol{w}} = (X^TX)^{-1}X^T\boldsymbol{y}$$

Closed Form Solution

1. Is X^TX invertible?
   - When $N \gg D + 1$, X^TX is (almost always) full rank and therefore, invertible!
   - If X^TX is not invertible (occurs when one of the features is a linear combination of the others), what does that imply about our problem?
2. If so, how computationally expensive is inverting X^TX?
   - $X^TX \in \mathbb{R}^{D+1 \times D+1}$ so inverting X^TX takes $O(D^3)$ time…
     - Computing X^TX takes $O(ND^2)$ time
   - What alternative optimization method(s) can we use to minimize the mean squared error?

Key Takeaways

- Decision tree and kNN regression
- Closed form solution for linear regression
  - Setting partial derivative/gradients to 0 and solving for critical points
  - Potential issues with the closed form solution: invertibility and computational c.sts