Machine Learning Department
School of Computer Science
Carnegie Mellon University

Stochastic Gradient Descent

+

Probabilistic Learning

(Binary Logistic Regression)

Matt Gormley
Lecture 9
Sep. 27, 2023

Reminders

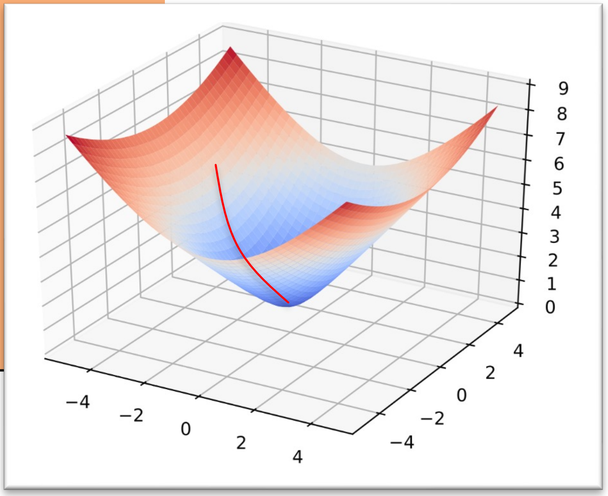
- Practice Problems 1
  - released on course website
- Exam 1: Thu, Sep. 28
  - Time: 6:30 – 8:30pm
  - Location: Your room/seat assignment will be announced on Piazza
- Homework 4: Logistic Regression
  - Out: Fri, Sep. 29
  - Due: Mon, Oct. 9 at 11:59pm

OPTIMIZATION METHOD #3: STOCHASTIC GRADIENT DESCENT

Gradient Descent

Algorithm 1 Gradient Descent

procedure GD($\mathcal{D}$, $\boldsymbol{\theta}^{(0)}$)
    $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta}^{(0)}$
    while not converged **do**
        $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \gamma \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$
    return $\boldsymbol{\theta}$

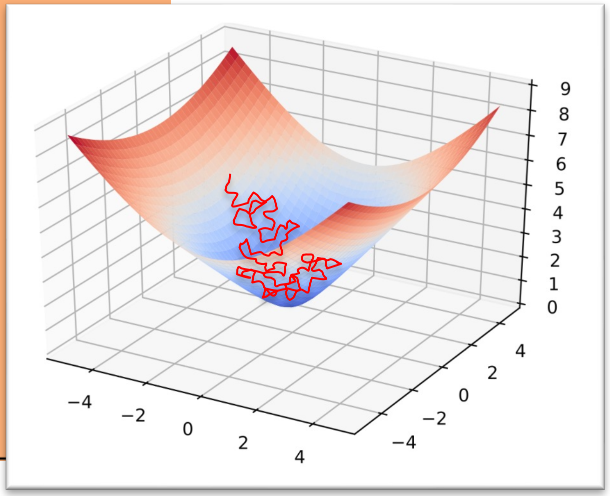


M

Stochastic Gradient Descent (SGD)

Algorithm 2 Stochastic Gradient Descent (SGD)

procedure SGD($\mathcal{D}, \boldsymbol{\theta}^{(0)}$)
    $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta}^{(0)}$
    while not converged **do**
        $i \sim$ Uniform$(\{1, 2, \ldots, N\})$
        $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \gamma \nabla_{\boldsymbol{\theta}} J^{(i)}(\boldsymbol{\theta})$
    return $\boldsymbol{\theta}$



per-example objective:

$$J^{(i)}(\boldsymbol{\theta})$$

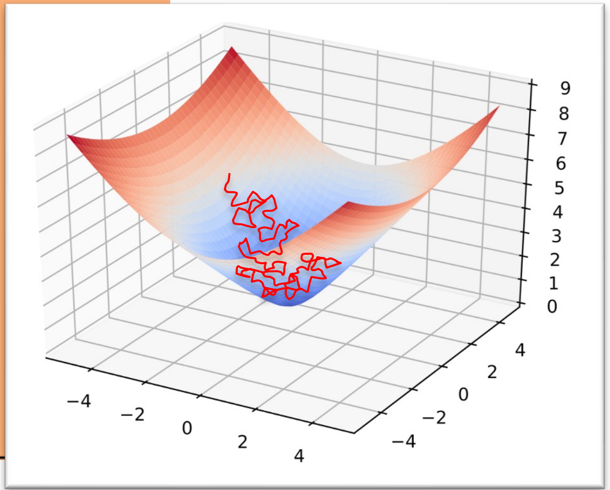
original objective:

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

Stochastic Gradient Descent (SGD)

Algorithm 2 Stochastic Gradient Descent (SGD)

procedure SGD($\mathcal{D}, \boldsymbol{\theta}^{(0)}$)
  $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta}^{(0)}$
  while not converged **do**
    for $i \in$ shuffle($\{1, 2, \ldots, N\}$) **do**
      $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \gamma \nabla_{\boldsymbol{\theta}} J^{(i)}(\boldsymbol{\theta})$
  return $\boldsymbol{\theta}$



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}).

per-example objective:

$$J^{(i)}(\boldsymbol{\theta})$$

original objective:

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

Why does SGD work?

Background: *Expectation of a function of a random variable*

For any discrete random variable X

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

Objective Function for SGD

We assume the form to be:

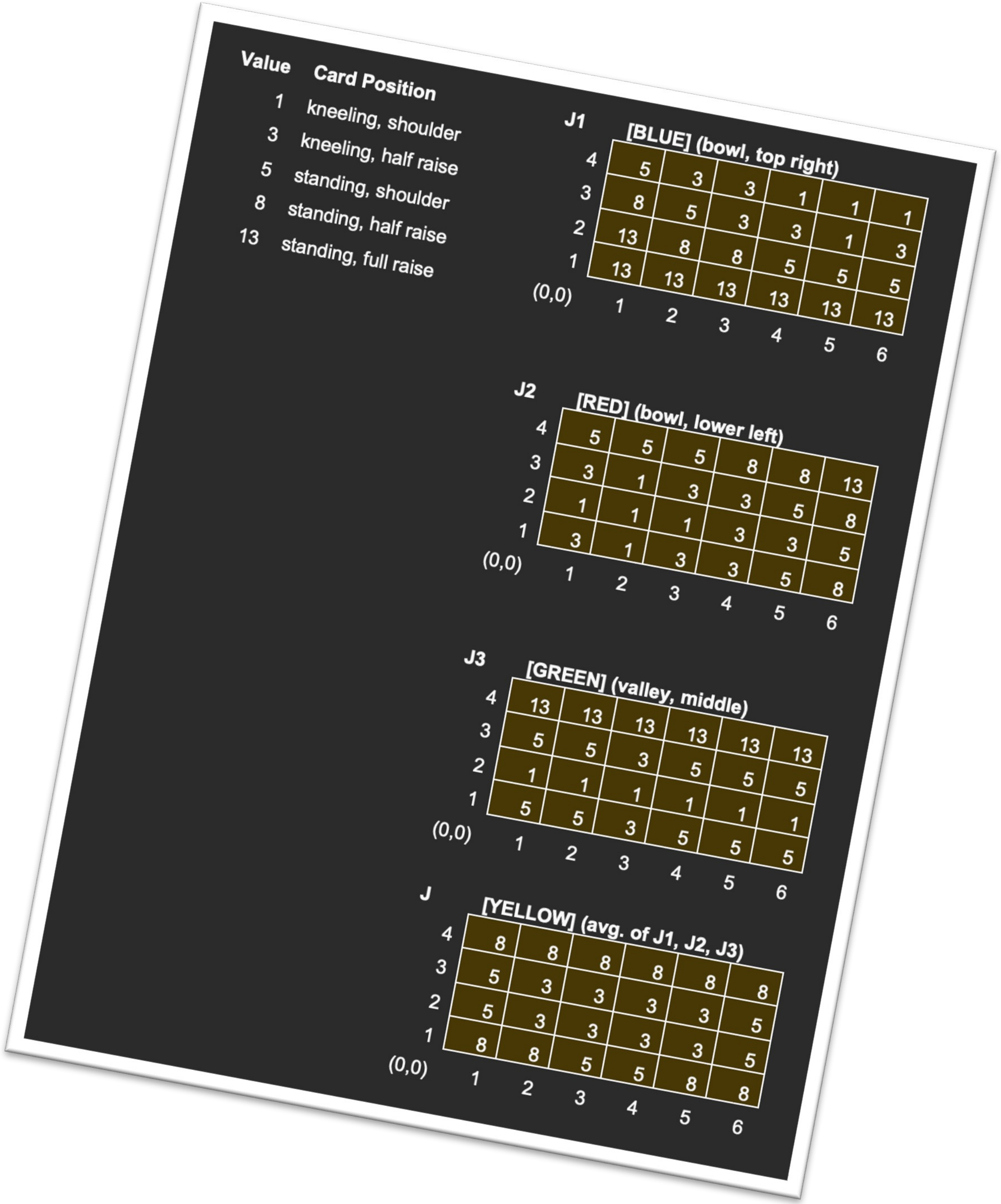
$$J(\boldsymbol{\theta}) = \frac{1}{N} \sum_{i=1}^{N} J^{(i)}(\boldsymbol{\theta})$$

Expectation of a Stochastic Gradient:

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

$$\begin{aligned} E\left[\nabla_{\boldsymbol{\theta}} J^{(i)}(\boldsymbol{\theta})\right] &= \sum_{i=1}^{N} \left(\text{probability of selecting } \boldsymbol{x}^{(i)}, y^{(i)}\right) \nabla_{\boldsymbol{\theta}} J^{(i)}(\boldsymbol{\theta}) \\ &= \sum_{i=1}^{N} \left(\frac{1}{N}\right) \nabla_{\boldsymbol{\theta}} J^{(i)}(\boldsymbol{\theta}) \\ &= \frac{1}{N} \sum_{i=1}^{N} \nabla_{\boldsymbol{\theta}} J^{(i)}(\boldsymbol{\theta}) \\ &= \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) \end{aligned}$$

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



Value	Card Position
1	kneeling, shoulder
3	kneeling, half raise
5	standing, shoulder
8	standing, half raise
13	standing, full raise

J1 [BLUE] (bowl, top right)

(0,0)	1	2	3	4	5	6
4	5	3	3	1	1	1
3	8	5	3	3	1	3
2	13	8	8	5	5	5
1	13	13	13	13	13	13

J2 [RED] (bowl, lower left)

(0,0)	1	2	3	4	5	6
4	5	5	5	8	8	13
3	3	1	3	3	5	8
2	1	1	1	3	3	5
1	3	1	3	3	5	8

J3 [GREEN] (valley, middle)

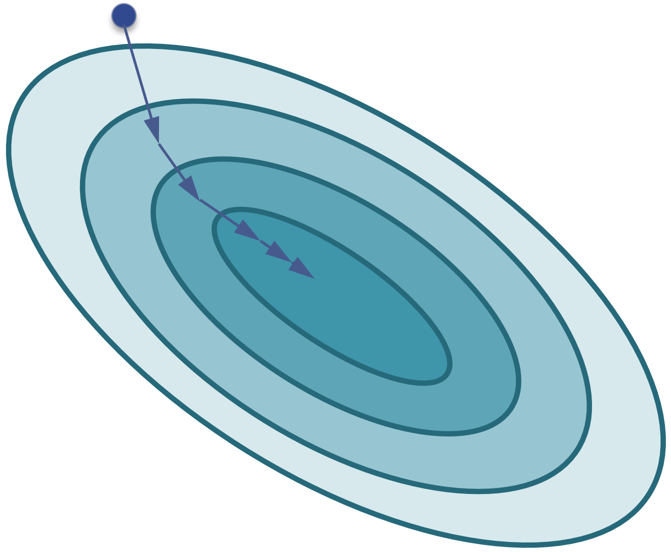
(0,0)	1	2	3	4	5	6
4	13	13	13	13	13	13
3	5	5	3	5	5	5
2	1	1	1	1	1	1
1	5	5	3	5	5	5

J [YELLOW] (avg. of J1, J2, J3)

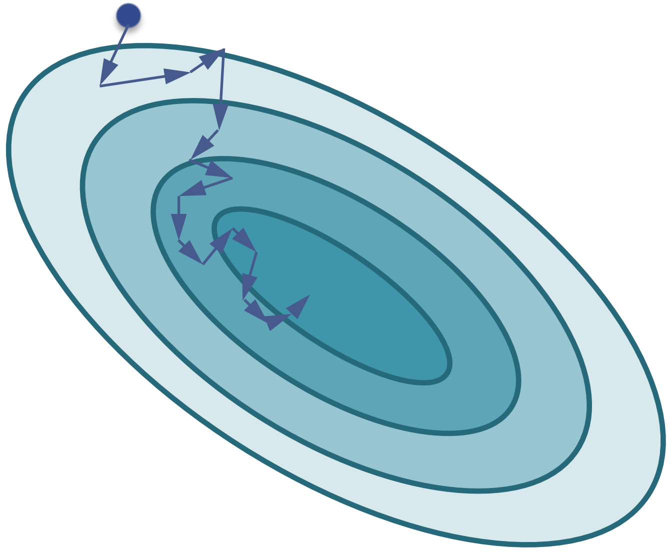
(0,0)	1	2	3	4	5	6
4	8	8	8	8	8	8
3	5	3	3	3	3	5
2	5	3	3	3	3	5
1	8	8	5	5	8	8

SGD VS. GRADIENT DESCENT

SGD vs. Gradient Descent



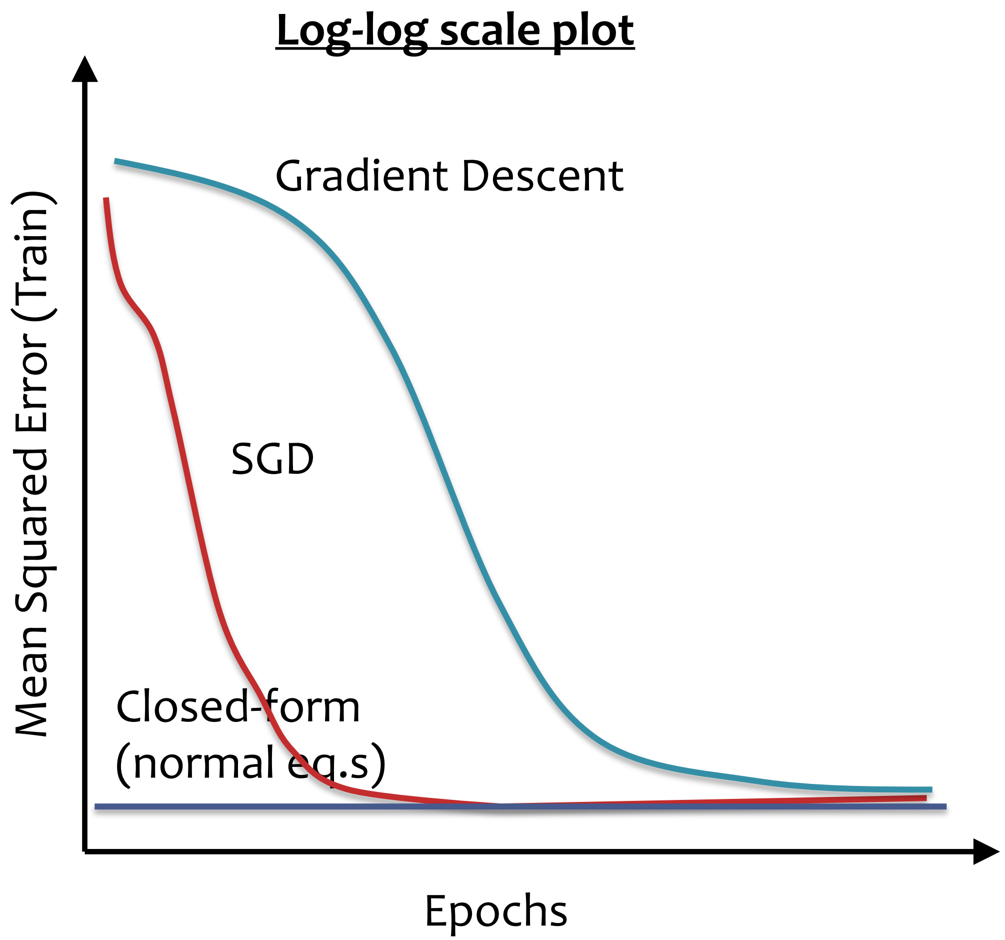
Gradient Descent



Stochastic Gradient Descent

SGD vs. Gradient Descent

- Empirical comparison:



- *Def*: an **epoch** is a single pass through the training data

1. For GD, only **one update** per epoch
2. 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 Approximation

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

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*
   - ...

$$\hat{\boldsymbol{\theta}} = \underset{\boldsymbol{\theta}}{\text{argmin}}\, J(\boldsymbol{\theta})$$

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

$$\hat{y} = h_{\hat{\boldsymbol{\theta}}}(\mathbf{x}) = \hat{\boldsymbol{\theta}}^T\mathbf{x}$$

Gradient Calculation for Linear Regression

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

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

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 $J^{(i)}(\boldsymbol{\theta})$ [used by SGD]

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

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

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)

procedure LMS($\mathcal{D}$, $\boldsymbol{\theta}^{(0)}$)
  $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta}^{(0)}$ ▷ Initialize parameters
  while not converged **do**
    for $i \in$ shuffle($\{1, 2, \ldots, N\}$) **do**
      $\mathbf{g} \leftarrow (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)})\mathbf{x}^{(i)}$ ▷ Compute gradient
      $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \gamma \mathbf{g}$ ▷ Update parameters
  return $\boldsymbol{\theta}$

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

procedure GDLR($\mathcal{D}$, $\boldsymbol{\theta}^{(0)}$)
    $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta}^{(0)}$ ▷ Initialize parameters
    while not converged **do**
        $\mathbf{g} \leftarrow \sum_{i=1}^{N} (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}) \mathbf{x}^{(i)}$ ▷ Compute gradient
        $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \gamma \mathbf{g}$ ▷ Update parameters
    return $\boldsymbol{\theta}$

Solving Linear Regression

Question:

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.

Answer:

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

Likelihood Function

One R.V.

Given N **independent, identically distributed (iid)** samples D = $\{x^{(1)}, x^{(2)}, \ldots, x^{(N)}\}$ from a discrete **random variable** X with probability mass function (*pmf*) $p(x|\theta)$ …

- Case 1: The **likelihood** function

  $$L(\theta) = p(x^{(1)}|\theta)\, p(x^{(2)}|\theta) \ldots\, p(x^{(N)}|\theta)$$

The **likelihood** tells us how likely one sample is relative to another

- Case 2: The **log-likelihood** function is

  $$\ell(\theta) = \log p(x^{(1)}|\theta) + \ldots + \log p(x^{(N)}|\theta)$$

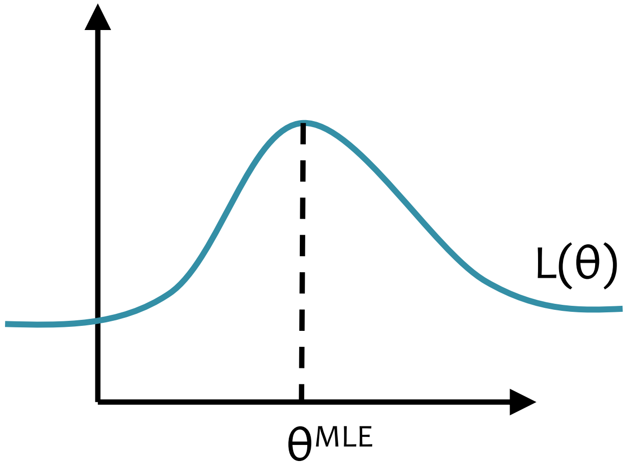
MLE

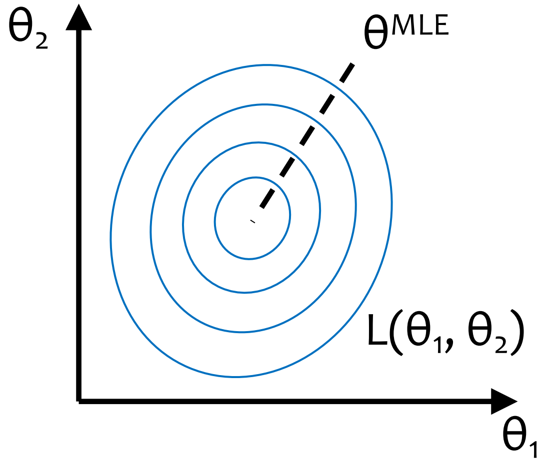
Suppose we have data $\mathcal{D} = \{x^{(i)}\}_{i=1}^{N}$

Principle of Maximum Likelihood Estimation:
Choose the parameters that maximize the likelihood of the data.

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

Maximum Likelihood Estimate (MLE)





Likelihood Function

Two R.V.s

Given N **iid** samples $D = \{(x^{(1)}, y^{(1)}), \ldots, (x^{(N)}, y^{(N)})\}$ from a pair of **random variables** X, Y where Y is **discrete** with probability mass function (pmf) $p(y \mid x, \theta)$

- Case 3: The **conditional likelihood** function:

$$L(\theta) = p(y^{(1)} \mid x^{(1)}, \theta) \ldots p(y^{(N)} \mid x^{(N)}, \theta)$$

- Case 4: The **conditional log-likelihood** function is

$$\ell(\theta) = \log p(y^{(1)} \mid x^{(1)}, \theta) + \ldots + \log p(y^{(N)} \mid x^{(N)}, \theta)$$

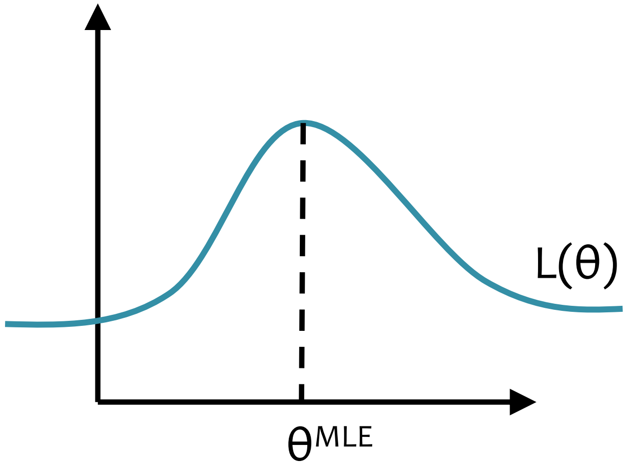
MLE

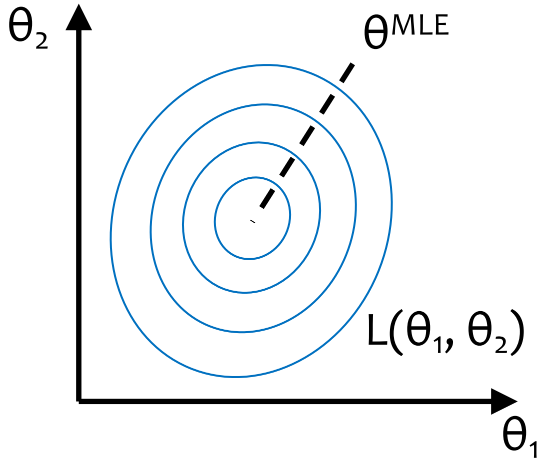
Suppose we have data $\mathcal{D} = \{(y^{(i)}, \mathbf{x}^{(i)})\}_{i=1}^{N}$

Principle of Maximum Likelihood Estimation:
Choose the parameters that maximize the conditional likelihood of the data.

$$\boldsymbol{\theta}^{\text{MLE}} = \underset{\boldsymbol{\theta}}{\text{argmax}} \prod_{i=1}^{N} p(y^{(i)} \mid \mathbf{x}^{(i)}, \boldsymbol{\theta})$$

Maximum Likelihood Estimate (MLE)





MLE

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

Principle of Maximum Likelihood Estimation:

Choose the parameters that maximize the conditional log-likelihood of the data.

$$\boldsymbol{\theta}^{\text{MLE}} = \underset{\boldsymbol{\theta}}{\text{argmax}} \prod_{i=1}^{N} p(y^{(i)} \mid \mathbf{x}^{(i)}, \boldsymbol{\theta})$$

$$= \underset{\boldsymbol{\theta}}{\text{argmax}} \sum_{i=1}^{N} \log p(y^{(i)} \mid \mathbf{x}^{(i)}, \boldsymbol{\theta})$$

MLE

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

Principle of Maximum Likelihood Estimation:

Choose the parameters that minimize the negative conditional log-likelihood of the data.

$$\boldsymbol{\theta}^{\text{MLE}} = \underset{\boldsymbol{\theta}}{\text{argmax}} \prod_{i=1}^{N} p(y^{(i)} \mid \mathbf{x}^{(i)}, \boldsymbol{\theta})$$

$$= \underset{\boldsymbol{\theta}}{\text{argmax}} \sum_{i=1}^{N} \log p(y^{(i)} \mid \mathbf{x}^{(i)}, \boldsymbol{\theta})$$

$$= \underset{\boldsymbol{\theta}}{\text{argmin}} - \sum_{i=1}^{N} \log p(y^{(i)} \mid \mathbf{x}^{(i)}, \boldsymbol{\theta})$$

MLE

What does maximizing likelihood accomplish?

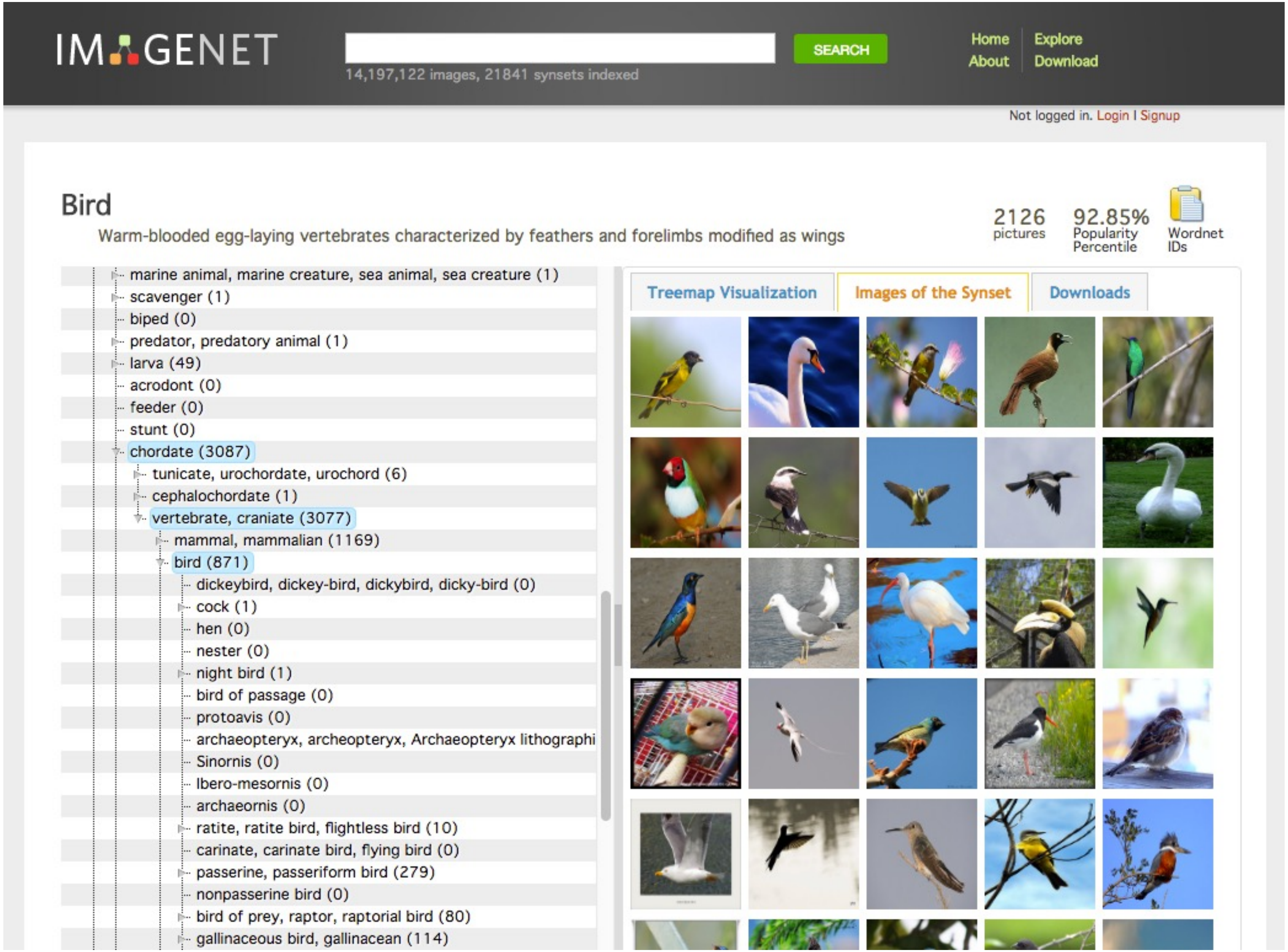
- There is only a finite amount of probability mass (i.e. sum-to-one constraint)
- MLE tries to allocate **as much** probability mass **as possible** to the things we have observed…

  …**at the expense** of the things we have **not** observed

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
Warm-blooded egg-laying vertebrates characterized by feathers and forelimbs modified as wings
2126 pictures
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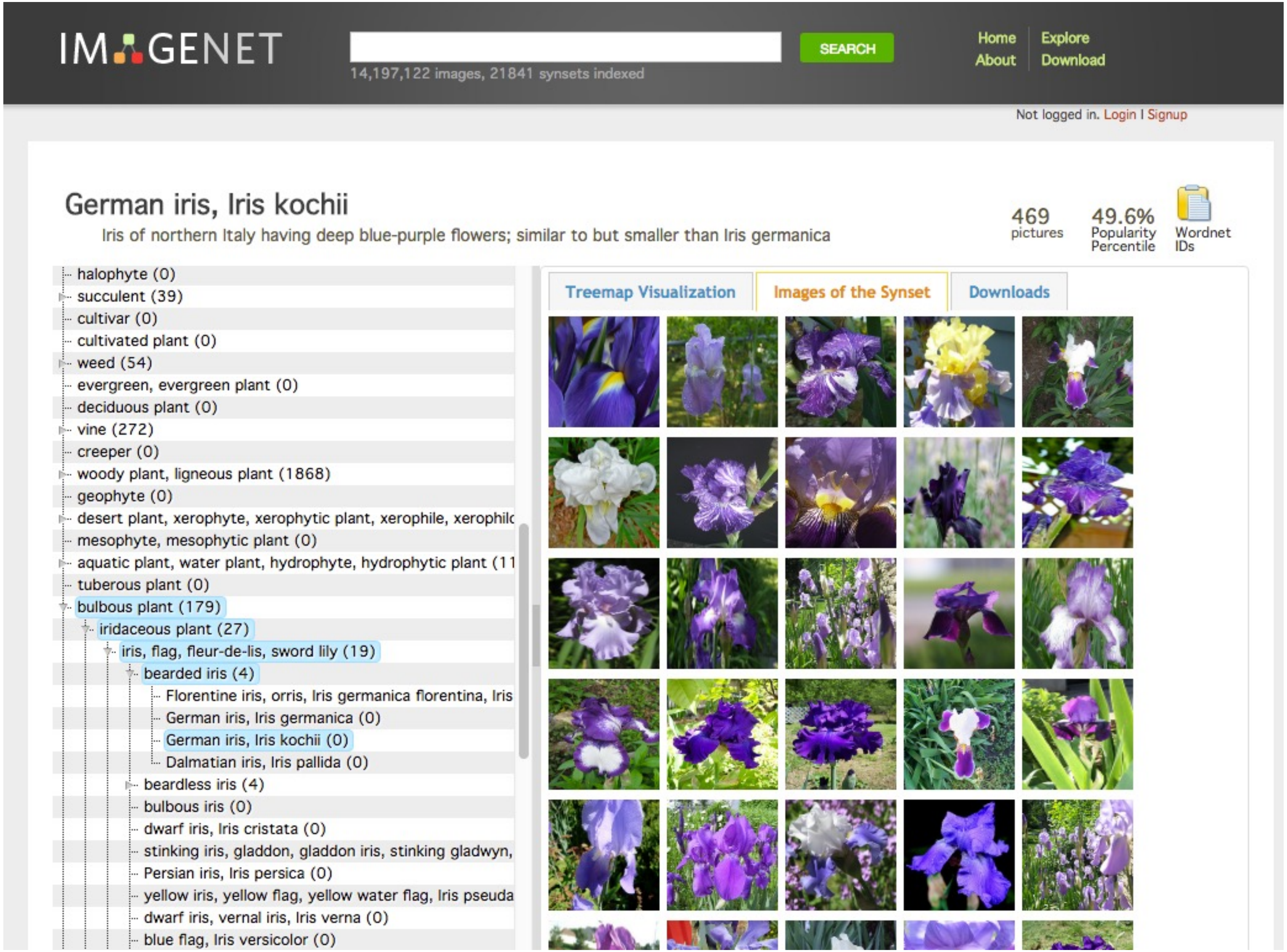
marine animal, marine creature, sea animal, sea creature (1)
scavenger (1)
biped (0)
predator, predatory animal (1)
larva (49)
acrodont (0)
feeder (0)
stunt (0)
chordate (3087)
tunicate, urochordate, urochord (6)
cephalochordate (1)
vertebrate, craniate (3077)
mammal, mammalian (1169)
bird (871)
dickeybird, dickey-bird, dickybird, dicky-bird (0)
cock (1)
hen (0)
nester (0)
night bird (1)
bird of passage (0)
protoavis (0)
archaeopteryx, archeopteryx, Archaeopteryx lithographi
Sinornis (0)
Ibero-mesornis (0)
archaeornis (0)
ratite, ratite bird, flightless bird (10)
carinate, carinate bird, flying bird (0)
passerine, passeriform bird (279)
nonpasserine bird (0)
bird of prey, raptor, raptorial bird (80)
gallinaceous bird, gallinacean (114)
Treemap Visualization
Images of the Synset
Downloads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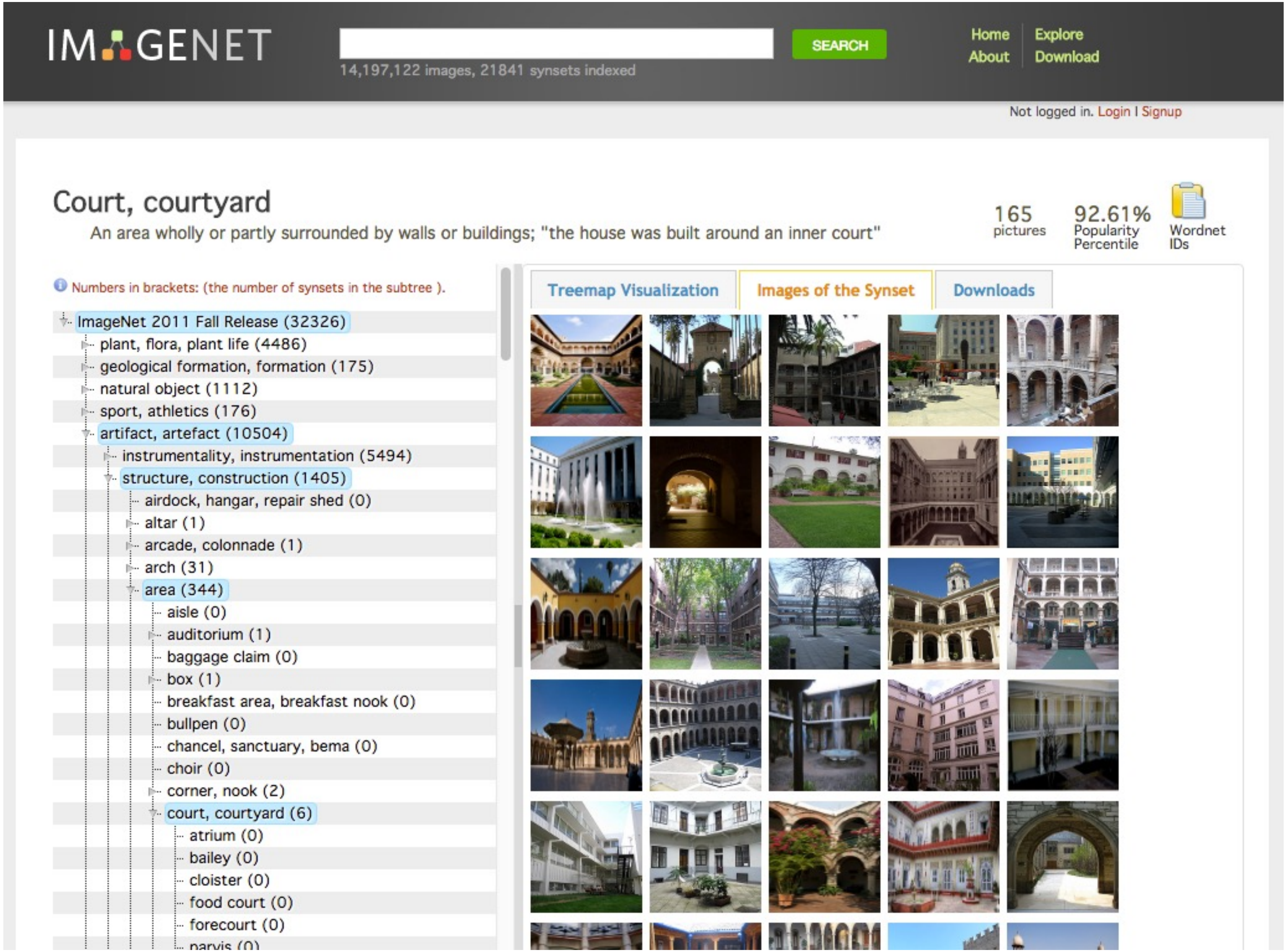
German iris, Iris kochii
Iris of northern Italy having deep blue-purple flowers; similar to but smaller than Iris germanica
469 pictures
49.6% Popularity Percentile
Wordnet IDs
halophyte (0)
succulent (39)
cultivar (0)
cultivated plant (0)
weed (54)
evergreen, evergreen plant (0)
deciduous plant (0)
vine (272)
creeper (0)
woody plant, ligneous plant (1868)
geophyte (0)
desert plant, xerophyte, xerophytic plant, xerophile, xerophilc
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)
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)
Treemap Visualization
Images of the Synset
Downloads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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
Wordnet IDs
Numbers in brackets: (the number of synsets in the subtree).
ImageNet 2011 Fall Release (32326)
plant, flora, plant life (4486)
geological formation, formation (175)
natural object (1112)
sport, athletics (176)
artifact, artefact (10504)
instrumentality, instrumentation (5494)
structure, construction (1405)
airdock, hangar, repair shed (0)
altar (1)
arcade, colonnade (1)
arch (31)
area (344)
aisle (0)
auditorium (1)
baggage claim (0)
box (1)
breakfast area, breakfast nook (0)
bullpen (0)
chancel, sanctuary, bema (0)
choir (0)
corner, nook (2)
court, courtyard (6)
atrium (0)
bailey (0)
cloister (0)
food court (0)
forecourt (0)
Treemap Visualization
Images of the Synset
Downloads

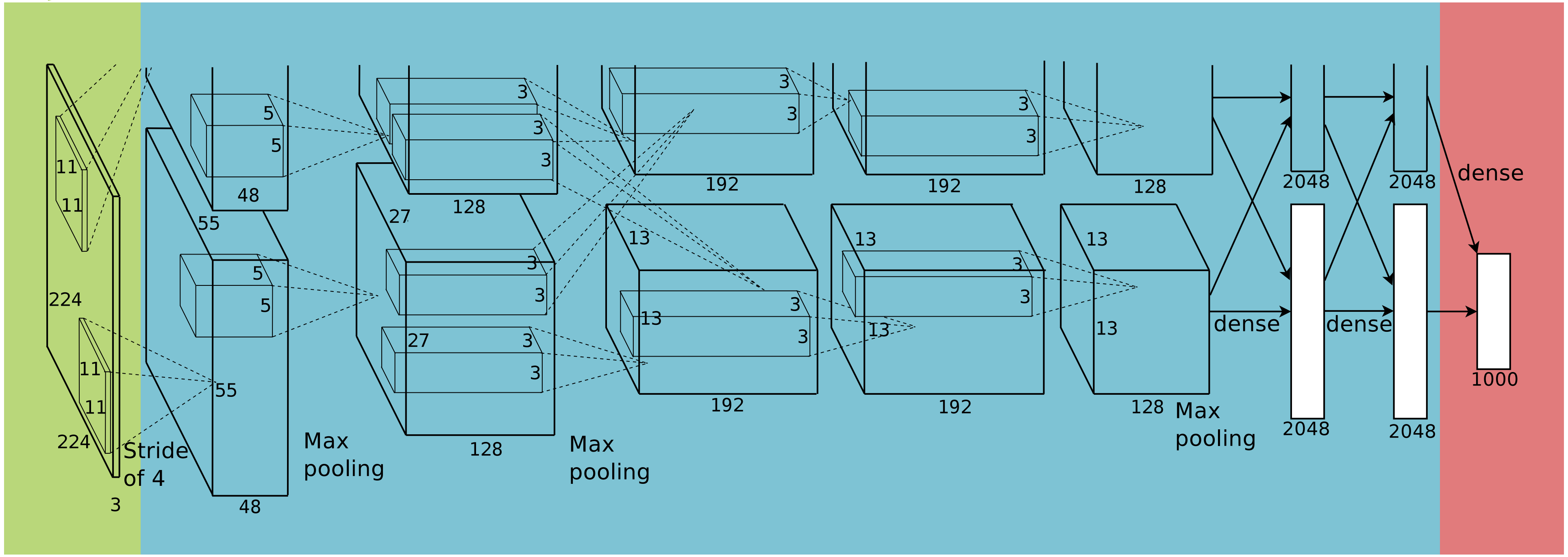
Example: Image Classification

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



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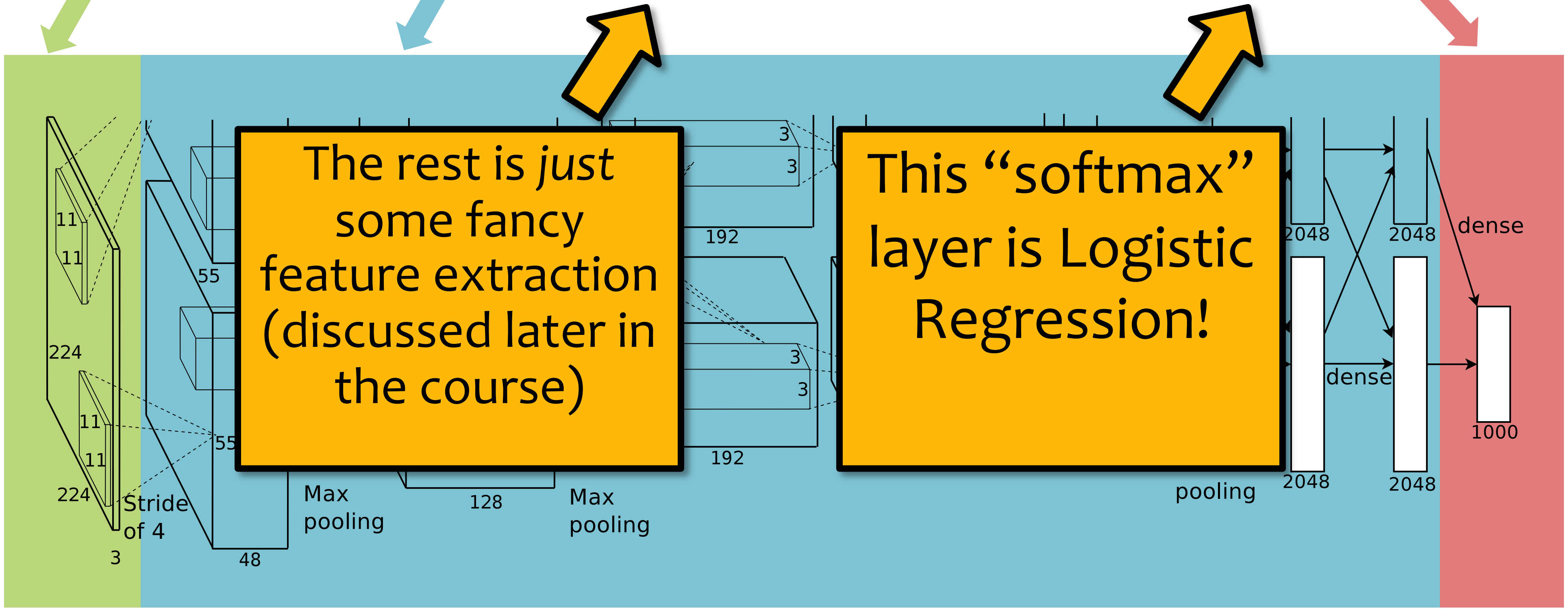
- Three fully connected layers

1000-way softmax



LOGISTIC REGRESSION

Logistic Regression

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

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

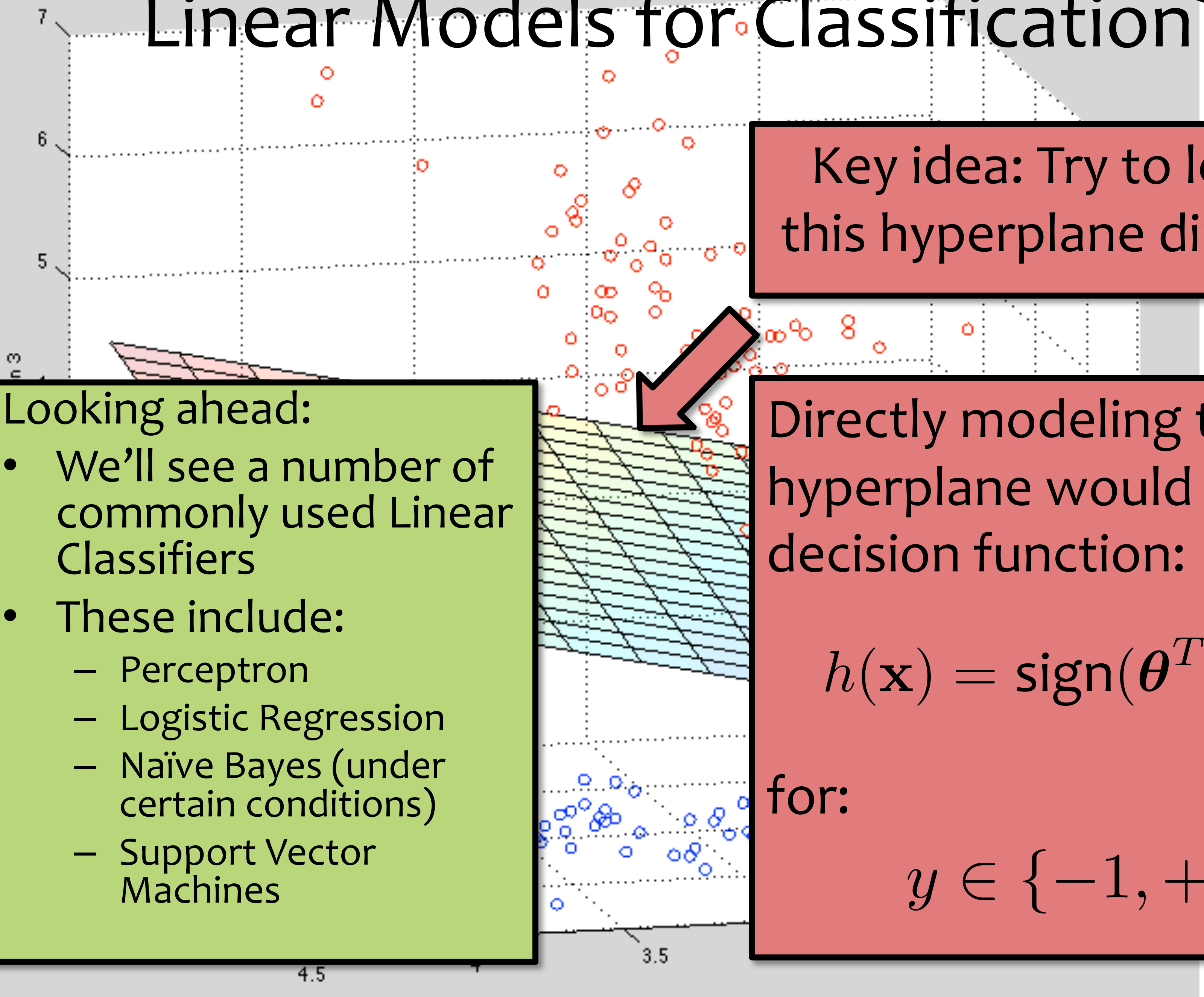
We are back to classification.

Despite the name logistic **regression.**

Linear Models for Classification

Recall…

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:

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

for:

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

Recall…

Background: Hyperplanes

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 to get **x'**!

Hyperplane (Definition 1):

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

Hyperplane (Definition 2):

$$\mathcal{H} = \{\mathbf{x}' : \boldsymbol{\theta}^T \mathbf{x}' = 0 \text{ and } x'_1 = 1\}$$

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

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

Half-spaces:

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

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

Using gradient descent for linear classifiers

Key idea behind today's lecture:

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

Optimization for Linear Classifiers

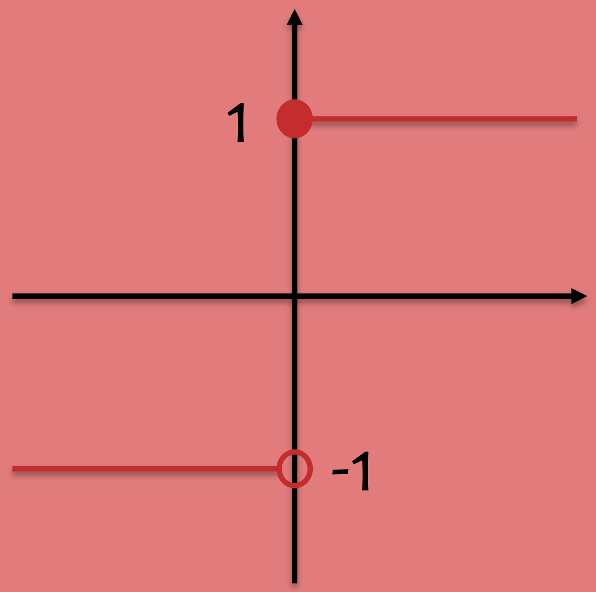
MSE for [your favorite model]

What is $\boldsymbol{\theta}^T \boldsymbol{x}$?

sign(·) vs. sigmoid(·)

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

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

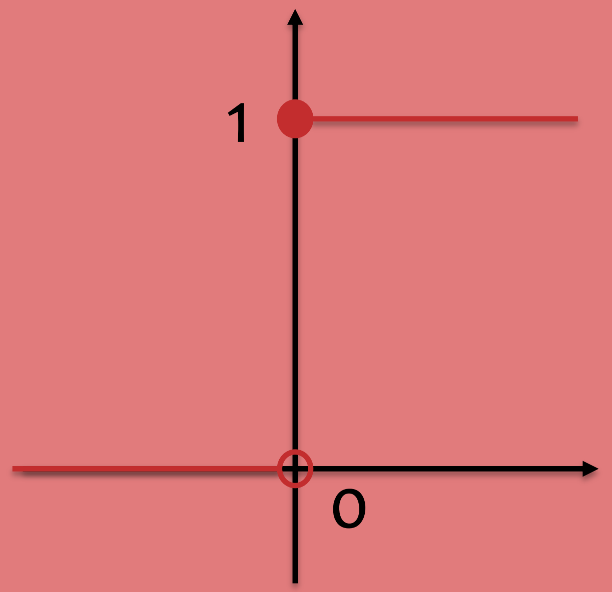


sign(u)

sign(·) vs. sigmoid(·)

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

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



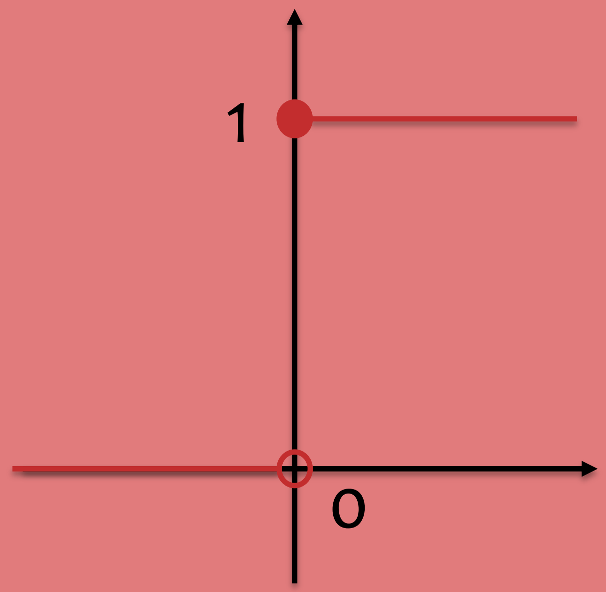
“sign”(u)

Goal: Learn a linear classifier with Gradient Descent

sign(·) vs. sigmoid(·)

But this decision function isn't differentiable…

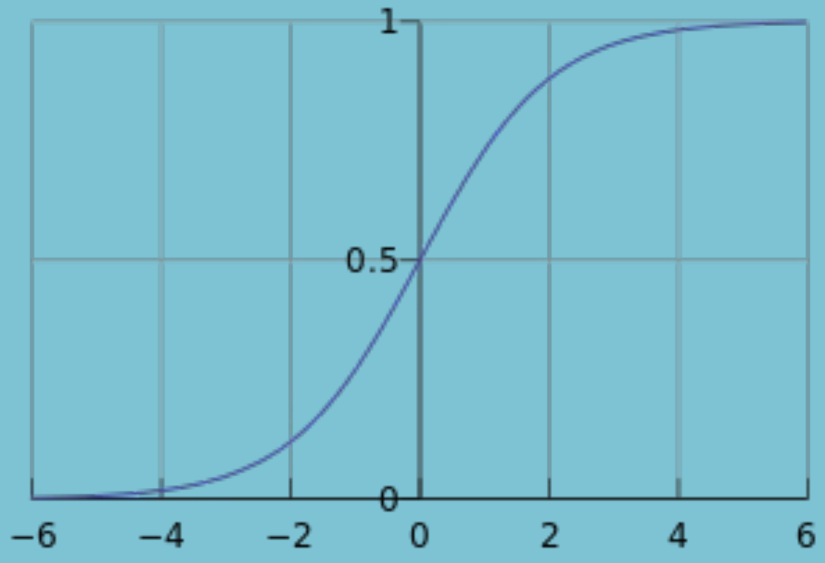
$$h(\mathbf{x}) = \text{"sign"}(\boldsymbol{\theta}^T \mathbf{x})$$



"sign"(u)

Use a differentiable function instead!

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



$$\text{logistic}(u) \equiv \frac{1}{1 + e^{-u}}$$

The *logistic* function is also called the *sigmoid* function.

Logistic Regression

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

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. $\boldsymbol{\theta}^* = \underset{\boldsymbol{\theta}}{\operatorname{argmin}}\, J(\boldsymbol{\theta})$

Prediction: Output is the most probable class.

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

Logistic Regression

1. Model

2. Objective

Logistic Regression

3A. Derivatives

3B. Gradients

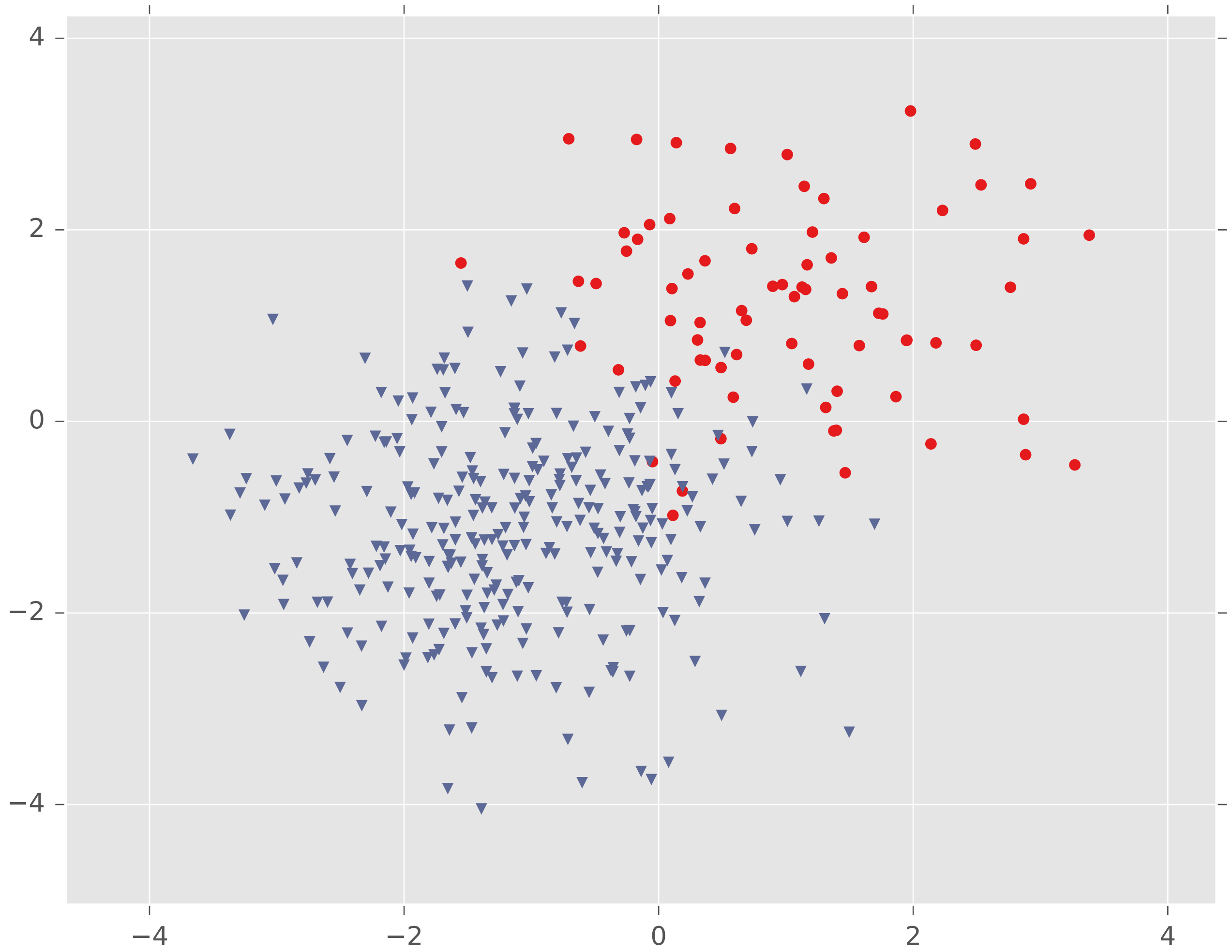
Logistic Regression

4. Optimization

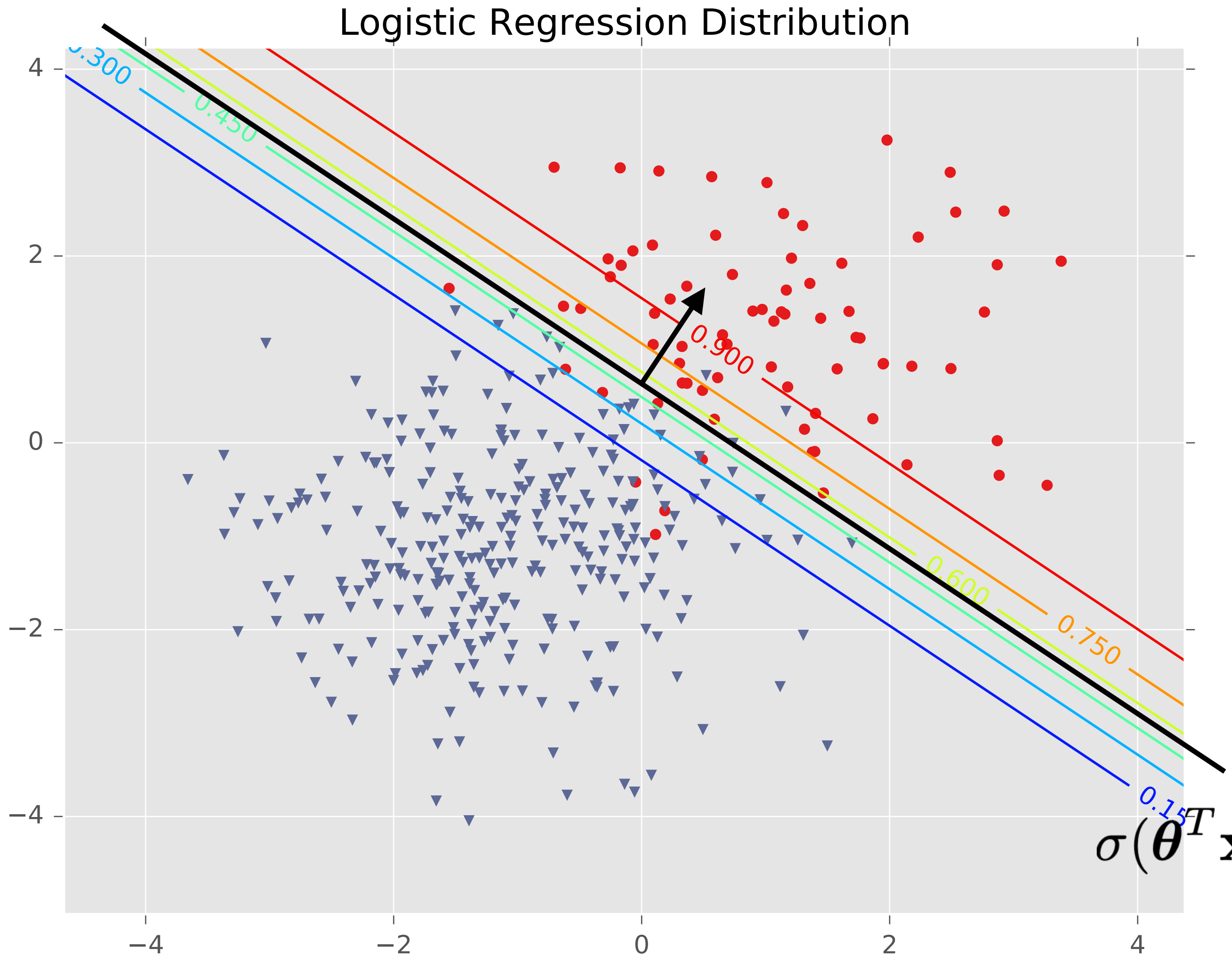
5. Prediction

LOGISTIC REGRESSION ON GAUSSIAN DATA

Logistic Regression

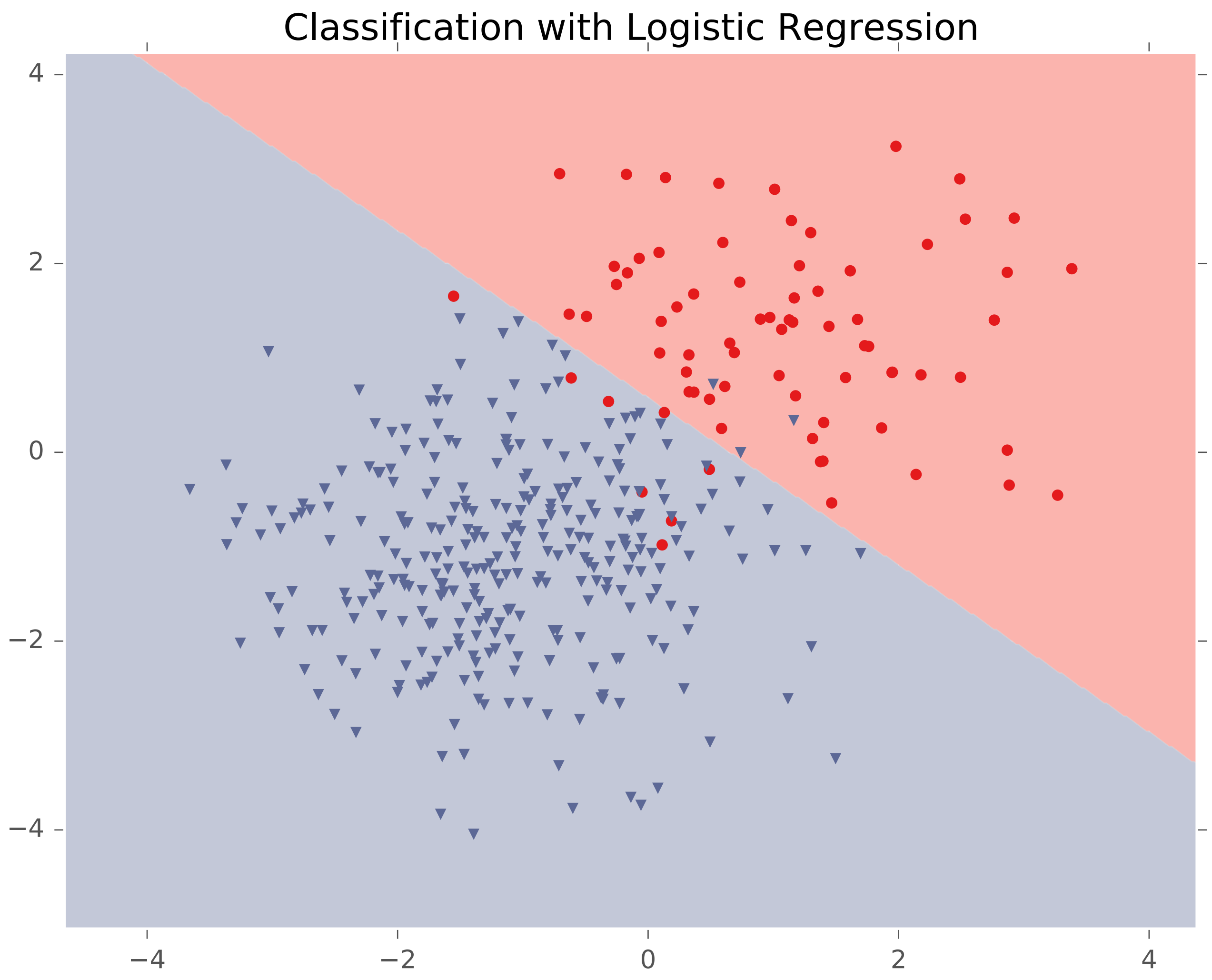


Logistic Regression



$$\sigma(\boldsymbol{\theta}^T \mathbf{x}) = 0.5$$

Logistic Regression



LEARNING LOGISTIC REGRESSION

SGD for Logistic Regression

Question:

Which of the following is a correct description of SGD for Logistic Regression?

Answer:

At each step (i.e. iteration) of SGD for Logistic Regression we…

A. (1) compute the gradient of the log-likelihood for all examples (2) update all the parameters using the gradient

B. (1) ask Matt for a description of SGD for Logistic Regression, (2) write it down, (3) report that answer

C. (1) compute the gradient of the log-likelihood for all examples (2) randomly pick an example (3) update only the parameters for that example

D. (1) randomly pick a parameter, (2) compute the partial derivative of the log-likelihood with respect to that parameter, (3) update that parameter for all examples

E. (1) randomly pick an example, (2) compute the gradient of the log-likelihood for that example, (3) update all the parameters using that gradient

F. (1) randomly pick a parameter and an example, (2) compute the gradient of the log-likelihood for that example with respect to that parameter, (3) update that parameter using that gradient

Maximum **Conditional** Likelihood Estimation

Learning: finds the parameters that minimize some objective function.

$$\boldsymbol{\theta}^* = \underset{\boldsymbol{\theta}}{\operatorname{argmin}}\, J(\boldsymbol{\theta})$$

We minimize the *negative* log conditional likelihood:

$$J(\boldsymbol{\theta}) = -\log \prod_{i=1}^{N} p_{\boldsymbol{\theta}}(y^{(i)}|\mathbf{x}^{(i)})$$

Why?

1. We can't maximize likelihood (as in Naïve Bayes) because we don't have a joint model p(x,y)
2. It worked well for Linear Regression (least squares is actually MCLE! more on this later…)

Maximum **Conditional** Likelihood Estimation

Learning: Four approaches to solving $\boldsymbol{\theta}^* = \underset{\boldsymbol{\theta}}{\text{argmin}}\, J(\boldsymbol{\theta})$

Approach 1: Gradient Descent
(take larger – more certain – steps opposite the gradient)

Approach 2: Stochastic Gradient Descent (SGD)
(take many small steps opposite the gradient)

Approach 3: Newton's Method
(use second derivatives to better follow curvature)

Approach 4: Closed Form???
(set derivatives equal to zero and solve for parameters)

Maximum **Conditional** Likelihood Estimation

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Approach 3: Newton's Method
(use second derivatives to better follow curvature)

~~**Approach 4:** Closed Form???
(set derivatives equal to zero and solve for parameters)~~

Logistic Regression does not have a closed form solution for MLE parameters.

Logistic Regression Objectives

You should be able to…

- Apply the principle of maximum likelihood estimation (MLE) to learn the parameters of a probabilistic model
- Given a discriminative probabilistic model, derive the conditional log-likelihood, its gradient, and the corresponding Bayes Classifier
- Explain the practical reasons why we work with the **log** of the likelihood
- Implement logistic regression for binary classification
- Prove that the decision boundary of binary logistic regression is linear