10-601 Introduction to Machine Learning

Machine Learning Department
School of Computer Science
Carnegie Mellon University

Logistic Regression

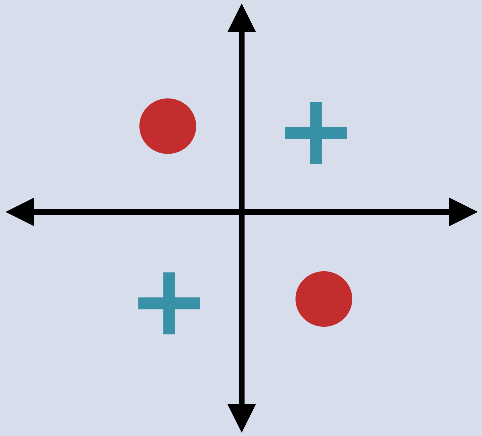
Matt Gormley
Lecture 9
Feb. 13, 2019

Q&A

Q: In recitation, we only covered the Perceptron mistake bound for **linearly separable data.** Isn't that an unrealistic setting?

A: Not at all! Even if your data isn't linearly separable to begin with, we can often add features to make it so.

x_1	x_2	y
+1	+1	+
+1	-1	-
-1	+1	-
-1	-1	+



Exercise: Add another feature to transform this nonlinearly separable data into linearly separable data.

Reminders

- Homework 3: KNN, Perceptron, Lin.Reg.
  - Out: Wed, Feb 6
  - Due: Fri, Feb 15 at 11:59pm
- Homework 4: Logistic Regression
  - Out: Fri, Feb 15
  - Due: Fri, Mar 1 at 11:59pm
- Midterm Exam 1
  - Thu, Feb 21, 6:30pm – 8:00pm
- Today's In-Class Poll
  - http://p9.mlcourse.org

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?

Bayes Optimal Classifier

Whiteboard

- Bayes Optimal Classifier
- Reducible / irreducible error
- Ex: Bayes Optimal Classifier for 0/1 Loss

Learning from Data (Frequentist)

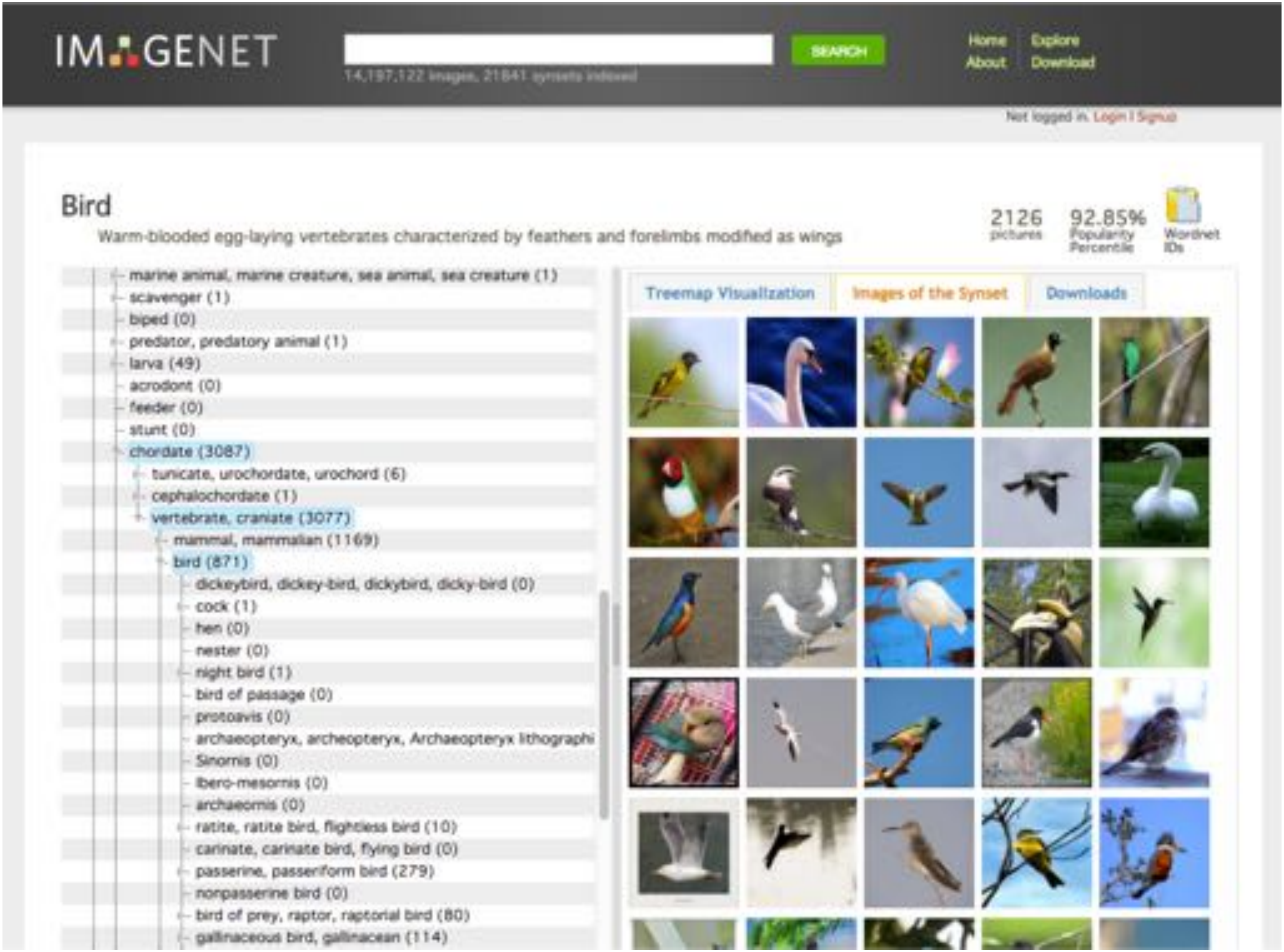
Whiteboard

- Principle of Maximum Likelihood Estimation (MLE)
- Strawmen:
  - Example: Bernoulli
  - Example: Gaussian
  - Example: Conditional #1
    (Bernoulli conditioned on Gaussian)
  - Example: Conditional #2
    (Gaussians conditioned on Bernoulli)

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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14,197,122 images, 21841 synsets indexed
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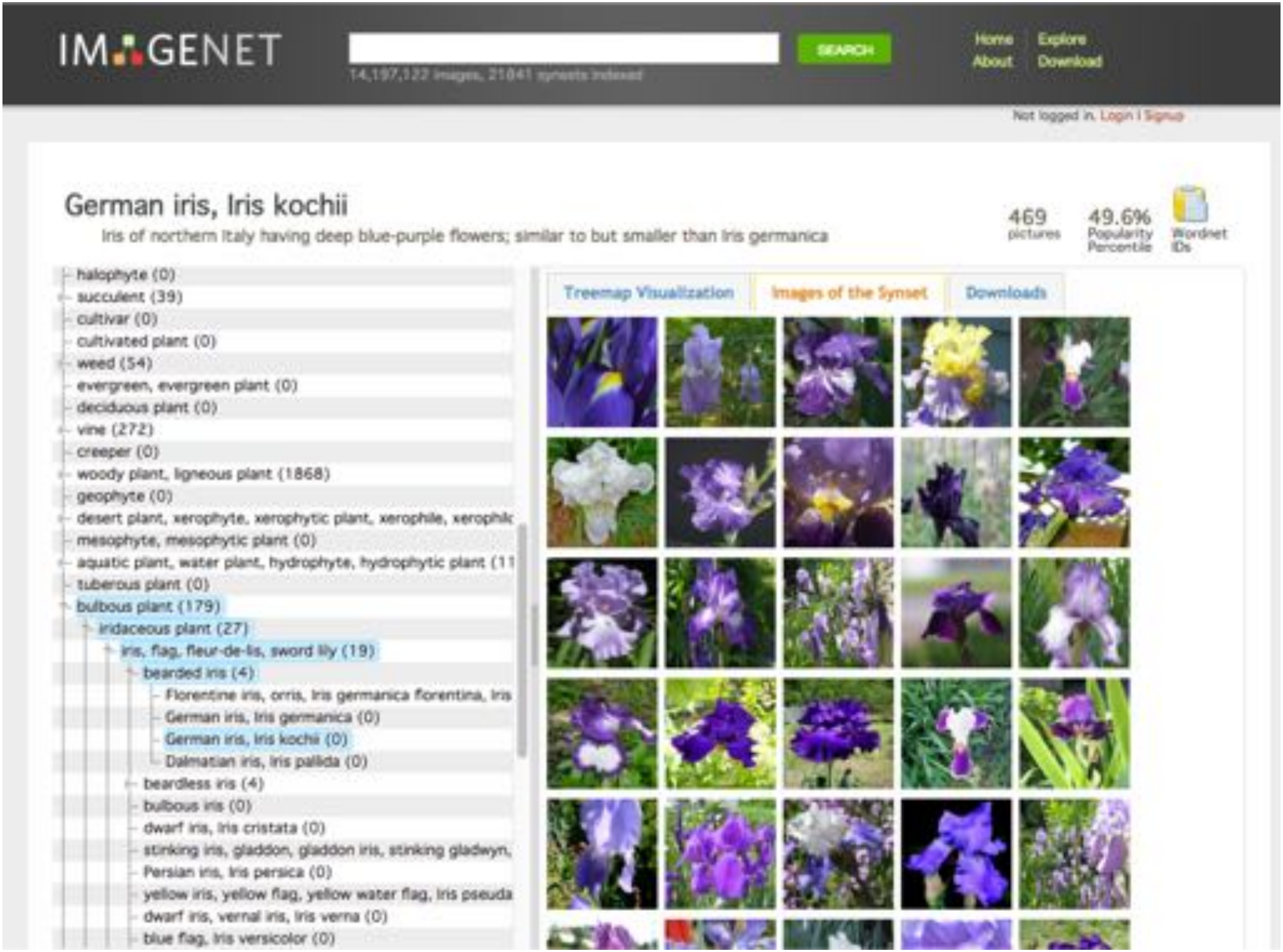
Bird
Warm-blooded egg-laying vertebrates characterized by feathers and forelimbs modified as wings
2126 pictures
92.85% Popularity Percentile
Wordnet IDs
marine animal, marine creature, sea animal, sea creature (1)
scavenger (1)
biped (0)
predator, predatory animal (1)
larva (49)
acrodont (0)
feeder (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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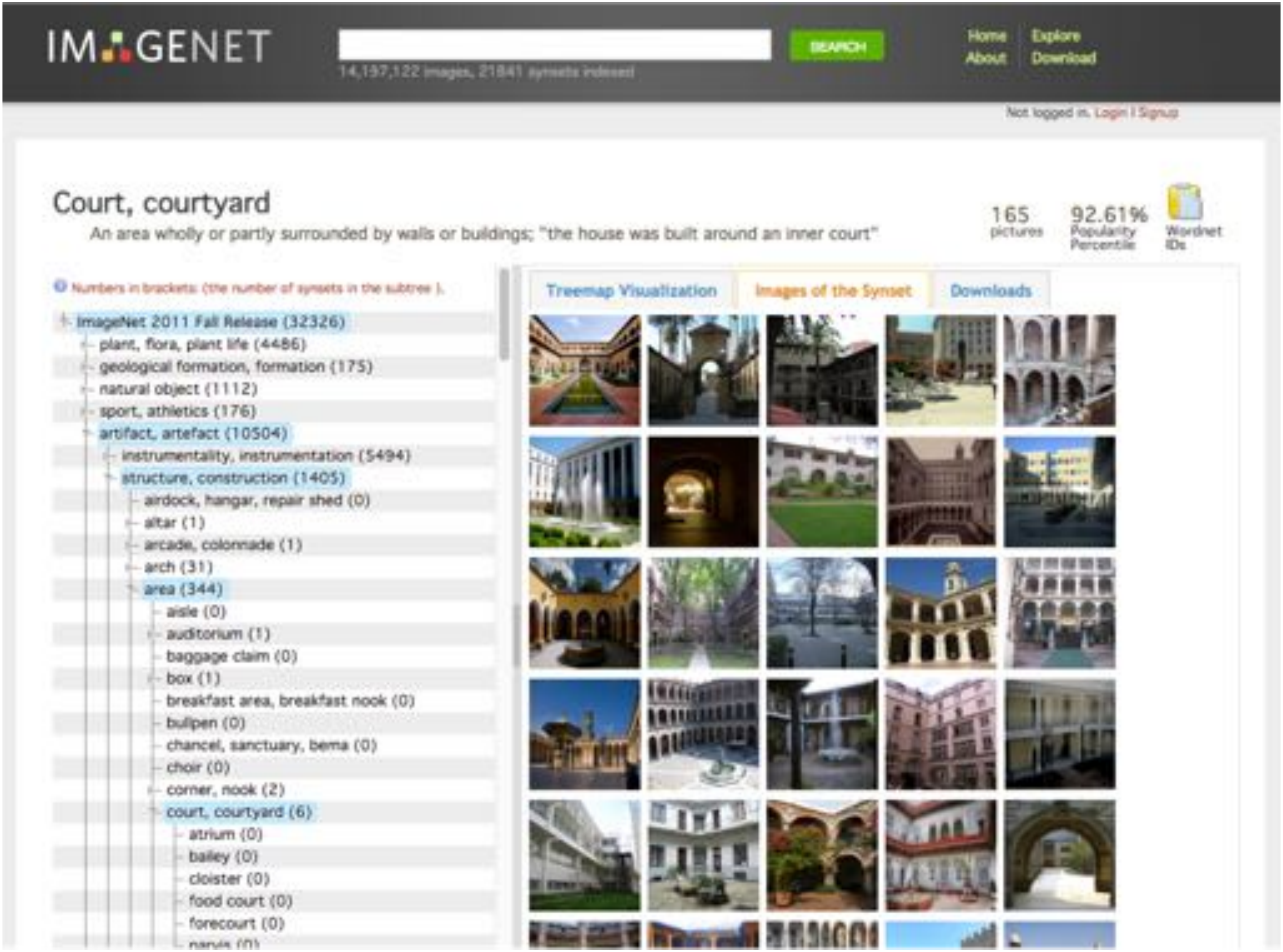
German iris, Iris kochii
Iris of northern Italy having deep blue-purple flowers; similar to but smaller than Iris germanica
469 pictures
49.6% Popularity Percentile
Wordnet IDs
halophyte (0)
succulent (39)
cultivar (0)
cultivated plant (0)
weed (54)
evergreen, evergreen plant (0)
deciduous plant (0)
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

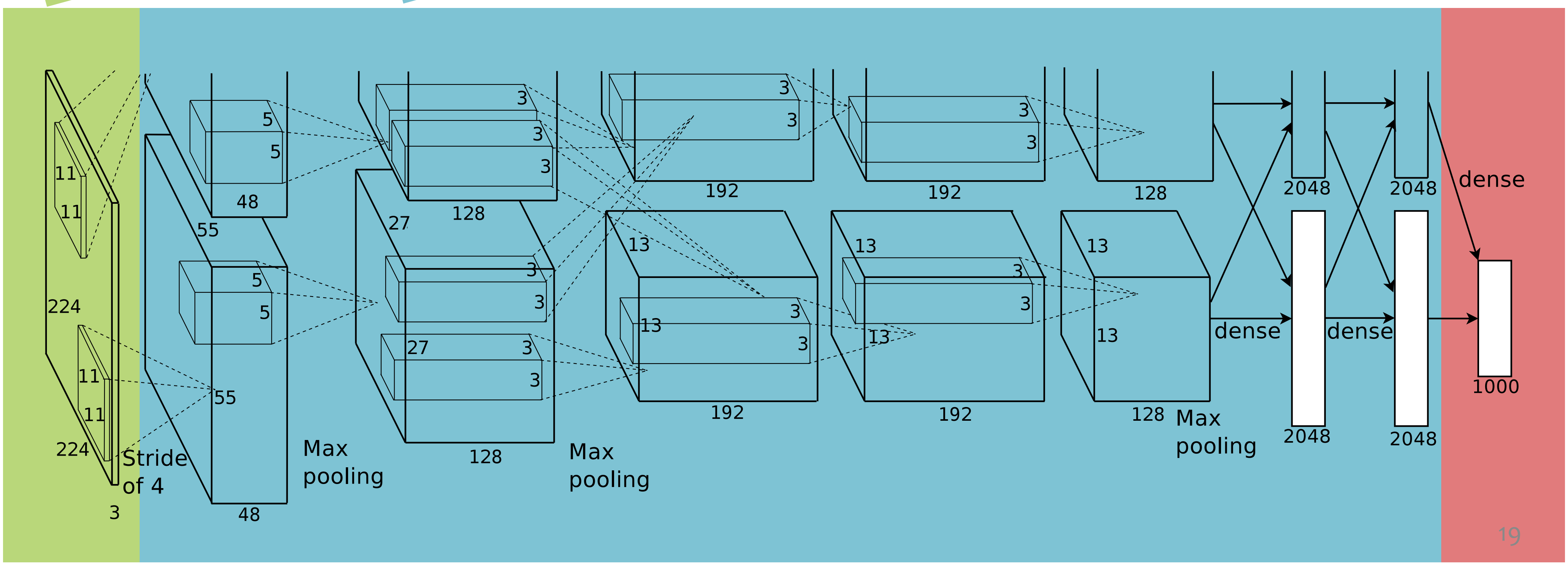
Example: Image Classification

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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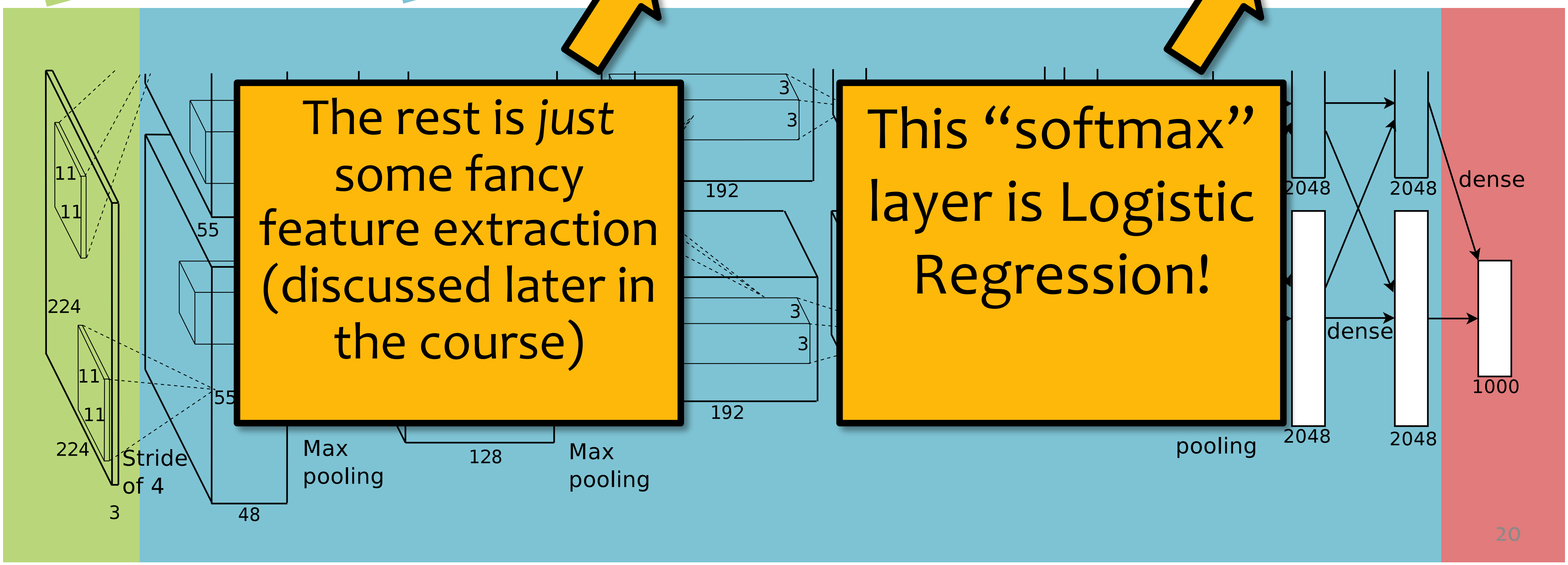


The rest is *just* some fancy feature extraction (discussed later in the course)

This "softmax" layer is Logistic Regression!

LOGISTIC REGRESSION

Logistic Regression

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

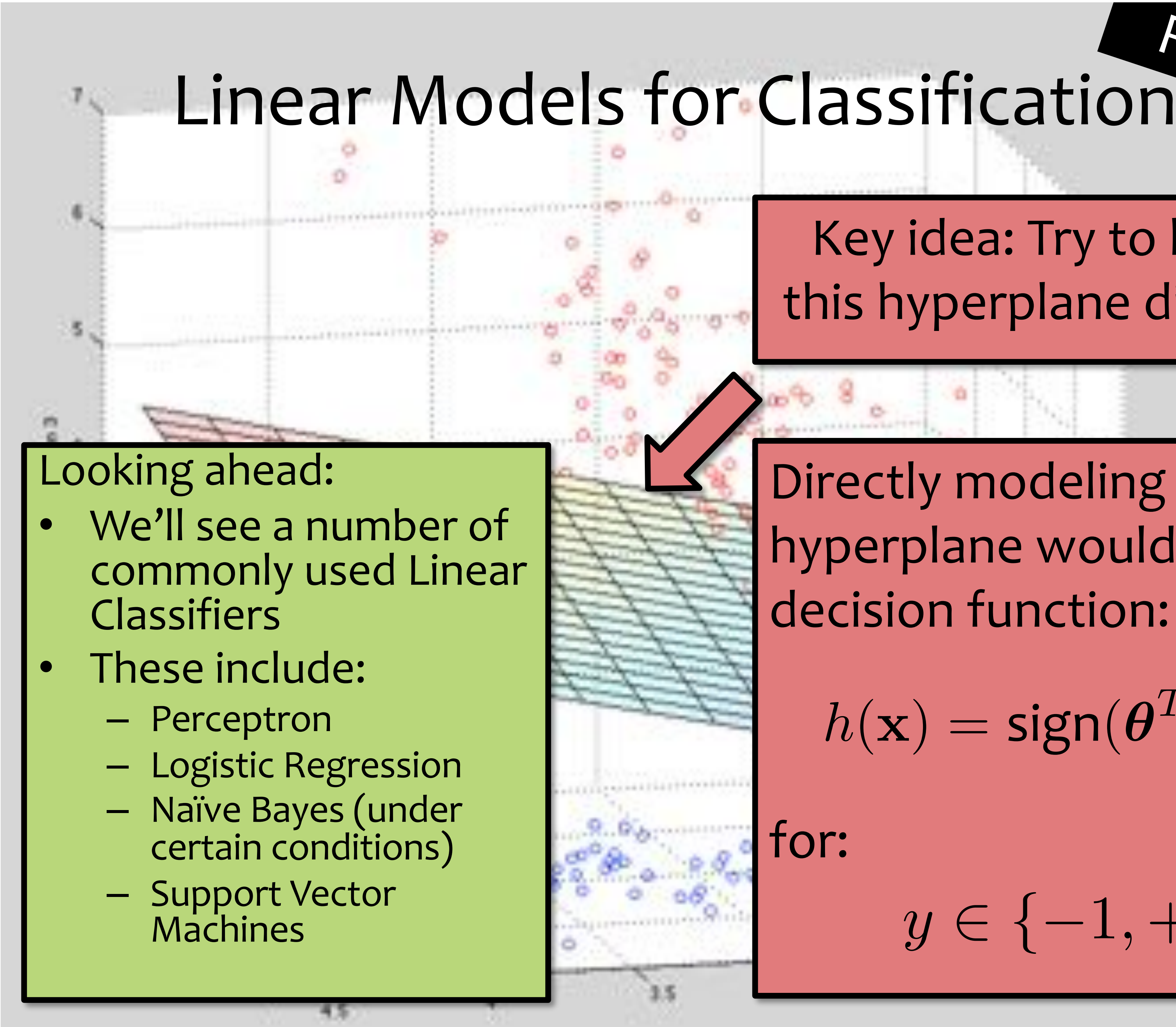
$$\mathcal{D} = \{\mathbf{x}^{(i)}, y^{(i)}\}_{i=1}^{N} \text{ where } \mathbf{x} \in \mathbb{R}^M \text{ and } y \in \{0, 1\}$$

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:

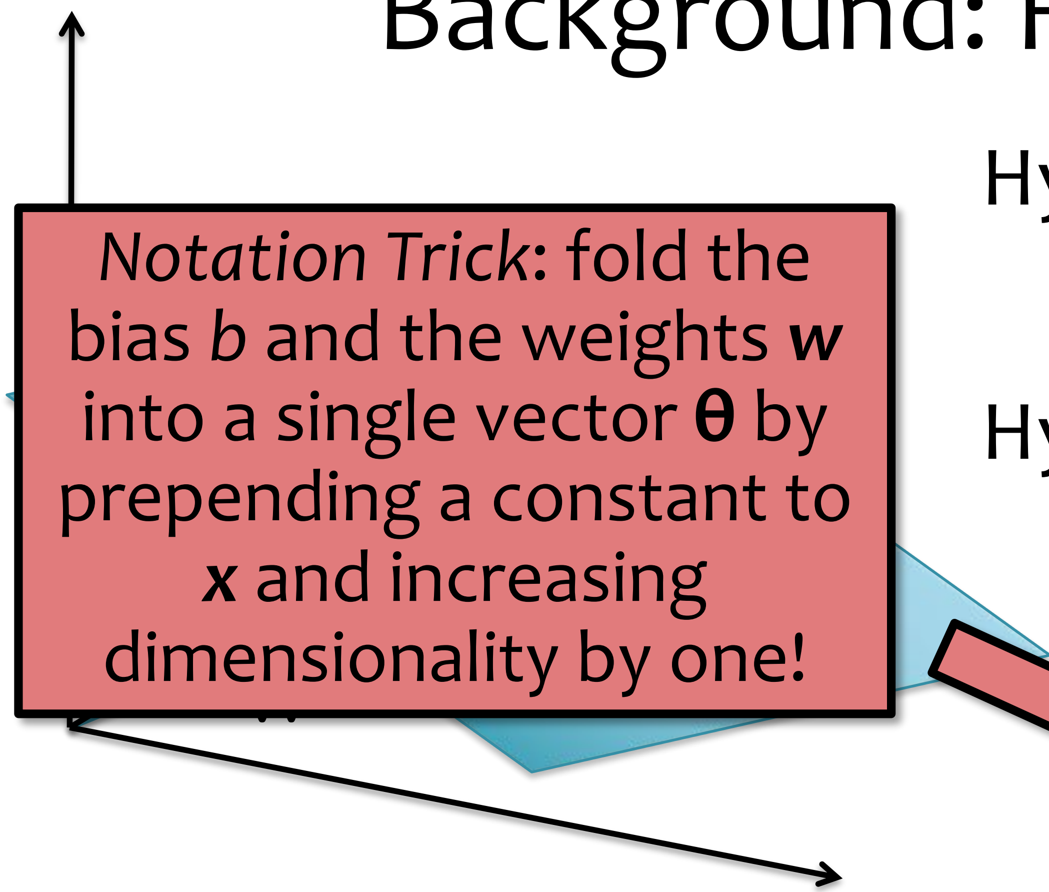
$$h(\mathbf{x}) = \text{sign}(\boldsymbol{\theta}^T \mathbf{x})$$

for:

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

Recall...

Background: Hyperplanes



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

Hyperplane (Definition 1):

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

Hyperplane (Definition 2):

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

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

Half-spaces:

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

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

Using gradient ascent for linear classifiers

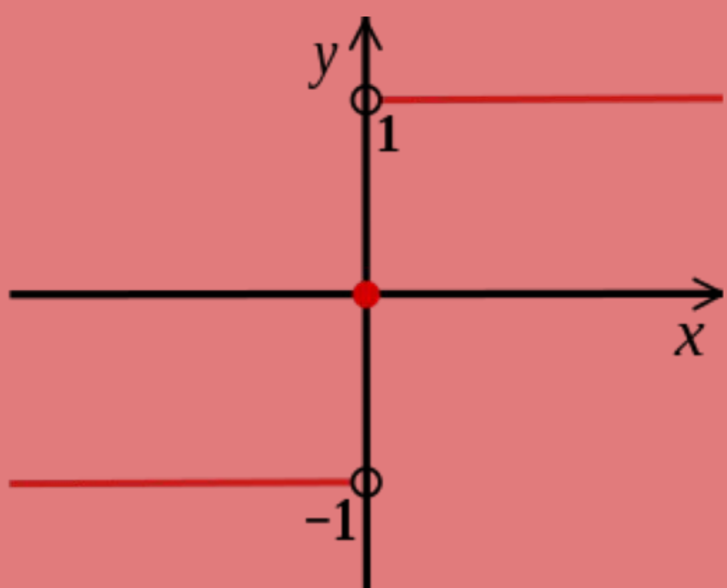
Key idea behind today's lecture:

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

Using gradient ascent for linear classifiers

This decision function isn't differentiable:

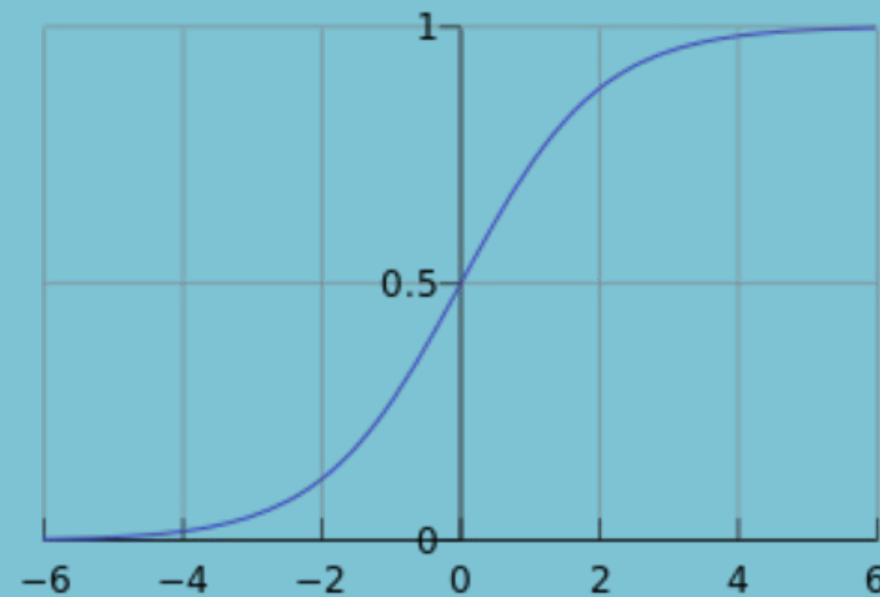
$$h(\mathbf{x}) = \text{sign}(\boldsymbol{\theta}^T \mathbf{x})$$



sign(x)

Use a differentiable function instead:

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



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

Using gradient ascent for linear classifiers

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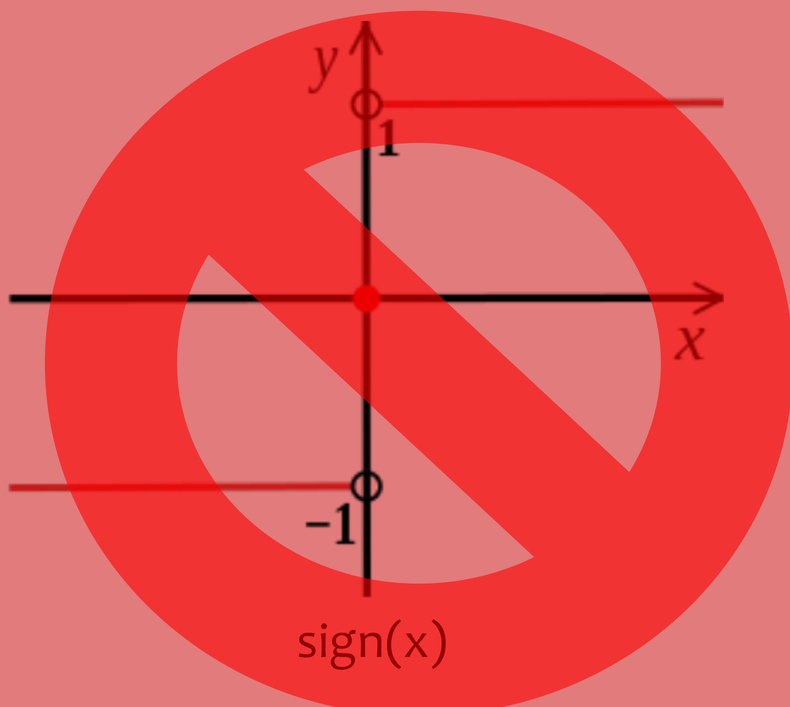

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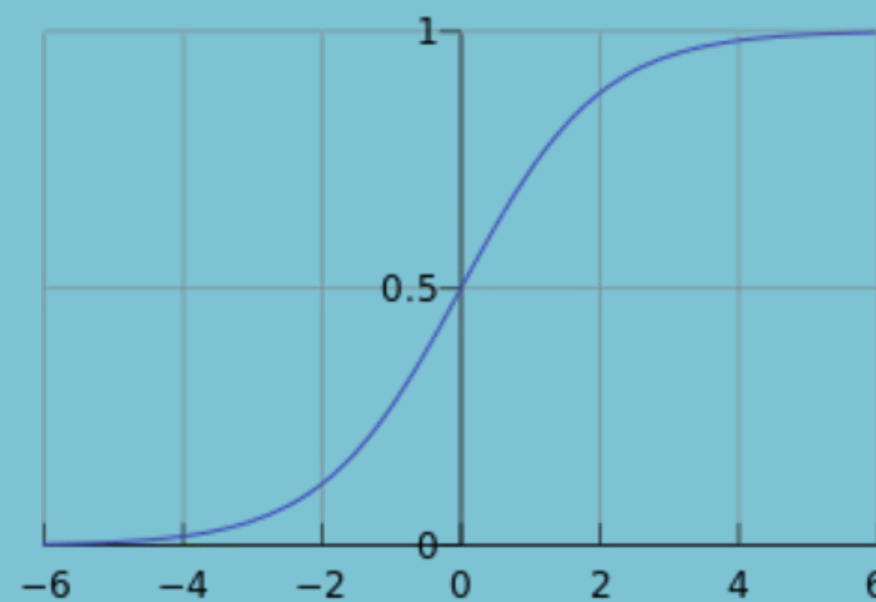

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Model: Logistic function applied to dot product of parameters with input vector.

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

Learning: finds the parameters that minimize some objective function.

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

Prediction: Output is the most probable class.

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

Logistic Regression

Whiteboard

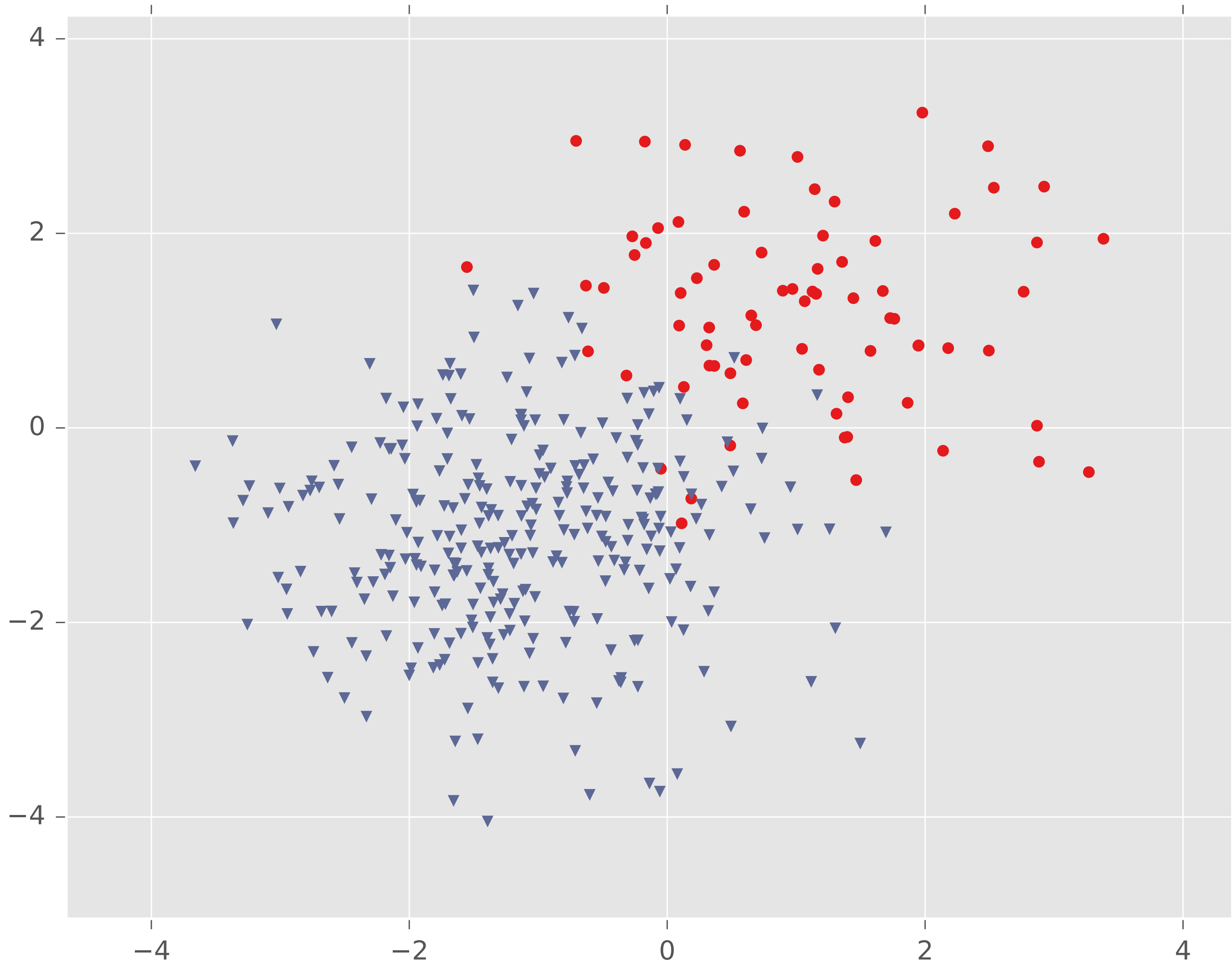
- Bernoulli interpretation
- Logistic Regression Model
- Decision boundary

Learning for Logistic Regression

Whiteboard

- Partial derivative for Logistic Regression
- Gradient for Logistic Regression

Logistic Regression



Logistic Regression

Logistic Regression

LEARNING LOGISTIC REGRESSION

Maximum **Conditional** Likelihood Estimation

Learning: finds the parameters that minimize some objective function.

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

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 MCLE)

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.

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

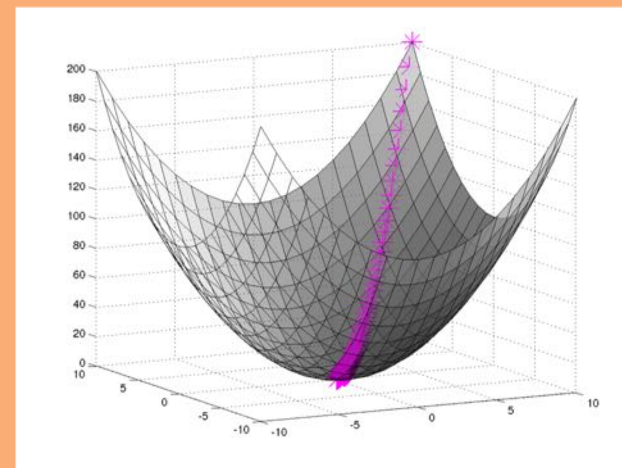
F. (1) randomly pick a parameter and an example, (2) compute the gradient of the log-likelihood for that example with respect to that parameter, (3) update that parameter using that gradient

Gradient Descent

Recall…

Algorithm 1 Gradient Descent

1: **procedure** $\text{GD}(\mathcal{D}, \boldsymbol{\theta}^{(0)})$
2: $\quad \boldsymbol{\theta} \leftarrow \boldsymbol{\theta}^{(0)}$
3: $\quad$ **while** not converged **do**
4: $\quad\quad \boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \lambda \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$
5: $\quad$ **return** $\boldsymbol{\theta}$



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

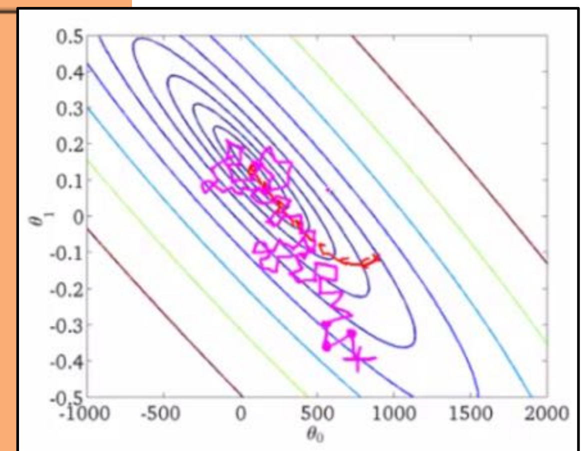
$$\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) = \begin{bmatrix} \frac{d}{d\theta_1} J(\boldsymbol{\theta}) \\ \frac{d}{d\theta_2} J(\boldsymbol{\theta}) \\ \vdots \\ \frac{d}{d\theta_M} J(\boldsymbol{\theta}) \end{bmatrix}$$

Stochastic Gradient Descent (SGD)

Recall…

Algorithm 1 Stochastic Gradient Descent (SGD)

```
procedure SGD(D, θ^(0))
    θ ← θ^(0)
    while not converged do
        for i ∈ shuffle({1, 2, ..., N}) do
            θ ← θ − λ ∇_θ J^(i)(θ)
    return θ
```



We can also apply SGD to solve the MCLE problem for Logistic Regression.

We need a per-example objective:

$$\text{Let } J(\boldsymbol{\theta}) = \textstyle\sum_{i=1}^{N} J^{(i)}(\boldsymbol{\theta})$$
$$\text{where } J^{(i)}(\boldsymbol{\theta}) = -\log p_{\boldsymbol{\theta}}(y^i|\mathbf{x}^i).$$

Mini-Batch SGD

- **Gradient Descent:**
  Compute true gradient exactly from all N examples
- **Mini-Batch SGD**:
  Approximate true gradient by the average gradient of K randomly chosen examples
- **Stochastic Gradient Descent (SGD)**:
  Approximate true gradient by the gradient of one randomly chosen example

Mini-Batch SGD

while not converged: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \lambda \mathbf{g}$

Three variants of first-order optimization:

Gradient Descent: $\mathbf{g} = \nabla J(\boldsymbol{\theta}) = \frac{1}{N} \sum_{i=1}^{N} \nabla J^{(i)}(\boldsymbol{\theta})$

SGD: $\mathbf{g} = \nabla J^{(i)}(\boldsymbol{\theta})$ where i sampled uniformly

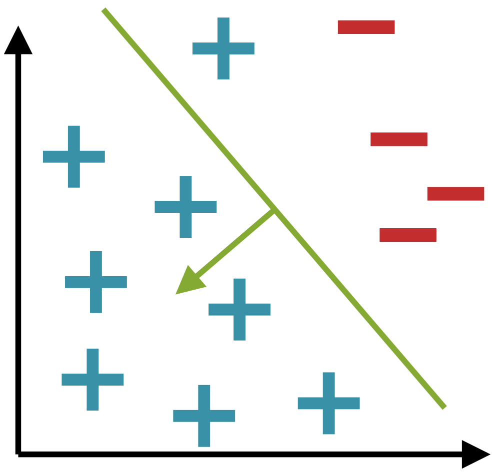
Mini-batch SGD: $\mathbf{g} = \frac{1}{S} \sum_{s=1}^{S} \nabla J^{(i_s)}(\boldsymbol{\theta})$ where i_s sampled uniformly $\forall s$

Logistic Regression vs. Perceptron

Question:

True or False: Just like Perceptron, **one step** (i.e. iteration) **of SGD for Logistic Regression** will result in a change to the parameters **only** if the current example is **incorrectly** classified.

Answer:



Summary

1. Discriminative classifiers directly model the **conditional**, $p(y|x)$
2. Logistic regression is a **simple linear classifier**, that retains a **probabilistic** semantics
3. Parameters in LR are learned by **iterative optimization** (e.g. SGD)

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 or multiclass classification
- Prove that the decision boundary of binary logistic regression is linear
- For linear regression, show that the parameters which minimize squared error are equivalent to those that maximize conditional likelihood