

#### 10-301/601 Introduction to Machine Learning

Machine Learning Department School of Computer Science Carnegie Mellon University

# Linear Regression

Matt Gormley Lecture 7 Sep. 20, 2022

### Reminders

- Homework 3: KNN, Perceptron, Lin.Reg.
  - Out: Wed, Sep. 21
  - Due: Wed, Sep. 28 at 11:59pm
  - (only two grace/late days permitted)
- Exam conflicts form

What type of conflict do you have? *
◯ Class
Conference
Interview
O Medical
Time Zone
Religious Obligation
O ther

### DECISION TREES WITH REAL-VALUED FEATURES

### Q&A

### **Q:** How do we learn a Decision Tree with realvalued features?

**A:** 



### Q&A

### **Q:** How do we learn a Decision Tree with realvalued features?

A: Make new discrete features out of the real-valued features and then learn the Decision Tree as normal! Here's an example...



### REGRESSION

# Regression

### Goal:

- Given a training dataset of pairs (x,y) where
  - **x** is a vector
  - y is a scalar
- Learn a function (aka. curve or line) y' = h(x) that best fits the training data

### **Example Applications:**

- Stock price prediction
- Forecasting epidemics
- Speech synthesis
- Generation of images (e.g. Deep Dream)







# K-NEAREST NEIGHBOR REGRESSION

## k-NN Regression

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**Example:** Dataset with only one feature x and one scalar output y

y



#### Algorithm 1: k=1 Nearest Neighbor Regression

- Train: store all (x, y) pairs
- Predict: pick the nearest x in training data and return its y

#### Algorithm 2: k=2 Nearest Neighbors Distance Weighted Regression

- Train: store all (x, y) pairs
- Predict: pick the nearest two instances x<sup>(n1)</sup> and x<sup>(n2)</sup> in training data and return the weighted average of their y values

## k-NN Regression

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**Example:** Dataset with only one feature x and one scalar output y

Algorithm 1: drawing the function is left as an exercise

y

# unction is left as (ercise

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### **DECISION TREE REGRESSION**

### **Decision Tree Regression**



### **Decision Tree Regression**

#### Dataset for Regression

Y	А	В	C	
4	1	0	0	
1	1	0	1	
3	1	0	0	
7	0	0	1	
5	1	1	0	
6	0	1	1	
8	1	1	0	
9	1		1	



During learning, choose the attribute that minimizes an appropriate splitting criterion (e.g. mean squared error, mean absolute error)

## LINEAR FUNCTIONS, RESIDUALS, AND MEAN SQUARED ERROR

### Linear Functions

<u>Def</u>: Regression is predicting real-valued outputs

$$\mathcal{D} = \left\{ \left( \mathbf{x}^{(i)}, y^{(i)} \right) \right\}_{i=1}^{n}$$
 with  $\mathbf{x}^{(i)} \in \mathbb{R}^{M}$ ,  $y^{(i)} \in \mathbb{R}$ 

**Common Misunderstanding:** Linear functions  $\neq$  Linear decision boundaries



### Linear Functions

<u>Def</u>: Regression is predicting real-valued outputs

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### **Common Misunderstanding:** Linear functions $\neq$ Linear decision boundaries



- $y = w_1 x_1 + w_2 x_2 + b$ 
  - A general linear function is  $y = \mathbf{w}^T \mathbf{x} + b$
  - A general linear decision boundary is  $y = \operatorname{sign}(\mathbf{w}^T\mathbf{x} + b)$

### **Regression Problems**

### Chalkboard

- Residuals
- Mean squared error

The Big Picture

### **OPTIMIZATION FOR ML**

### **Unconstrained Optimization**

• Def: In **unconstrained optimization**, we try minimize (or maximize) a function with *no* constraints on the inputs to the function



# Optimization for ML

Not quite the same setting as other fields...

- Function we are optimizing might not be the true goal
  - (e.g. likelihood vs generalization error)
- Precision might not matter
   (e.g. data is noisy, so optimal up to 1e-16 might not help)
- Stopping early can help generalization error (i.e. "early stopping" is a technique for regularization – discussed more next time)

# min vs. argmin



 $v^* = min_x f(x)$  $x^* = argmin_x f(x)$ 

- Q1. 1. Question: What is  $v^*$ ?
- O₂. Question: What is x\*?

### min vs. argmin



$$v^* = min_x f(x)$$
  
 $x^* = argmin_x f(x)$ 

### 1. Question: What is v\*?

 $v^* = 1$ , the minimum value of the function

2. Question: What is x\*?

x\* = 0, the argument that yields the minimum value

### **OPTIMIZATION METHOD #0: RANDOM GUESSING**

### Notation Trick: Folding in the Intercept Term



$$\mathbf{x}' = [1, x_1, x_2, \dots, x_M]^T$$
$$\boldsymbol{\theta} = [b, w_1, \dots, w_M]^T$$

Notation Trick: fold the bias b and the weights w into a single vector **θ** by prepending a constant to x and increasing dimensionality by one!

$$h_{\mathbf{w},b}(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b$$
$$h_{\boldsymbol{\theta}}(\mathbf{x}') = \boldsymbol{\theta}^T \mathbf{x}'$$

This convenience trick allows us to more compactly talk about linear functions as a simple dot product (without explicitly writing out the intercept term every time).

# Linear Regression as Function $\mathcal{D} = \{\mathbf{x}^{(i)}, y^{(i)}\}_{i=1}^{N}$ where $\mathbf{x} \in \mathbb{R}^{M}$ and $y \in \mathbb{R}$ Approximation

1. Assume  ${\mathcal D}$  generated as:

 $\mathbf{x}^{(i)} \sim p^*(\cdot)$   $y^{(i)} = h^*(\mathbf{x}^{(i)})$ 

2. Choose hypothesis space,  $\mathcal{H}$ : all linear functions in M-dimensional space

$$\mathcal{H} = \{h_{\boldsymbol{\theta}} : h_{\boldsymbol{\theta}}(\mathbf{x}) = \boldsymbol{\theta}^T \mathbf{x}, \boldsymbol{\theta} \in \mathbb{R}^M\}$$

3. Choose an objective function: *mean squared error (MSE)* 

$$J(\boldsymbol{\theta}) = \frac{1}{N} \sum_{i=1}^{N} e_i^2$$
$$= \frac{1}{N} \sum_{i=1}^{N} \left( y^{(i)} - h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) \right)^2$$
$$= \frac{1}{N} \sum_{i=1}^{N} \left( y^{(i)} - \boldsymbol{\theta}^T \mathbf{x}^{(i)} \right)^2$$

- 4. Solve the unconstrained optimization problem via favorite method:
  - gradient descent
  - closed form
  - stochastic gradient descent
  - ...

$$\hat{\boldsymbol{ heta}} = \operatorname*{argmin}_{\boldsymbol{ heta}} J(\boldsymbol{ heta})$$

5. Test time: given a new x, make prediction  $\hat{y}$ 

$$\hat{y} = h_{\hat{oldsymbol{ heta}}}(\mathbf{x}) = \hat{oldsymbol{ heta}}^T \mathbf{x}$$

### **Contour Plots**

#### **Contour Plots**

- Each level curve labeled 1. with value
- Value label indicates the 2. value of the function for all points lying on that level curvé
- Just like a topographical map, but for a function 3.



 $J(\mathbf{\theta}) = J(\theta_1, \theta_2) = (10(\theta_1 - 0.5))^2 + (6(\theta_1 - 0.4))^2$ 1.0 000.00 30,000 10.000 0.8 -15.000 20.000 15.000 0.6 20.000 000  $\theta_2$ 0.4 5.000 . 0.2 0.0 -0.6 0.0 0.2 0.4

 $\theta_1$ 

1.0

0.8

# Optimization by Random Guessing

#### Optimization Method #0: Random Guessing

- 1. Pick a random  $\theta$
- 2. Evaluate  $J(\theta)$
- 3. Repeat steps 1 and 2 many times
- Return θ that gives smallest J(θ)

 $J(\mathbf{\theta}) = J(\theta_1, \theta_2) = (10(\theta_1 - 0.5))^2 + (6(\theta_1 - 0.4))^2$ 



# Optimization by Random Guessing

#### Optimization Method #0: Random Guessing

- 1. Pick a random  $\theta$
- 2. Evaluate  $J(\theta)$
- 3. Repeat steps 1 and 2 many times
- Return θ that gives smallest J(θ)

#### For Linear Regression:

• **objective function** is Mean Squared Error (MSE)

• MSE = J(
$$\boldsymbol{\Theta}$$
,  $\boldsymbol{D}$   
= J( $\boldsymbol{\Theta}_1$ ,  $\boldsymbol{\Theta}_2$ ) =  $\frac{1}{N} \sum_{i=1}^{N} (y^{(i)} - \boldsymbol{\theta}^T \mathbf{x}^{(i)})^2$ 

- contour plot: each line labeled with MSE – lower means a better fit
- minimum corresponds to parameters (w,b) = (θ<sub>1</sub>, θ<sub>2</sub>) that best fit some training dataset



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### **Counting Butterflies**



# Linear Regression in High Dimensions

- In our discussions of linear regression, we will always assume there is just one output, y
- But our inputs will usually have many features:

$$\mathbf{x} = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_M]^T$$

- For example:
  - suppose we had a drone take pictures of each section of forest
  - each feature could correspond to a pixel in this image such that  $x_m = 1$  if the pixel is orange and  $x_m = 0$  otherwise
  - the output y would be the number of butterflies in each picture





## Linear Regression by Rand. Guessing

#### Optimization Method #0: Random Guessing

- 1. Pick a random  $\theta$
- 2. Evaluate  $J(\theta)$
- 3. Repeat steps 1 and 2 many times
- 4. Return  $\boldsymbol{\theta}$  that gives smallest J( $\boldsymbol{\theta}$ )



#### For Linear Regression:

- target function h\*(x) is unknown
- only have access to h\*(x) through training examples (x<sup>(i)</sup>,y<sup>(i)</sup>)
- want h(x; θ<sup>(t)</sup>) that best approximates h\*(x)
- enable generalization w/inductive bias that restricts hypothesis class to linear functions

#### Linear Regression by Rand. Guessing $J(\boldsymbol{\theta}) = J(\boldsymbol{\theta}_1, \boldsymbol{\theta}_2) = \frac{1}{N} \sum_{i=1}^{N} \left( y^{(i)} - \boldsymbol{\theta}^T \mathbf{x}^{(i)} \right)^2$ **Optimization Method #0:** 1.0 **Random Guessing** 000.00 ,30,000 10.000 Pick a random $\theta$ 1. 0.8 -Evaluate $J(\boldsymbol{\theta})$ 2. Repeat steps 1 and 2 many 3. 15.000 15.000 20.000 times 20.000 . Return **\theta** that gives $\theta_2$ 4. smallest $J(\theta)$ 0.4 $y = h^*(x)$ 5.000 h(x; **θ**<sup>(4)</sup>) (unknown) 0.2 h(x; **θ**<sup>(2)</sup>) 0 0.0 0.2 0.4 0.6 0.8 1.0 $\theta_1$ W 6 > $\theta_{2}$ $J(\theta_1, \theta_2)$ θ t 0.2 0.2 10.4 1 h(x; **θ**<sup>(1)</sup>) 2 0.3 0.7 7.2 0.6 3 1.0 0.4 16.2 4 0.9 0.7Х

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### OPTIMIZATION METHOD #1: GRADIENT DESCENT

### Optimization for ML

### Chalkboard

- Derivatives
- Gradient

# **Topographical Maps**



# **Topographical Maps**















### Gradient Descent

Chalkboard

- Gradient Descent Algorithm
- Details: starting point, stopping criterion, line search

### Gradient Descent

Algorithm 1 Gradient Descent

1: procedure 
$$GD(\mathcal{D}, \boldsymbol{\theta}^{(0)})$$

- 2:  $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta}^{(0)}$
- 3: while not converged do 4:  $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \boldsymbol{\gamma} \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$

5: return  $\theta$ 



In order to apply GD to Linear Regression all we need is the **gradient** of the objective function (i.e. vector of partial derivatives).

$$\begin{bmatrix} \frac{d}{d\theta_1} J(\boldsymbol{\theta}) \\ \frac{d}{d\theta_2} J(\boldsymbol{\theta}) \\ \vdots \\ \frac{d}{d\theta_M} J(\boldsymbol{\theta}) \end{bmatrix}$$

 $\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) =$ 

### Gradient Descent

Algorithm 1 Gradient Descent

1: procedure 
$$GD(\mathcal{D}, \boldsymbol{\theta}^{(0)})$$

- 2:  $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta}^{(0)}$
- 3: while not converged do 4:  $\theta \leftarrow \theta - \gamma \nabla_{\theta} J(\theta)$

5: return  $\theta$ 



There are many possible ways to detect **convergence**. For example, we could check whether the L2 norm of the gradient is below some small tolerance.

 $||\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})||_2 \leq \epsilon$ 

Alternatively we could check that the reduction in the objective function from one iteration to the next is small.

## GRADIENT DESCENT FOR LINEAR REGRESSION

#### 

1. Assume  $\mathcal{D}$  generated as:

 $\begin{aligned} \mathbf{x}^{(i)} &\sim p^*(\cdot) \\ y^{(i)} &= h^*(\mathbf{x}^{(i)}) \end{aligned}$ 

2. Choose hypothesis space,  $\mathcal{H}$ : all linear functions in *M*-dimensional space

$$\mathcal{H} = \{h_{\boldsymbol{\theta}} : h_{\boldsymbol{\theta}}(\mathbf{x}) = \boldsymbol{\theta}^T \mathbf{x}, \boldsymbol{\theta} \in \mathbb{R}^M\}$$

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- 4. Solve the unconstrained optimization problem via favorite method:
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$$\hat{\boldsymbol{ heta}} = \operatorname*{argmin}_{\boldsymbol{ heta}} J(\boldsymbol{ heta})$$

5. Test time: given a new x, make prediction  $\hat{y}$ 

$$\hat{y} = h_{\hat{oldsymbol{ heta}}}(\mathbf{x}) = \hat{oldsymbol{ heta}}^T \mathbf{x}$$

# Linear Regression by Gradient Desc.

#### Optimization Method #1: Gradient Descent

- 1. Pick a random  $\theta$
- 2. Repeat:
  a. Evaluate gradient ∇J(θ)
  b. Step opposite gradient
- Return θ that gives smallest J(θ)



### Linear Regression by Gradient Desc.

#### Optimization Method #1: Gradient Descent

- 1. Pick a random  $\theta$
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<i>(</i> )	t	$\theta_1$	θ2	$J(\theta_1, \theta_2)$
0'	1	0.01	0.02	25.2
$\Theta_{(s)}$	2	0.30	0.12	8.7
63	3	0.51	0.30	1.5
Ð <sup>(4)</sup>	4	0.59	0.43	0.2

### Linear Regression by Gradient Desc. $J(\theta) = J(\theta_1, \theta_2) = \frac{1}{N} \sum_{i=1}^{N} (y^{(i)} - \theta^T \mathbf{x}^{(i)})^2$

#### Optimization Method #1: Gradient Descent

- 1. Pick a random  $\theta$
- 2. Repeat:
  a. Evaluate gradient ∇J(θ)
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>



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4

0.51

0.59

0.30

0.43

1.5

0.2





# **Optimization for Linear Regression**

### Chalkboard

- Computing the gradient for Linear Regression
- Gradient Descent for Linear Regression

### Gradient Calculation for Linear Regression

Derivative of 
$$J^{(i)}(\boldsymbol{\theta})$$
:  

$$\frac{d}{d\theta_k} J^{(i)}(\boldsymbol{\theta}) = \frac{d}{d\theta_k} \frac{1}{2} (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)})^2$$

$$= \frac{1}{2} \frac{d}{d\theta_k} (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)})^2$$

$$= (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}) \frac{d}{d\theta_k} (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)})$$

$$= (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}) \frac{d}{d\theta_k} \left( \sum_{j=1}^K \theta_j x_j^{(i)} - y^{(i)} \right)^2$$

$$= (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}) x_k^{(i)}$$

Derivative of  $J(\boldsymbol{\theta})$ :

$$\begin{aligned} \frac{d}{d\theta_k} J(\boldsymbol{\theta}) &= \sum_{i=1}^N \frac{d}{d\theta_k} J^{(i)}(\boldsymbol{\theta}) \\ &= \sum_{i=1}^N (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}) x_k^{(i)} \end{aligned}$$

Gradient of 
$$J(\boldsymbol{\theta})$$
 [used by Gradient Descent]  

$$\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) = \begin{bmatrix} \frac{d}{d\theta_1} J(\boldsymbol{\theta}) \\ \frac{d}{d\theta_2} J(\boldsymbol{\theta}) \\ \vdots \\ \frac{d}{d\theta_M} J(\boldsymbol{\theta}) \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^N (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}) x_1^{(i)} \\ \sum_{i=1}^N (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}) x_2^{(i)} \\ \vdots \\ \sum_{i=1}^N (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}) \mathbf{x}^{(i)} \end{bmatrix}$$

$$= \sum_{i=1}^N (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}) \mathbf{x}^{(i)}$$

# GD for Linear Regression

Gradient Descent for Linear Regression repeatedly takes steps opposite the gradient of the objective function



### **Regression Loss Functions**

### **In-Class Exercise:**

Which of the following could be used as loss functions for training a linear regression model?

Select all that apply.

A. 
$$\ell(\hat{y}, y) = (\hat{y})^2$$
  
B.  $\ell(\hat{y}, y) = |\hat{y} - y|$   
C.  $\ell(\hat{y}, y) = \frac{1}{2}(\hat{y} - y)^2$   
D.  $\ell(\hat{y}, y) = \frac{1}{4}(\hat{y} - y)^4$   
E.  $\ell(\hat{y}, y) = \begin{cases} \frac{1}{2}(\hat{y} - y)^2 & \text{if } |\hat{y} - y| \le \delta \\ \delta |\hat{y} - y| - \frac{1}{2}\delta^2 & \text{otherwise} \end{cases}$   
F.  $\ell(\hat{y}, y) = \log(\cosh(\hat{y} - y))$ 

### CONVEXITY



Suppose we have a function  $f(x) : \mathcal{X} \to \mathcal{Y}$ .

- The value  $x^*$  is a **global minimum** of f iff  $f(x^*) \leq f(x), \forall x \in \mathcal{X}$ .
- The value  $x^*$  is a **local minimum** of f iff  $\exists \epsilon$  s.t.  $f(x^*) \leq f(x), \forall x \in [x^* \epsilon, x^* + \epsilon]$ .



 Each local minimum is a global minimum

#### **Nonconvex Function**



- A nonconvex function is not convex
- Each **local minimum** is **not** necessarily a **global minimum**

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#### **Convex Function**



 Each local minimum is a global minimum

#### **Nonconvex Function**



- A nonconvex function is not convex
- Each **local minimum** is **not** necessarily a **global minimum**

 $x_2$ 



 $x_1$ 

 $tx_1 + (1-t)x_2$ 

Each local minimum of a convex function is also a global minimum.

A strictly convex function has a unique global minimum.

## CONVEXITY AND LINEAR REGRESSION

### Convexity and Linear Regression

The **Mean Squared Error** function, which we minimize for learning the parameters of Linear Regression, **is convex**!

... but in the general case it is **not** strictly convex.

### Gradient Descent & Convexity

- Gradient descent is a local optimization algorithm
- If the function is nonconvex, it will find a local minimum, not necessarily a global minimum
- If the function is convex, it will find a global minimum

