



10-301/10-601 Introduction to Machine Learning

Machine Learning Department School of Computer Science Carnegie Mellon University

Stochastic Gradient Descent

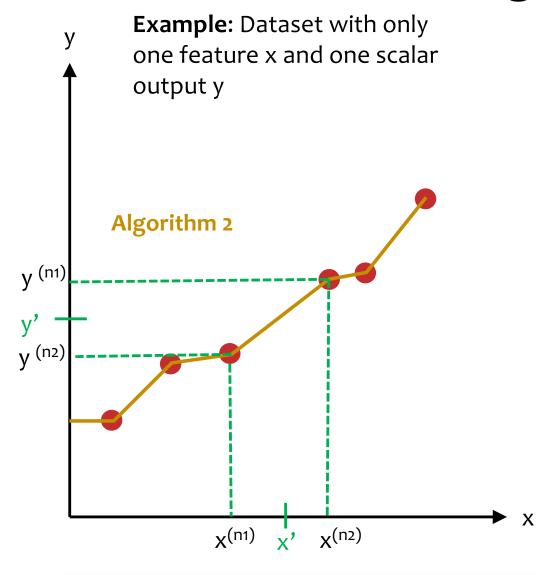


Probabilistic Learning

(Binary Logistic Regression)

Matt Gormley Lecture 9 Feb. 15, 2023

k-NN Regression



This version is incorrect.

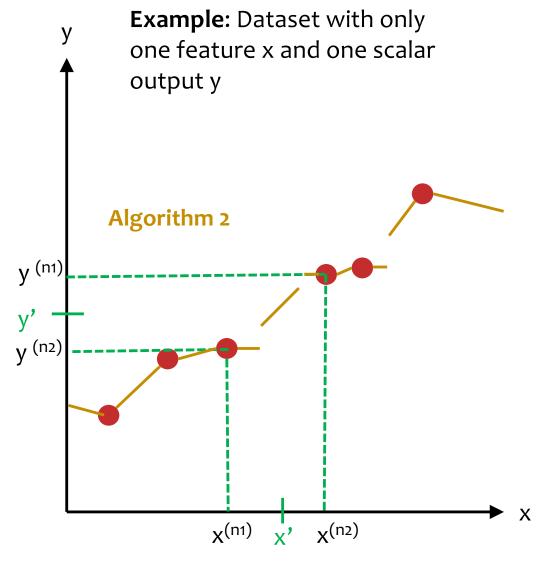
Algorithm 1: k=1 Nearest Neighbor Regression

- 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⁽ⁿ¹⁾ and x⁽ⁿ²⁾ in training data and return the weighted average of their y values

k-NN Regression



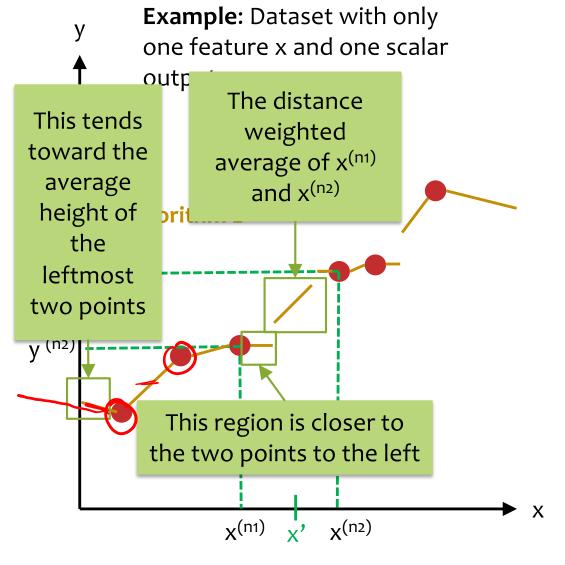
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Reminders

- Practice Problems 1
 - released on course website
- Exam 1: Thu, Feb. 16
 - Time: 6:30 8:30pm
 - Location: Your room/seat assignment will be announced on Piazza
- Homework 4: Logistic Regression
 - Out: Fri, Feb 17
 - Due: Sun, Feb. 26 at 11:59pm

OPTIMIZATION METHOD #3: STOCHASTIC GRADIENT DESCENT

Gradient Descent

Algorithm 1 Gradient Descent

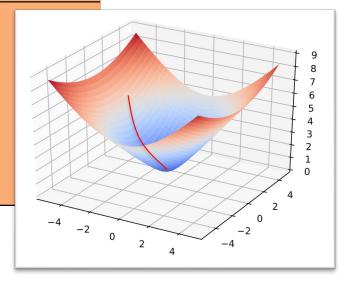
1: **procedure** $GD(\mathcal{D}, \boldsymbol{\theta}^{(0)})$

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 θ



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:

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

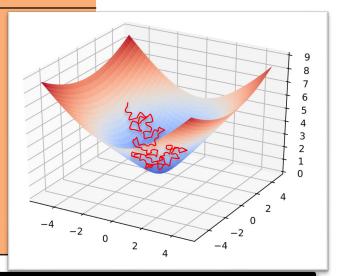
original objective:

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

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}).

Background: Probability

Expectation of a function of a random variable

For any discrete random variable X

$$E_X[f(X)] = \sum_{x \in \mathcal{X}} P(X = x) f(x)$$

• If the example is sampled uniformly at random, the expected value of the pointwise gradient is the same as the full gradient!

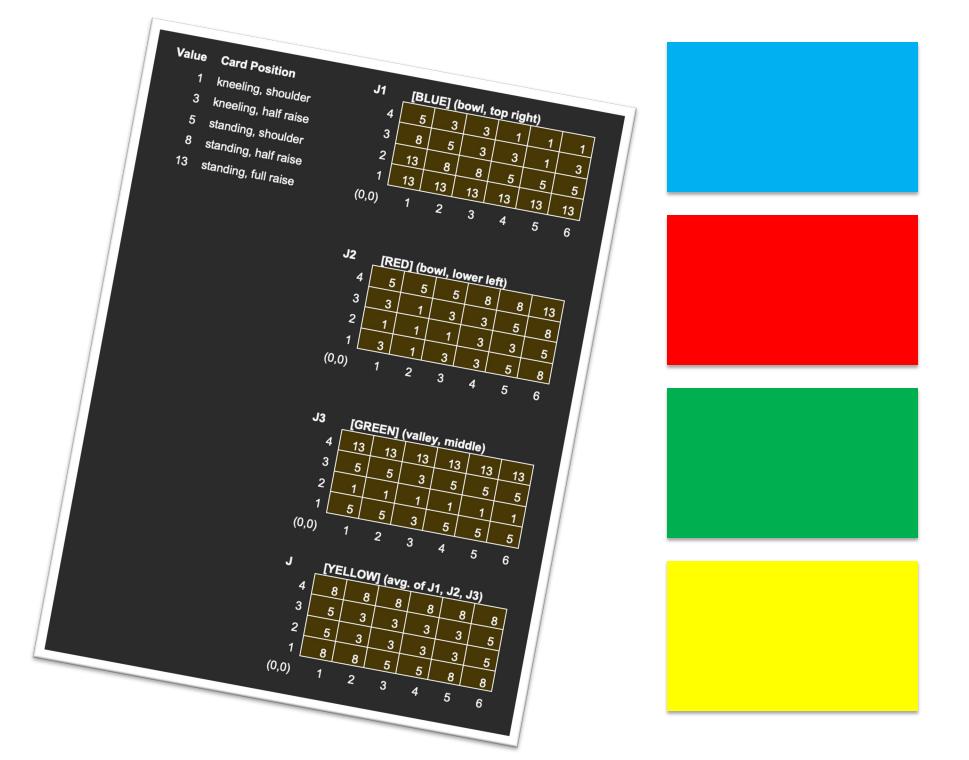
$$E[f(i)] = \sum_{i=1}^{N} (\text{probability of selecting } x^{(i)}, y^{(i)}) \nabla_{\theta} J^{(i)}(\theta)$$

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

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

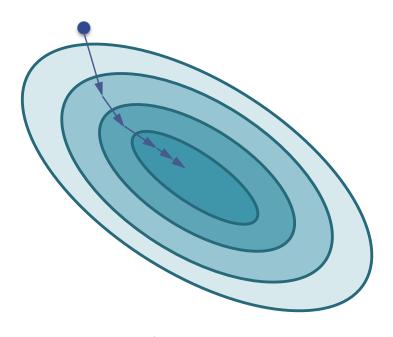
$$= \nabla_{\theta} J(\theta)$$

 In practice, the data set is randomly shuffled then looped through so that each data point is used equally often

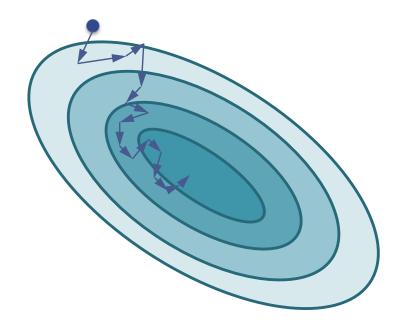


SGD VS. GRADIENT DESCENT

SGD vs. Gradient Descent



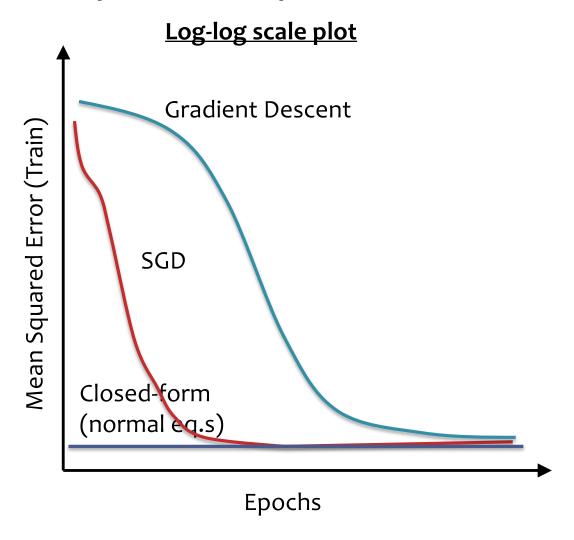
Gradient Descent



Stochastic Gradient Descent

SGD vs. Gradient Descent

• Empirical comparison:



- 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

SGD vs. Gradient Descent

Theoretical comparison:

Define convergence to be when $J(\boldsymbol{\theta}^{(t)}) - J(\boldsymbol{\theta}^*) < \epsilon$

Method	Steps to Convergence	Computation per Step
Gradient descent	$O(\log 1/\epsilon)$	O(NM)
SGD	$o(1/\epsilon)$	O(M)

(with high probability under certain assumptions)

Main Takeaway: SGD has much slower asymptotic convergence (i.e. it's slower in theory), but is often much faster in practice.

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

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

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

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

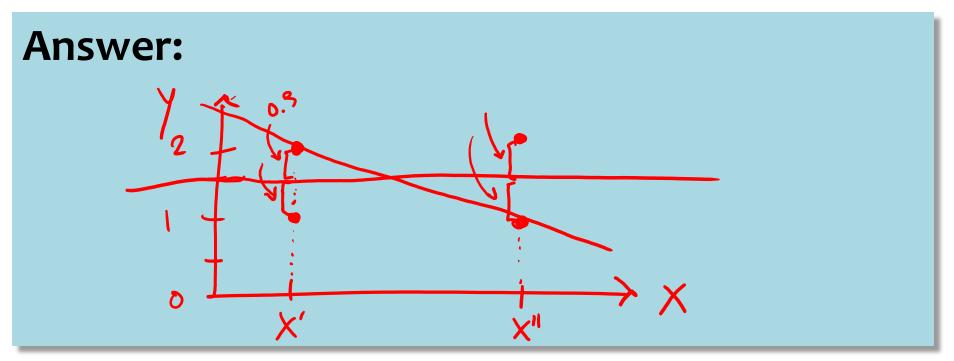
return θ

6:

Solving Linear Regression

Question: Q1 A=toxic B=Tre C=False

True or False: If Mean Squared Error (i.e. $\frac{1}{N} \sum_{i=1}^{N} (y^{(i)} - h(\mathbf{x}^{(i)}))^2$) has a unique minimizer (i.e. argmin), then Mean Absolute Error (i.e. $\frac{1}{N} \sum_{i=1}^{N} |y^{(i)} - h(\mathbf{x}^{(i)})|$) must also have a unique minimizer.



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

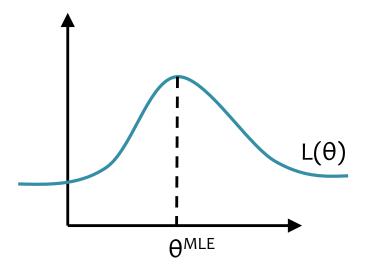
Suppose we have data $\mathcal{D} = \{x^{(i)}\}_{i=1}^{N}$

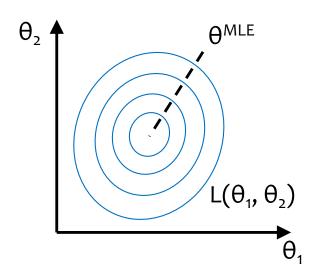
Principle of Maximum Likelihood Estimation:

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

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

Maximum Likelihood Estimate (MLE)





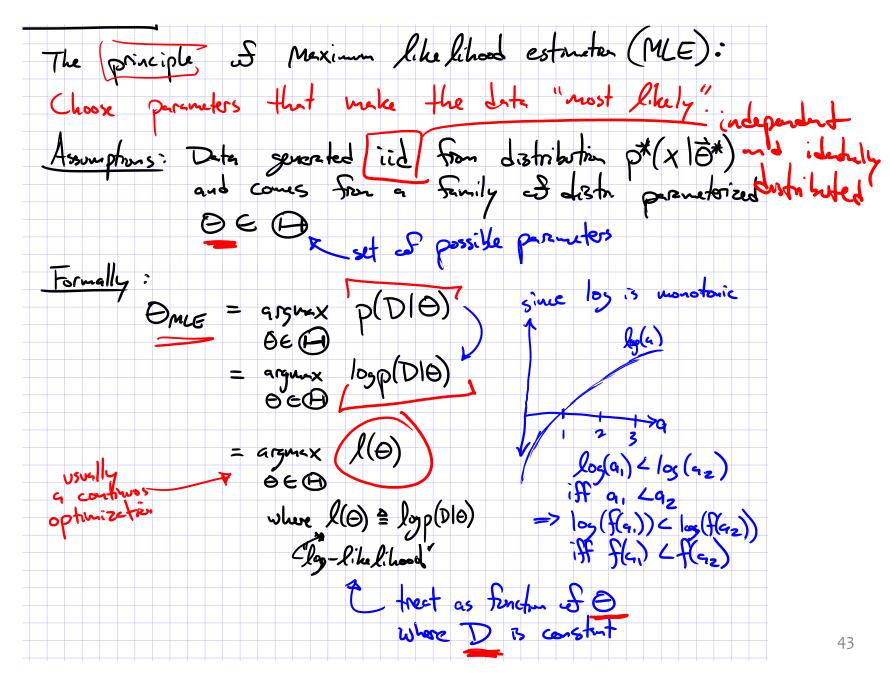
MLE

What does maximizing likelihood accomplish?

- There is only a finite amount of probability mass (i.e. sum-to-one constraint) $\leq \frac{P(K=x)}{2} = 1$
- 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/

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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)		1. 1. 1	
scavenger (1)	Treemap Visualization	Images of the Synset	Downloads
- biped (0)			
predator, predatory animal (1)		Maria M	F 1
- larva (49)			
- acrodont (0)			
- feeder (0)	No.		1
- stunt (0)			
r- chordate (3087)			
tunicate, urochordate, urochord (6)			
rephalochordate (1)			
vertebrate, craniate (3077)	725,704	X	
mammal, mammalian (1169)			
†- bird (871)	A STATE OF THE STA		
- dickeybird, dickey-bird, dickybird, dicky-bird (0)			
r cock (1)			
- hen (0)			HS
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⊩ night bird (1)		350	100 A 100 B
- bird of passage (0)	To State of the second	463	0 (4)
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archaeopteryx, archeopteryx, Archaeopteryx lithographi			
- Sinornis (0)			
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- archaeornis (0)	the state of the s	N/A	1 3.5
ratite, ratite bird, flightless bird (10)		~	-//
- carinate, carinate bird, flying bird (0)			
passerine, passeriform bird (279)			200
nonpasserine bird (0)	OF THE REAL PROPERTY.	. 1	
i⊸ bird of prey, raptor, raptorial bird (80)		720	
gallinaceous bird, gallinacean (114)	建筑		

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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 (3	9)
- cultivar (0)	
 cultivated pla 	ant (0)
weed (54)	
- evergreen, e	vergreen plant (0)
- deciduous pla	ant (0)
vine (272)	
- creeper (0)	
woody plant,	ligneous plant (1868)
geophyte (0)	
	xerophyte, xerophytic plant, xerophile, xerophile mesophytic plant (0)
	, water plant, hydrophyte, hydrophytic plant (11
- tuberous plan	
bulbous plant	
	g, fleur-de-lis, sword lily (19)
bea	rded iris (4)
	Florentine iris, orris, Iris germanica florentina, Iris
	German iris, Iris germanica (0)
	German iris, Iris kochii (0)
1	Dalmatian iris, Iris pallida (0)
⊩ bea	rdless iris (4)
bulk	oous iris (0)
dwa	arf iris, Iris cristata (0)
stin	king iris, gladdon, gladdon iris, stinking gladwyn,
Per	sian iris, Iris persica (0)
- yell	ow iris, yellow flag, yellow water flag, Iris pseuda
dwa	arf iris, vernal iris, Iris verna (0)
blue	e flag, Iris versicolor (0)



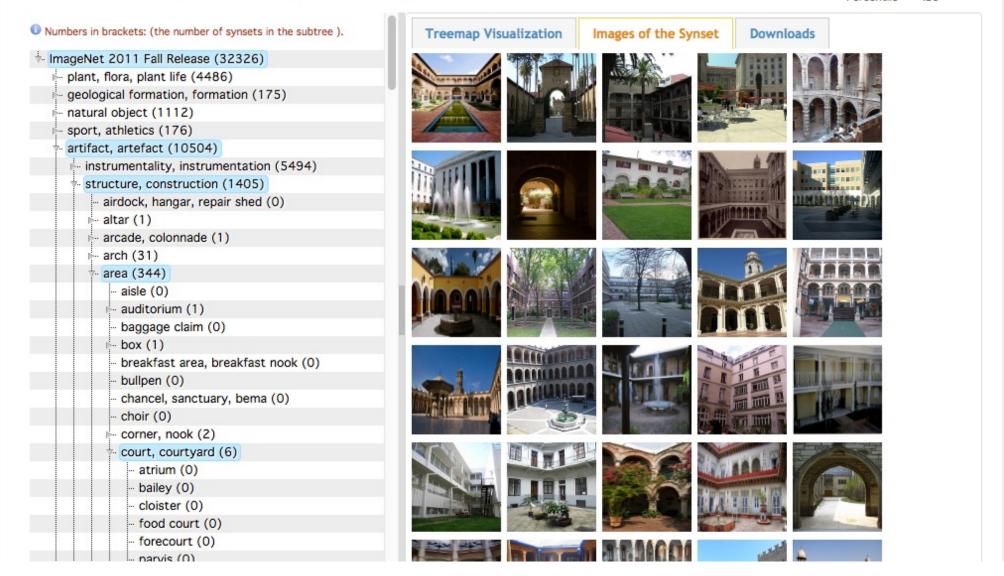
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Court, courtyard

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

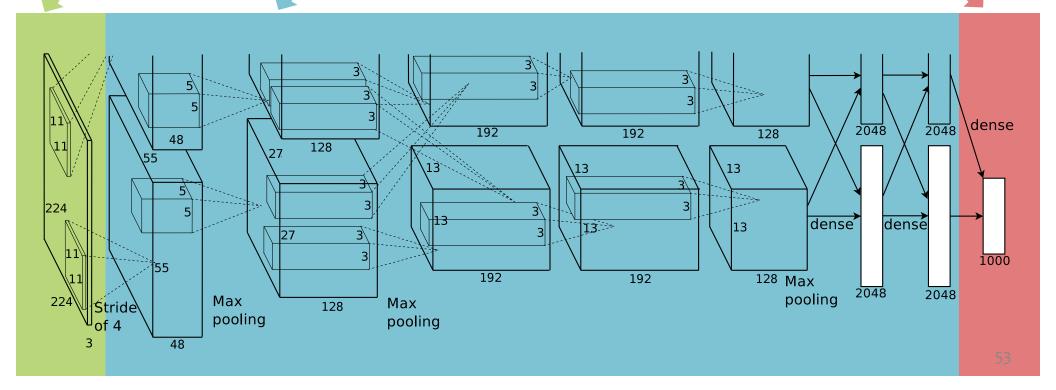
CNN for Image Classification

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

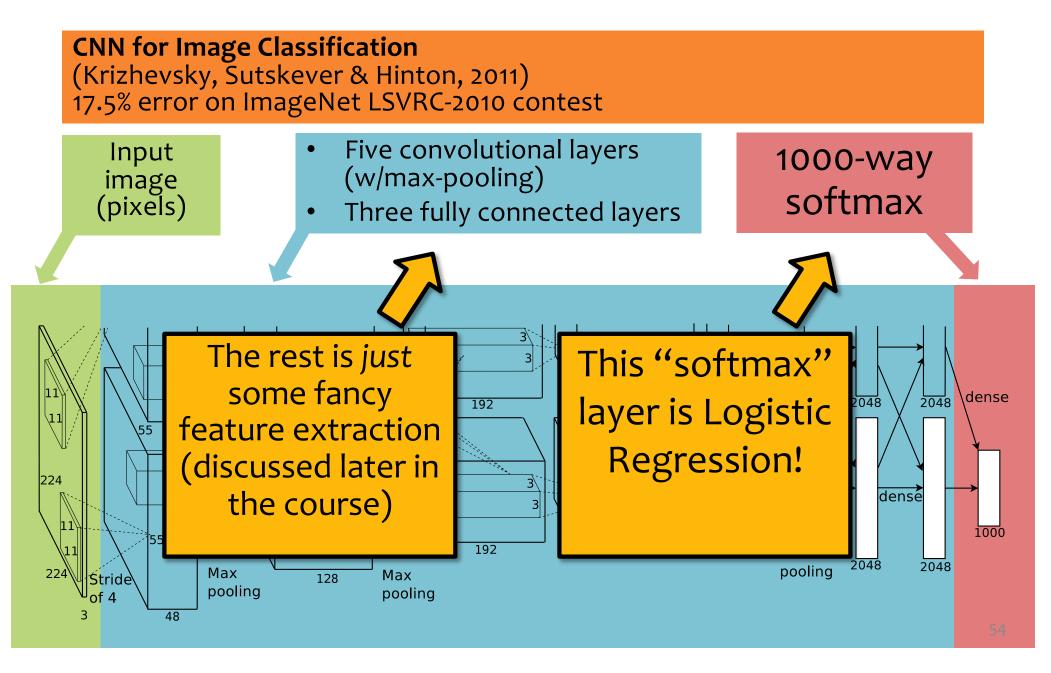
Input image (pixels)

- 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'!

Hyperplane (Definition 1):

$$\mathcal{H} = \{ \mathbf{x} : \mathbf{w}^T \mathbf{x} + b = 0 \}$$

Hyperplane (Definition 2):

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

and
$$x_0' = 1\}$$
 $oldsymbol{ heta} = [b, w_1, \dots, w_M]^T$

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

Half-spaces:

$$\mathcal{H}^+ = \{\mathbf{x} : \boldsymbol{\theta}^T \mathbf{x} > 0 \text{ and } x_0^1 = 1\}$$

$$\mathcal{H}^- = \{\mathbf{x} : \boldsymbol{\theta}^T \mathbf{x} < 0 \text{ and } x_0^1 = 1\}$$

Key idea behind today's lecture:

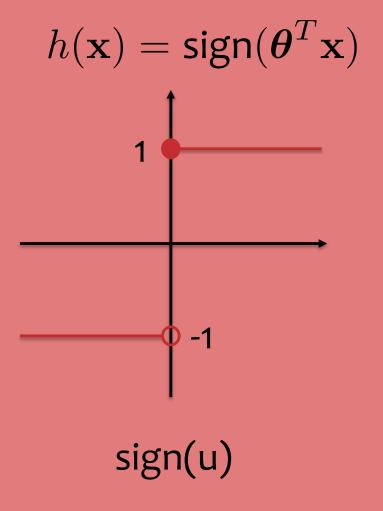
- 1. Define a linear classifier (logistic regression)
- Define an objective function (likelihood)
- Optimize it with gradient descent to learn parameters
- 4. Predict the class with highest probability under the model

Optimization for Linear Classifiers

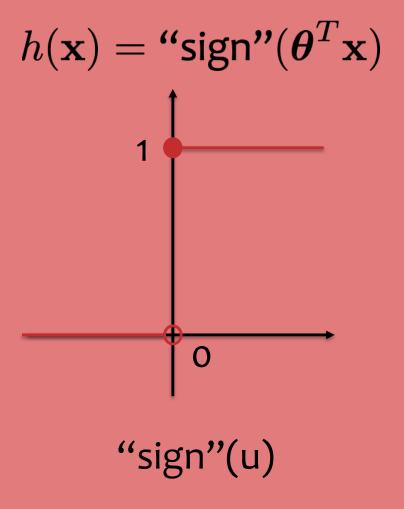
Whiteboard

- 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 $y \in \{0,1\}$



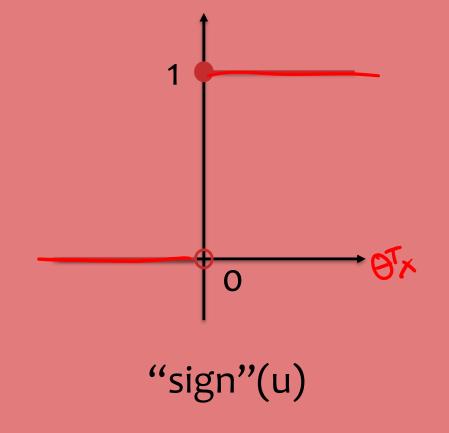
Suppose we wanted to learn a linear classifier, but instead of predicting $y \in \{-1,+1\}$ we wanted to predict $y \in \{0,1\}$



Goal: Learn a linear classifier with Gradient Descent

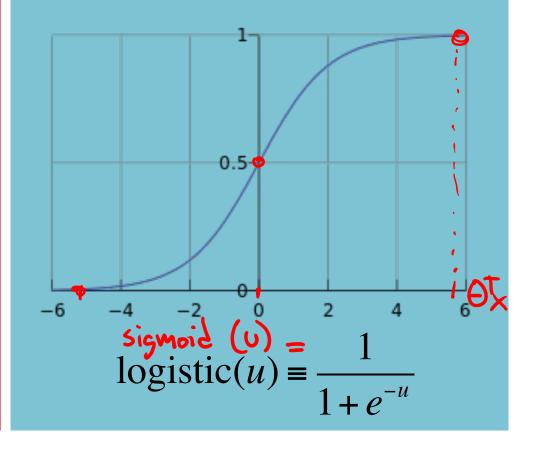
But this decision function isn't differentiable...

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



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.

th 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. ${m heta}^* = \mathop{\rm argmin}_{m heta} J({m heta})$

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