



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

Machine Learning Department School of Computer Science Carnegie Mellon University

### **Stochastic Gradient Descent**



## **Probabilistic Learning**

(Binary Logistic Regression)

Matt Gormley Lecture 9 Feb. 16, 2022

### Reminders

- Practice for Exam 1
  - Mock Exam 1
    - Due: Wed, Feb. 16 at 11:59pm
    - See <u>@683</u> for participation point details
  - Practice Problems 1 released on course website
- Exam 1: Thu, Feb. 17
  - Time: 6:30 8:30pm
  - Location: Your room/seat assignment will be announced on Piazza
- Homework 4: Logistic Regression
  - Out: Fri, Feb 18
  - Due: Sun, Feb. 27 at 11:59pm

## OPTIMIZATION METHOD #3: STOCHASTIC GRADIENT DESCENT

### **Gradient Descent**

### Algorithm 1 Gradient Descent

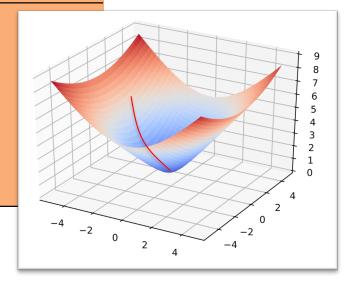
1: **procedure**  $GD(\mathcal{D}, \boldsymbol{\theta}^{(0)})$ 

2:  $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta}^{(0)}$ 

3: **while** not converged **do** 

4:  $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \boldsymbol{\gamma} \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$ 

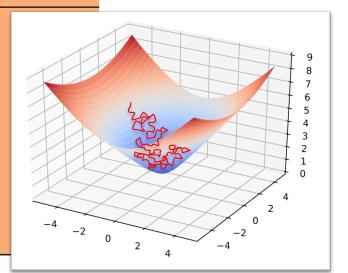
5: return  $\theta$ 



## Stochastic Gradient Descent (SGD)

### Algorithm 2 Stochastic Gradient Descent (SGD)

```
1: \operatorname{procedure} \operatorname{SGD}(\mathcal{D}, \boldsymbol{\theta}^{(0)})
2: \boldsymbol{\theta} \leftarrow \boldsymbol{\theta}^{(0)}
3: \operatorname{while} \operatorname{not} \operatorname{converged} \operatorname{do}
4: i \sim \operatorname{Uniform}(\{1, 2, \dots, N\})
5: \boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \gamma \nabla_{\boldsymbol{\theta}} J^{(i)}(\boldsymbol{\theta})
6: \operatorname{return} \boldsymbol{\theta}
```



### per-example objective:

$$J^{(i)}(oldsymbol{ heta})$$

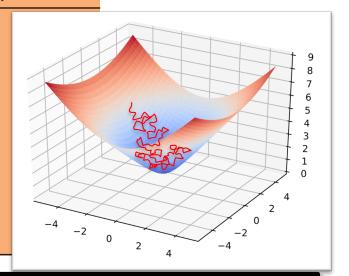
original objective:

$$J(\boldsymbol{\theta}) = \sum_{i=1}^{N} J^{(i)}(\boldsymbol{\theta})$$

## Stochastic Gradient Descent (SGD)

### Algorithm 2 Stochastic Gradient Descent (SGD)

```
1: procedure SGD(\mathcal{D}, \theta^{(0)})
2: \theta \leftarrow \theta^{(0)}
3: while not converged do
4: for i \in \text{shuffle}(\{1, 2, \dots, N\}) do
5: \theta \leftarrow \theta - \gamma \nabla_{\theta} J^{(i)}(\theta)
6: return \theta
```



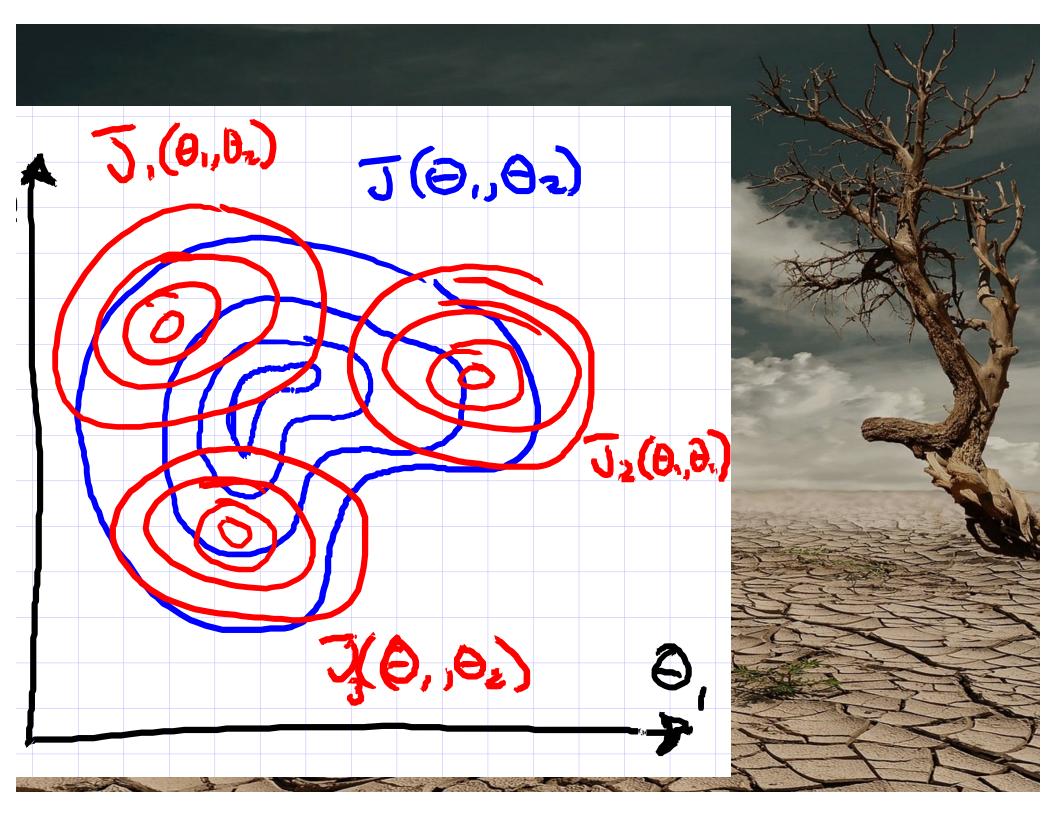
per-example objective:

$$J^{(i)}(oldsymbol{ heta})$$

original objective:

$$J(\boldsymbol{\theta}) = \sum_{i=1}^{N} J^{(i)}(\boldsymbol{\theta})$$

In practice, it is common to implement SGD using sampling without replacement (i.e. shuffle({1,2,... N}), even though most of the theory is for sampling with replacement (i.e. Uniform({1,2,... N}).



### Why does SGD work?

### Whiteboard

Example of SGD on simple 2D function

## Why does SGD work?

$$\frac{dJ(\vec{\Theta})}{d\theta_j} = \frac{1}{N} \sum_{i=1}^{N} \frac{d}{d\theta_j} \left( J_i(\vec{\Theta}) \right)$$

$$\sqrt{J(\vec{\Theta})} = \frac{1}{N} \sum_{i=1}^{N} \sqrt{J_i(\vec{\Theta})}$$

$$j_{i} = \frac{1}{N} \sum_{i=1}^{N} \sqrt{J_i(\vec{\Theta})}$$

Recall: for any discrete r.v. 
$$X$$

$$E_{X}[f(x)] \triangleq \sum_{x} P(x=x)f(x)$$

Qibbat is the expectal value of a randomly chosen 
$$\nabla J_i(\Theta)$$
?

Let  $I \sim U_{ni} Sorm(\{1,...,U\})$ 

$$\Rightarrow P(I=i) = \frac{1}{N} \text{ if } ie\{1,...N\}$$

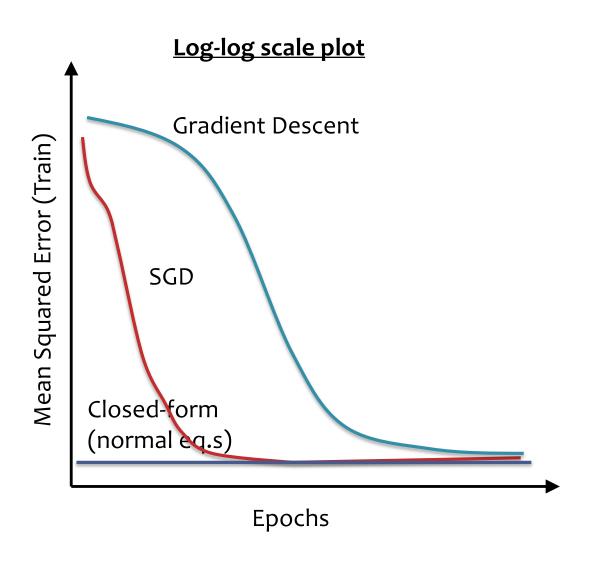
$$E_{I}[\nabla J_{I}(\vec{\Theta})] = \bigotimes_{i=1}^{N} P(I=i) \nabla J_{i}(\vec{\Theta})$$

$$= \frac{1}{N} \bigotimes_{i=1}^{N} \nabla J_{i}(\vec{\Theta})$$

$$= \nabla J(\vec{\Theta})$$

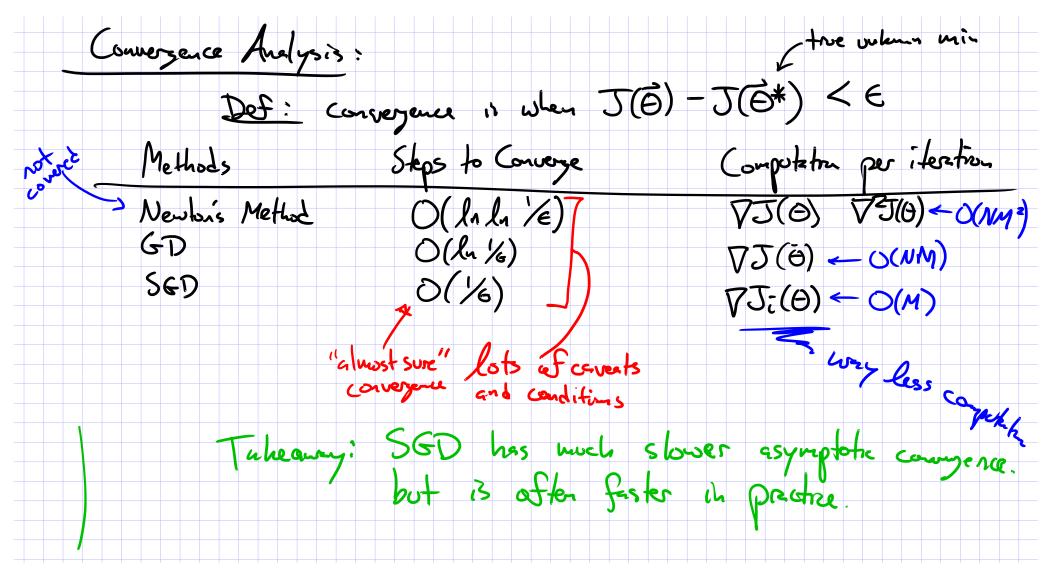
## LINEAR REGRESSION: PRACTICALITIES

## **Empirical Convergence**



- Def: an epoch is a single pass through the training data
- For GD, only one update per epoch
- For SGD, N updates
   per epoch
   N = (# train examples)
- SGD reduces MSE much more rapidly than GD
- For GD / SGD, training MSE is initially large due to uninformed initialization

## Convergence of Optimizers



## SGD FOR LINEAR REGRESSION

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

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

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

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

### Gradient Calculation for Linear Regression

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

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

#### Derivative of $J(\theta)$ :

$$egin{aligned} rac{d}{d heta_k}J(oldsymbol{ heta}) &= \sum_{i=1}^N rac{d}{d heta_k}J^{(i)}(oldsymbol{ heta}) \ &= \sum_{i=1}^N (oldsymbol{ heta}^T\mathbf{x}^{(i)} - y^{(i)})x_k^{(i)} \end{aligned}$$

Gradient of 
$$J^{(i)}(\theta)$$
 [used by SGD] 
$$\nabla_{\theta}J^{(i)}(\theta) = \begin{bmatrix} \frac{\frac{d}{d\theta_{1}}}{J^{(i)}(\theta)} \\ \frac{\frac{d}{d\theta_{2}}}{J^{(i)}(\theta)} \end{bmatrix} = \begin{bmatrix} (\theta^{T}\mathbf{x}^{(i)} - y^{(i)})x_{1}^{(i)} \\ (\theta^{T}\mathbf{x}^{(i)} - y^{(i)})x_{2}^{(i)} \\ \vdots \\ (\theta^{T}\mathbf{x}^{(i)} - y^{(i)})x_{N}^{(i)} \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{N} (\theta^{T}\mathbf{x}^{(i)} - y^{(i)})x_{1}^{(i)} \\ \sum_{i=1}^{N} (\theta^{T}\mathbf{x}^{(i)} - y^{(i)})x_{N}^{(i)} \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{N} (\theta^{T}\mathbf{x}^{(i)} - y^{(i)})x_{1}^{(i)} \\ \sum_{i=1}^{N} (\theta^{T}\mathbf{x}^{(i)} - y^{(i)})x_{N}^{(i)} \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{N} (\theta^{T}\mathbf{x}^{(i)} - y^{(i)})x_{1}^{(i)} \\ \sum_{i=1}^{N} (\theta^{T}\mathbf{x}^{(i)} - y^{(i)})x_{N}^{(i)} \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{N} (\theta^{T}\mathbf{x}^{(i)} - y^{(i)})x_{1}^{(i)} \\ \sum_{i=1}^{N} (\theta^{T}\mathbf{x}^{(i)} - y^{(i)})x_{1}^{(i)} \end{bmatrix}$$

$$\begin{split} & \text{Gradient of } J(\boldsymbol{\theta}) & \left[ \text{used by Gradient Descent} \right] \\ & \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) = \begin{bmatrix} \frac{d}{d\theta_1} J(\boldsymbol{\theta}) \\ \frac{d}{d\theta_2} J(\boldsymbol{\theta}) \\ \vdots \\ \frac{d}{d\theta_M} J(\boldsymbol{\theta}) \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^N (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}) x_1^{(i)} \\ \sum_{i=1}^N (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}) x_2^{(i)} \\ \vdots \\ \sum_{i=1}^N (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}) \mathbf{x}_N^{(i)} \end{bmatrix} \\ & = \sum_{i=1}^N (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}) \mathbf{x}^{(i)} \end{aligned}$$

## SGD for Linear Regression

SGD applied to Linear Regression is called the "Least Mean Squares" algorithm

```
Algorithm 1 Least Mean Squares (LMS)
  1: procedure LMS(\mathcal{D}, \boldsymbol{\theta}^{(0)})
            \boldsymbol{\theta} \leftarrow \boldsymbol{\theta}^{(0)}
                                                                              ▷ Initialize parameters
  2:
           while not converged do
  3:
                   for i \in \mathsf{shuffle}(\{1, 2, \dots, N\}) do
  4:
                        \mathbf{g} \leftarrow (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}) \mathbf{x}^{(i)}
                                                                                  5:
                        \theta \leftarrow \theta - \gamma \mathbf{g}

    □ Update parameters

  6:
            return \theta
  7:
```

## GD for Linear Regression

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

## Algorithm 1 GD for Linear Regression 1: procedure GDLR( $\mathcal{D}$ , $\theta^{(0)}$ ) 2: $\theta \leftarrow \theta^{(0)}$ $\triangleright$ Initialize parameters

3: **while** not converged **do** 

4: 
$$\mathbf{g} \leftarrow \sum_{i=1}^{N} (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}) \mathbf{x}^{(i)}$$
 > Compute gradient  
5:  $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \gamma \mathbf{g}$  > Update parameters

6: return  $\theta$ 

## Linear Regression Objectives

#### You should be able to...

- Design k-NN Regression and Decision Tree Regression
- Implement learning for Linear Regression using three optimization techniques: (1) closed form, (2) gradient descent, (3) stochastic gradient descent
- Choose a Linear Regression optimization technique that is appropriate for a particular dataset by analyzing the tradeoff of computational complexity vs. convergence speed
- Distinguish the three sources of error identified by the bias-variance decomposition: bias, variance, and irreducible error.

### Optimization Objectives

### You should be able to...

- Apply gradient descent to optimize a function
- Apply stochastic gradient descent (SGD) to optimize a function
- Apply knowledge of zero derivatives to identify a closed-form solution (if one exists) to an optimization problem
- Distinguish between convex, concave, and nonconvex functions
- Obtain the gradient (and Hessian) of a (twice) differentiable function

### PROBABILISTIC LEARNING

## Probabilistic Learning

### **Function Approximation**

Previously, we assumed that our output was generated using a deterministic target function:

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

$$y^{(i)} = c^*(\mathbf{x}^{(i)})$$

Our goal was to learn a hypothesis h(x) that best approximates c\*(x)

### **Probabilistic Learning**

Today, we assume that our output is **sampled** from a conditional **probability distribution**:

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

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

Our goal is to learn a probability distribution p(y|x) that best approximates  $p^*(y|x)$ 

## Robotic Farming

	Deterministic	Probabilistic
Classification (binary output)	Is this a picture of a wheat kernel?	Is this plant drought resistant?
Regression (continuous output)	How many wheat kernels are in this picture?	What will the yield of this plant be?





## MAXIMUM LIKELIHOOD ESTIMATION

### MLE

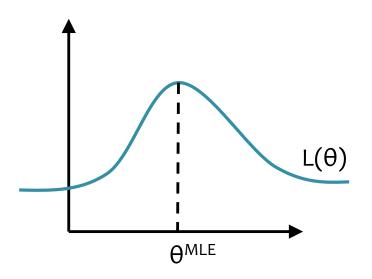
Suppose we have data  $\mathcal{D} = \{x^{(i)}\}_{i=1}^{N}$ 

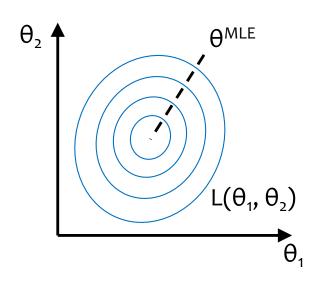
### Principle of Maximum Likelihood Estimation:

Choose the parameters that maximize the likelihood of the data. N

$$\boldsymbol{\theta}^{\mathsf{MLE}} = \operatorname*{argmax}_{\boldsymbol{\theta}} \prod_{i=1} p(\mathbf{x}^{(i)} | \boldsymbol{\theta})$$

Maximum Likelihood Estimate (MLE)





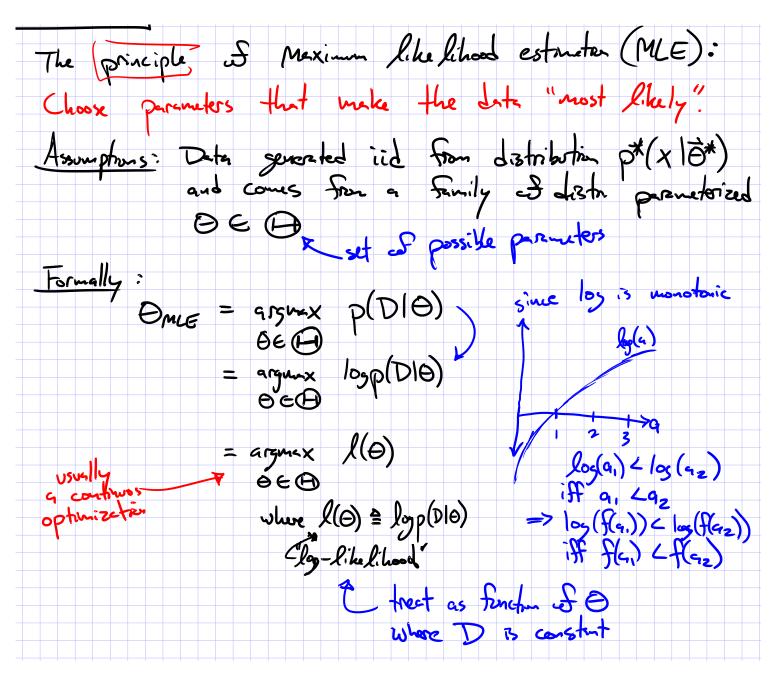
### MLE

What does maximizing likelihood accomplish?

- There is only a finite amount of probability mass (i.e. sum-to-one constraint)
- MLE tries to allocate as much probability mass as possible to the things we have observed...

... at the expense of the things we have not observed

### Maximum Likelihood Estimation



## MOTIVATION: LOGISTIC REGRESSION

## Example: Image Classification

- ImageNet LSVRC-2010 contest:
  - Dataset: 1.2 million labeled images, 1000 classes
  - Task: Given a new image, label it with the correct class
  - Multiclass classification problem
- Examples from http://image-net.org/

Not logged in. Login I Signup

#### Bird

IM. GENET

Warm-blooded egg-laying vertebrates characterized by feathers and forelimbs modified as wings

2126 pictures

92.85% Popularity Percentile



	marine animal, marine creature, sea animal, sea creature (1)		
	- scavenger (1)	Treemap Visualization	Image
	biped (0)		
	- predator, predatory animal (1)		4
	⊩ larva (49)		-
	- acrodont (0)		- 8
	- feeder (0)	100	
	- stunt (0)		_
	chordate (3087)		
	tunicate, urochordate, urochord (6)		
	cephalochordate (1)		
	vertebrate, craniate (3077)		
	mammal, mammalian (1169)		
	†- bird (871)		
	dickeybird, dickey-bird, dickybird, dicky-bird (0)	N .	
	cock (1)		
	hen (0)		
	- nester (0)		
	i- night bird (1)		
	- bird of passage (0)		
	- protoavis (0)		
	- archaeopteryx, archeopteryx, Archaeopteryx lithographi	Ho of	-
	- Sinornis (0)		No.
	- Ibero-mesornis (0)		_
	- archaeornis (0)	10 PA / 19 PA	
	- carinate, carinate bird, flying bird (0)	ALL STATES	
	passerine, passeriform bird (279)	A CONTRACTOR OF THE PARTY OF TH	
	nonpasserine bird (0) bird of prey, raptor, raptorial bird (80)	000000	~
	gallinaceous bird, gallinacean (114)		925
	gainiaceous bird, gainiacean (114)		



Not logged in. Login I Signup

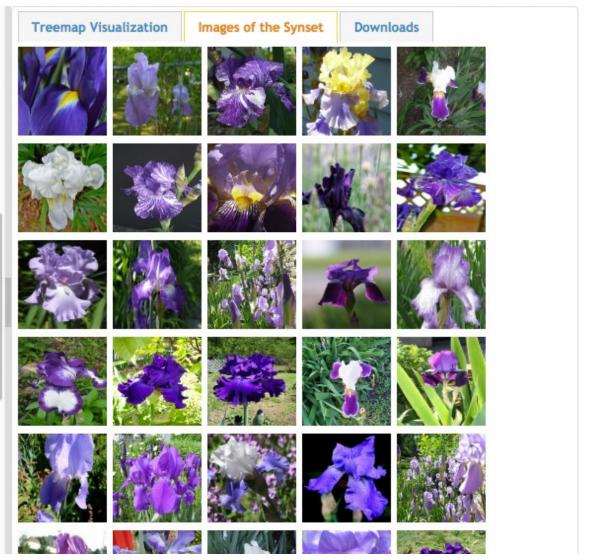
#### German iris, Iris kochii

Iris of northern Italy having deep blue-purple flowers; similar to but smaller than Iris germanica

469 pictures 49.6% Popularity Percentile



halophyte (0)		
succulent (39)		
- cultivar (0)		
- cultivated plant (0)		
- weed (54)		
evergreen, evergreen plant (0)		
- deciduous plant (0)		
→ vine (272)		
- creeper (0)		
woody plant, ligneous plant (1868)		
geophyte (0)		
desert plant, xerophyte, xerophytic plant, xerophile, xerophile		
mesophyte, mesophytic plant (0)		
aquatic plant, water plant, hydrophyte, hydrophytic plant (11		
tuberous plant (0)		
bulbous plant (179)		
iridaceous plant (27)		
iris, flag, fleur-de-lis, sword lily (19)  iris, flag, fleur-de-lis, sword lily (19)		
bearded iris (4)		
Florentine iris, orris, Iris germanica florentina, Iris		
- German iris, Iris germanica (0)		
German iris, Iris kochii (0)		
Dalmatian iris, Iris pallida (0)		
- beardless iris (4)		
- bulbous iris (0)		
- dwarf iris, Iris cristata (0)		
stinking iris, gladdon, gladdon iris, stinking gladwyn,		
- Persian iris, Iris persica (0)		
yellow iris, yellow flag, yellow water flag, Iris pseuda		
- dwarf iris, vernal iris, Iris verna (0)		
blue flag, Iris versicolor (0)		



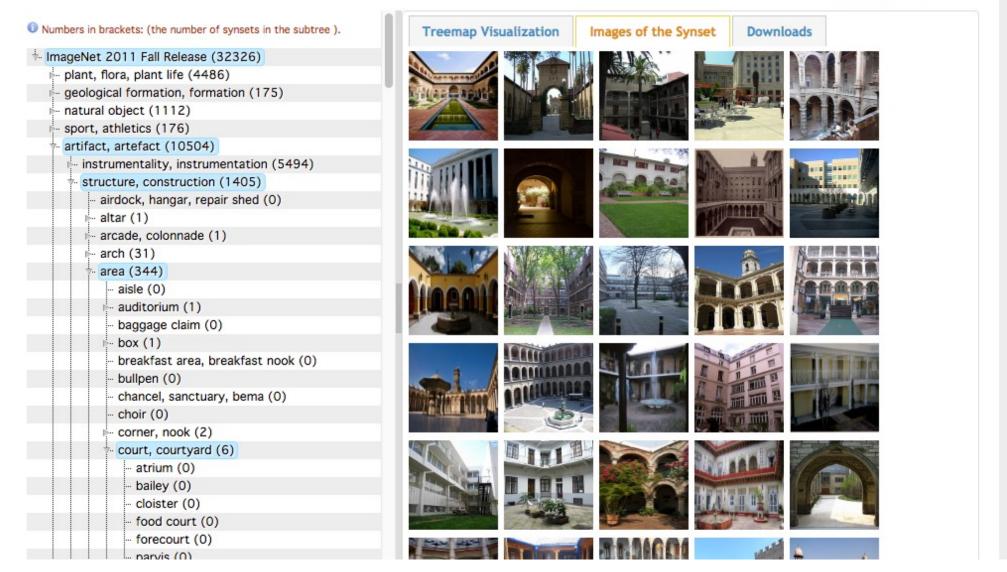
#### Court, courtyard

**IM** GENET

An area wholly or partly surrounded by walls or buildings; "the house was built around an inner court"

165 pictures 92.61% Popularity Percentile





## Example: Image Classification

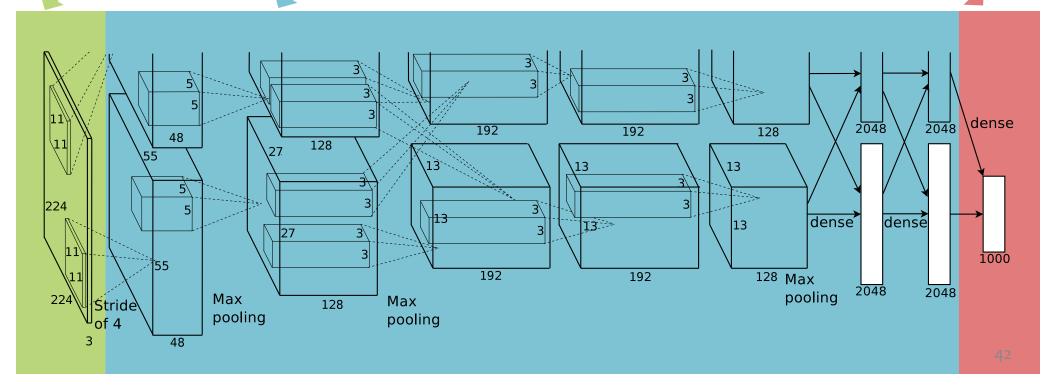
#### **CNN for Image Classification**

(Krizhevsky, Sutskever & Hinton, 2011) 17.5% error on ImageNet LSVRC-2010 contest

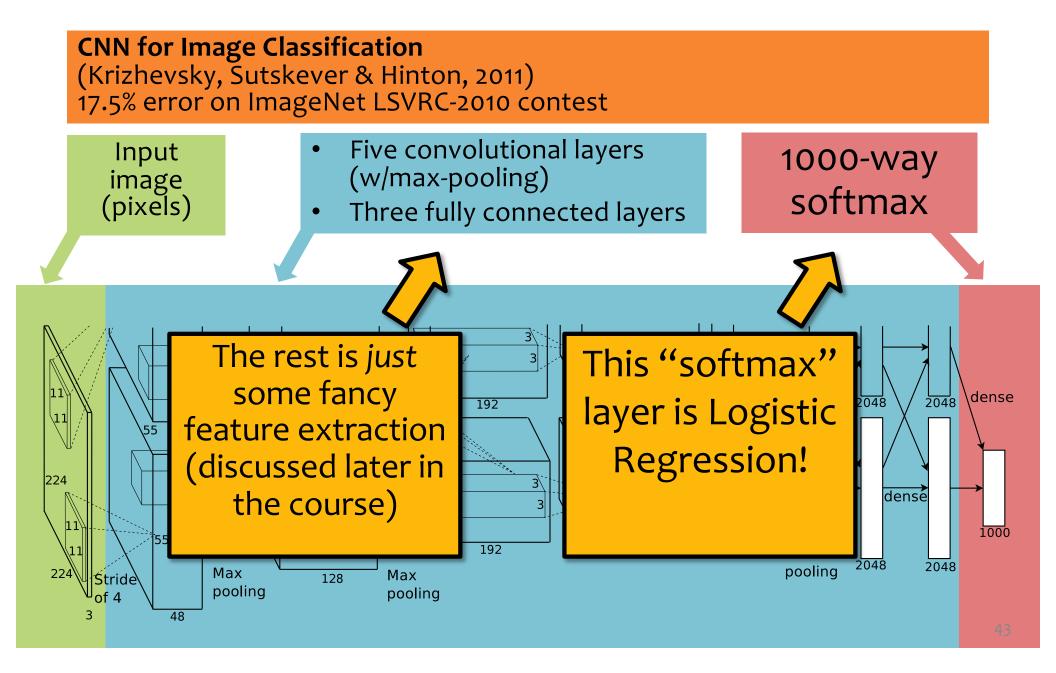
Input image (pixels)

- Five convolutional layers (w/max-pooling)
- Three fully connected layers

1000-way softmax



## Example: Image Classification



### **LOGISTIC REGRESSION**

## Logistic Regression

**Data:** Inputs are continuous vectors of length M. Outputs are discrete.

$$\mathcal{D} = \{\mathbf{x}^{(i)}, y^{(i)}\}_{i=1}^N$$
 where  $\mathbf{x} \in \mathbb{R}^M$  and  $y \in \{0, 1\}$ 



We are back to classification.

Despite the name logistic regression.

## Linear Models for Classification

Key idea: Try to learn this hyperplane directly

### Looking ahead:

- We'll see a number of commonly used Linear Classifiers
- These include:
  - Perceptron
  - Logistic Regression
  - Naïve Bayes (under certain conditions)
  - Support Vector Machines

Directly modeling the hyperplane would use a decision function:

$$h(\mathbf{x}) = \operatorname{sign}(\boldsymbol{\theta}^T \mathbf{x})$$

$$y \in \{-1, +1\}$$

## Background: Hyperplanes

Notation Trick: fold the bias b and the weights w into a single vector  $\boldsymbol{\theta}$  by prepending a constant to x and increasing dimensionality by one to get x'!

Half-spaces:

Hyperplane (Definition 1):

$$\mathcal{H} = \{\mathbf{x} : \mathbf{w}^T \mathbf{x} = b\}$$

Hyperplane (Definition 2):

$$\mathcal{H} = \{\mathbf{x}': \boldsymbol{\theta}^T \mathbf{x}' = 0$$

and 
$$x_1' = 1$$

$$\boldsymbol{\theta} = [b, w_1, \dots, w_M]^T$$

$$\mathbf{x'} = [1, x_1, \dots, x_M]^T$$

$$\mathcal{H}^+ = \{\mathbf{x} : \boldsymbol{\theta}^T \mathbf{x} > 0 \text{ and } x_1 = 1\}$$

$$\mathcal{H}^- = \{\mathbf{x} : \boldsymbol{\theta}^T \mathbf{x} < 0 \text{ and } x_1 = 1\}$$

### Key idea behind today's lecture:

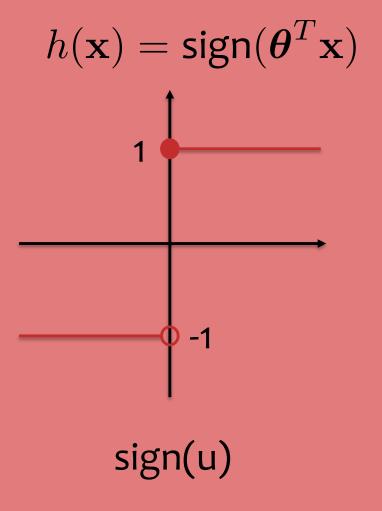
- Define a linear classifier (logistic regression)
- Define an objective function (likelihood)
- Optimize it with gradient descent to learn parameters
- 4. Predict the class with highest probability under the model

### Optimization for Linear Classifiers

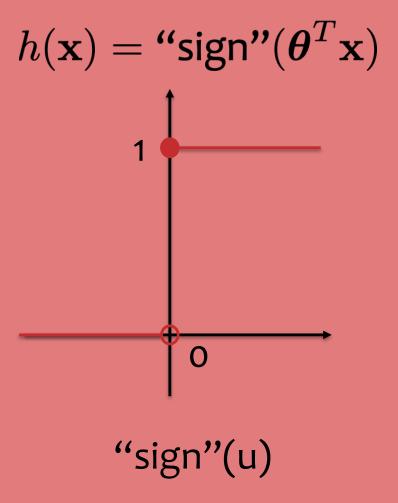
### Whiteboard

- Strawman: Mean squared error for Perceptron!
- What does  $\theta^T \mathbf{x}$  tell us about  $\mathbf{x}$ ?

Suppose we wanted to learn a linear classifier, but instead of predicting  $y \in \{-1,+1\}$  we wanted to predict  $y \in \{0,1\}$ 



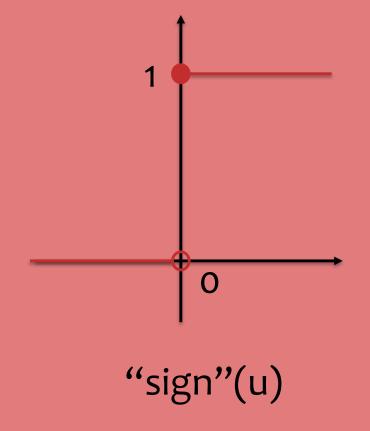
Suppose we wanted to learn a linear classifier, but instead of predicting  $y \in \{-1,+1\}$  we wanted to predict  $y \in \{0,1\}$ 



Goal: Learn a linear classifier with Gradient Descent

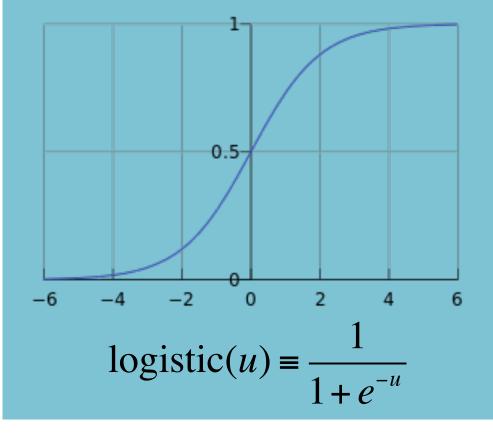
But this decision function isn't differentiable...

$$h(\mathbf{x}) = \text{"sign"}(\boldsymbol{\theta}^T \mathbf{x})$$



Use a differentiable function instead!

$$p_{\theta}(y = 1|\mathbf{x}) = \frac{1}{1 + \exp(-\boldsymbol{\theta}^T \mathbf{x})}$$



## Logistic Regression

**Data:** Inputs are continuous vectors of length M. Outputs are discrete.

$$\mathcal{D} = \{\mathbf{x}^{(i)}, y^{(i)}\}_{i=1}^N$$
 where  $\mathbf{x} \in \mathbb{R}^M$  and  $y \in \{0, 1\}$ 

**Model:** Logistic function applied to dot product of parameters with input vector.

$$p_{\boldsymbol{\theta}}(y=1|\mathbf{x}) = \frac{1}{1 + \exp(-\boldsymbol{\theta}^T \mathbf{x})}$$

**Learning:** finds the parameters that minimize some objective function.  ${m heta}^* = rgmin J({m heta})$ 

**Prediction:** Output is the most probable class.

$$\hat{y} = \operatorname*{argmax} p_{\boldsymbol{\theta}}(y|\mathbf{x})$$
$$y \in \{0,1\}$$

## **Logistic Regression**

### Whiteboard

- Logistic Regression Model
- Partial derivative for logistic regression
- Gradient for logistic regression
- Decision boundary