

10-301/601: Introduction to Machine Learning

Lecture 9 – Logistic Regression

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9/28/22

Q & A:

Where does the $O(n^3)$ computational complexity for matrix inversion come from?

- And that other number you quoted for that matter?

Matrix inversion	One $n \times n$ matrix	One $n \times n$ matrix	Gauss–Jordan elimination	$O(n^3)$
			Strassen algorithm	$O(n^{2.807})$
			Coppersmith–Winograd algorithm	$O(n^{2.376})$
			Optimized CW-like algorithms	$O(n^{2.373})$

Front Matter

- Announcements:
 - HW3 released 9/21, due 9/28 (today!) at 11:59 PM
 - **Only two grace days allowed on HW3**
 - HW3 exit poll has also been released: you have until one week from the due date to complete it
- Exam 1 on 10/4 (one week from yesterday) from 6:30 PM - 8:30 PM
 - Exam 1 practice problems released on the course website, under [Coursework](#)
- Lecture instead of recitation this Friday (9/30)

Probabilistic Learning

- Previously:
 - (Unknown) Target function, $c^*: \mathcal{X} \rightarrow \mathcal{Y}$
 - Classifier, $h: \mathcal{X} \rightarrow \mathcal{Y}$
 - Goal: find a classifier, h , that best approximates c^*
- Now:
 - (Unknown) Target *distribution*, $y \sim p^*(Y|\mathbf{x})$
 - Distribution, $p(Y|\mathbf{x})$
 - Goal: find a distribution, p , that best approximates p^*

Likelihood

- Given N independent, identically distribution (iid) samples $\mathcal{D} = \{x^{(1)}, \dots, x^{(N)}\}$ of a random variable X
 - If X is discrete with probability mass function (pmf) $p(X|\theta)$, then the *likelihood* of $\mathcal{D}$ is

$$L(\theta) = \prod_{i=1}^N p(x^{(i)}|\theta)$$

- If X is continuous with probability density function (pdf) $f(X|\theta)$, then the *likelihood* of $\mathcal{D}$ is

$$L(\theta) = \prod_{i=1}^N f(x^{(i)}|\theta)$$

Log-Likelihood

- Given N independent, identically distribution (iid) samples $\mathcal{D} = \{x^{(1)}, \dots, x^{(N)}\}$ of a random variable X
 - If X is discrete with probability mass function (pmf) $p(X|\theta)$, then the *log-likelihood* of $\mathcal{D}$ is

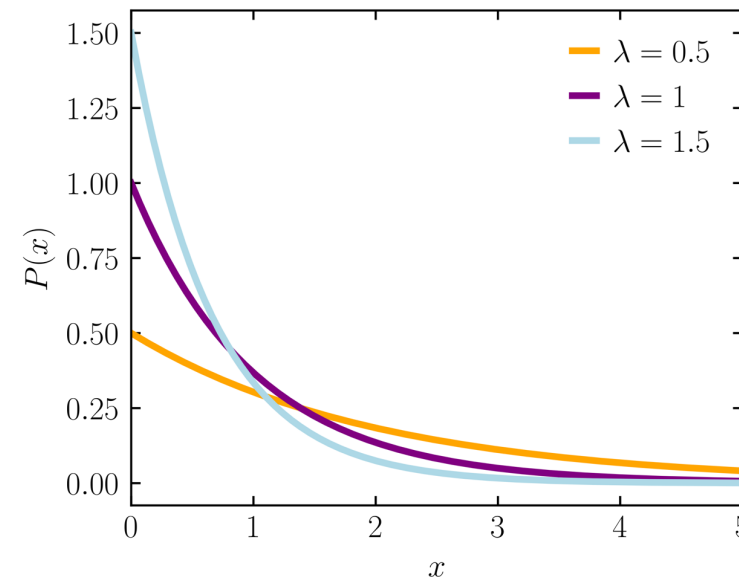
$$\ell(\theta) = \log \prod_{i=1}^N p(x^{(i)}|\theta) = \sum_{i=1}^N \log p(x^{(i)}|\theta)$$

- If X is continuous with probability density function (pdf) $f(X|\theta)$, then the *log-likelihood* of $\mathcal{D}$ is

$$\ell(\theta) = \log \prod_{i=1}^N f(x^{(i)}|\theta) = \sum_{i=1}^N \log f(x^{(i)}|\theta)$$

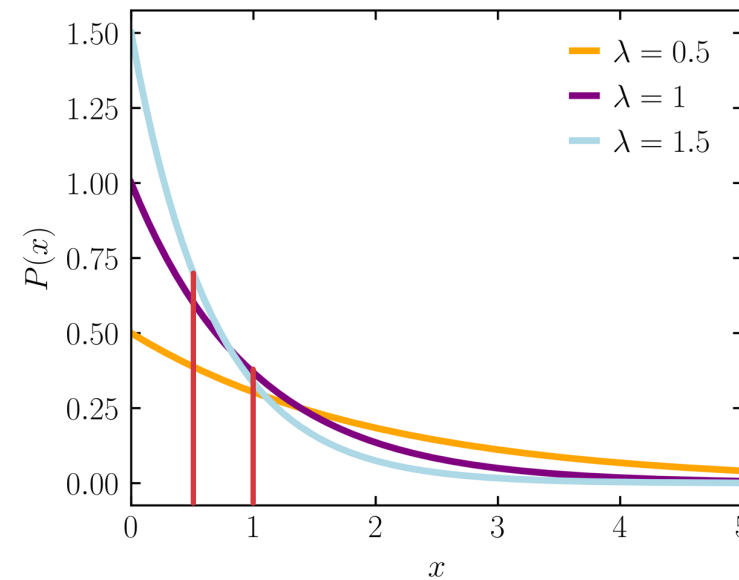
Maximum Likelihood Estimation (MLE)

- Insight: every valid probability distribution has a finite amount of probability mass as it must sum/integrate to 1
- Idea: set the parameter(s) so that the likelihood of the samples is maximized
- Intuition: assign as much of the (finite) probability mass to the observed data *at the expense of unobserved data*
- Example: the exponential distribution



Maximum Likelihood Estimation (MLE)

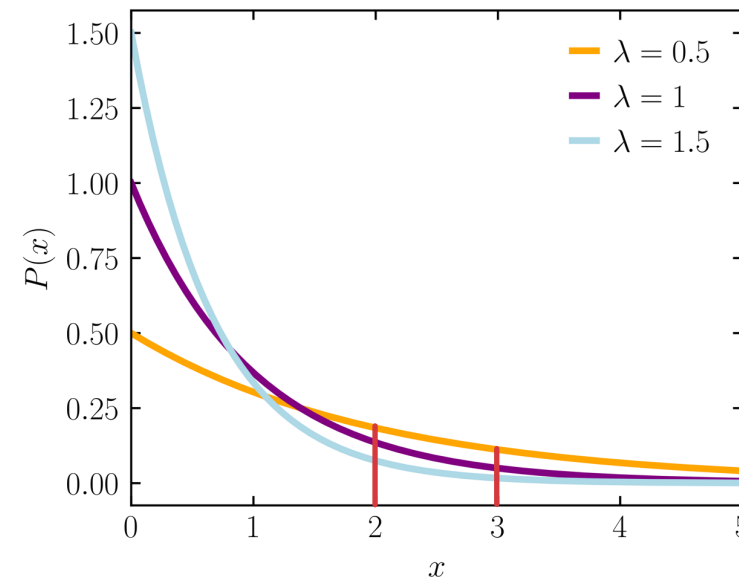
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- Example: the exponential distribution



$$\{x^{(1)} = 0.5, x^{(2)} = 1\}$$

Maximum Likelihood Estimation (MLE)

- Insight: every valid probability distribution has a finite amount of probability mass as it must sum/integrate to 1
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- Example: the exponential distribution



$$\{x^{(1)} = 2, x^{(2)} = 3\}$$

Exponential Distribution MLE

- The pdf of the exponential distribution is

$$f(x|\lambda) = \lambda e^{-\lambda x}$$

- Given N iid samples $\{x^{(1)}, \dots, x^{(N)}\}$, the likelihood is

$$L(\lambda) = \prod_{i=1}^N f(x^{(i)}|\lambda) = \prod_{i=1}^N \lambda e^{-\lambda x^{(i)}}$$

Exponential Distribution MLE

- The pdf of the exponential distribution is

$$f(x|\lambda) = \lambda e^{-\lambda x}$$

- Given N iid samples $\{x^{(1)}, \dots, x^{(N)}\}$, the log-likelihood is

$$\begin{aligned}\ell(\lambda) &= \sum_{i=1}^N \log f(x^{(i)}|\lambda) = \sum_{i=1}^N \log \lambda e^{-\lambda x^{(i)}} \\ &= \sum_{i=1}^N \log \lambda + \log e^{-\lambda x^{(i)}} = N \log \lambda - \lambda \sum_{i=1}^N x^{(i)}\end{aligned}$$

Okay, but now what?

How do we actually find the best value for the parameter, λ ?

- The pdf of the exponential distribution is

$$f(x|\lambda) = \lambda e^{-\lambda x}$$

- Given N iid samples $\{x^{(1)}, \dots, x^{(N)}\}$, the log-likelihood is

$$\ell(\lambda) = \sum_{i=1}^N \log f(x^{(i)}|\lambda) = \sum_{i=1}^N \log \lambda e^{-\lambda x^{(i)}}$$

$$= \sum_{i=1}^N \log \lambda + \log e^{-\lambda x^{(i)}} = N \log \lambda - \lambda \sum_{i=1}^N x^{(i)}$$

Exponential Distribution MLE

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$$= \sum_{i=1}^N \log \lambda + \log e^{-\lambda x^{(i)}} = N \log \lambda - \lambda \sum_{i=1}^N x^{(i)}$$

- Taking the partial derivative and setting it equal to 0 gives

$$\frac{\partial \ell}{\partial \lambda} = \frac{N}{\lambda} - \sum_{i=1}^N x^{(i)}$$

Exponential Distribution MLE

- The pdf of the exponential distribution is

$$f(x|\lambda) = \lambda e^{-\lambda x}$$

- Given N iid samples $\{x^{(1)}, \dots, x^{(N)}\}$, the log-likelihood is

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$$= \sum_{i=1}^N \log \lambda + \log e^{-\lambda x^{(i)}} = N \log \lambda - \lambda \sum_{i=1}^N x^{(i)}$$

- Taking the partial derivative and setting it equal to 0 gives

$$\frac{N}{\hat{\lambda}} - \sum_{i=1}^N x^{(i)} = 0 \rightarrow \frac{N}{\hat{\lambda}} = \sum_{i=1}^N x^{(i)} \rightarrow \hat{\lambda} = \frac{N}{\sum_{i=1}^N x^{(i)}}$$

Building a Probabilistic Classifier

- Define a decision rule
 - Given a test data point $\mathbf{x}'$, predict its label $\hat{y}$ using the posterior distribution $P(Y = y|\mathbf{x}')$
 - Common choice: $\hat{y} = \underset{y}{\operatorname{argmax}} P(Y = y|\mathbf{x}')$
- Idea: model $P(Y|\mathbf{x})$ as some parametric function of $\mathbf{x}$

Modelling the Posterior

- Suppose we have binary labels $y \in \{0,1\}$ and D -dimensional inputs $\mathbf{x} = [1, x_1, \dots, x_D]^T \in \mathbb{R}^{D+1}$

- **Assume**

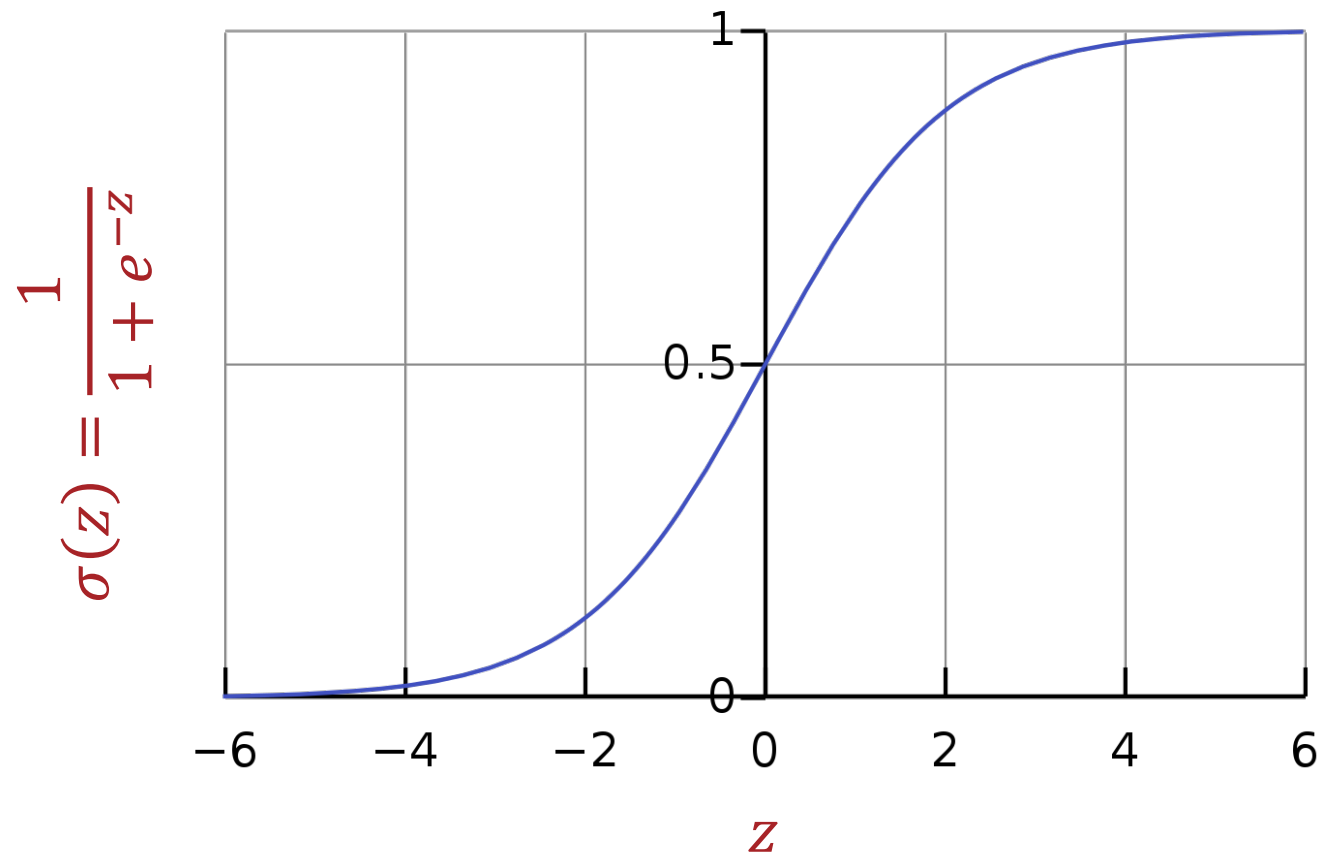
1 prepended to $\mathbf{x}$

$$P(Y = 1|\mathbf{x}, \boldsymbol{\theta}) = \sigma(\boldsymbol{\theta}^T \mathbf{x}) = \frac{1}{1 + \exp(-\boldsymbol{\theta}^T \mathbf{x})} = \frac{\exp(\boldsymbol{\theta}^T \mathbf{x})}{\exp(\boldsymbol{\theta}^T \mathbf{x}) + 1}$$

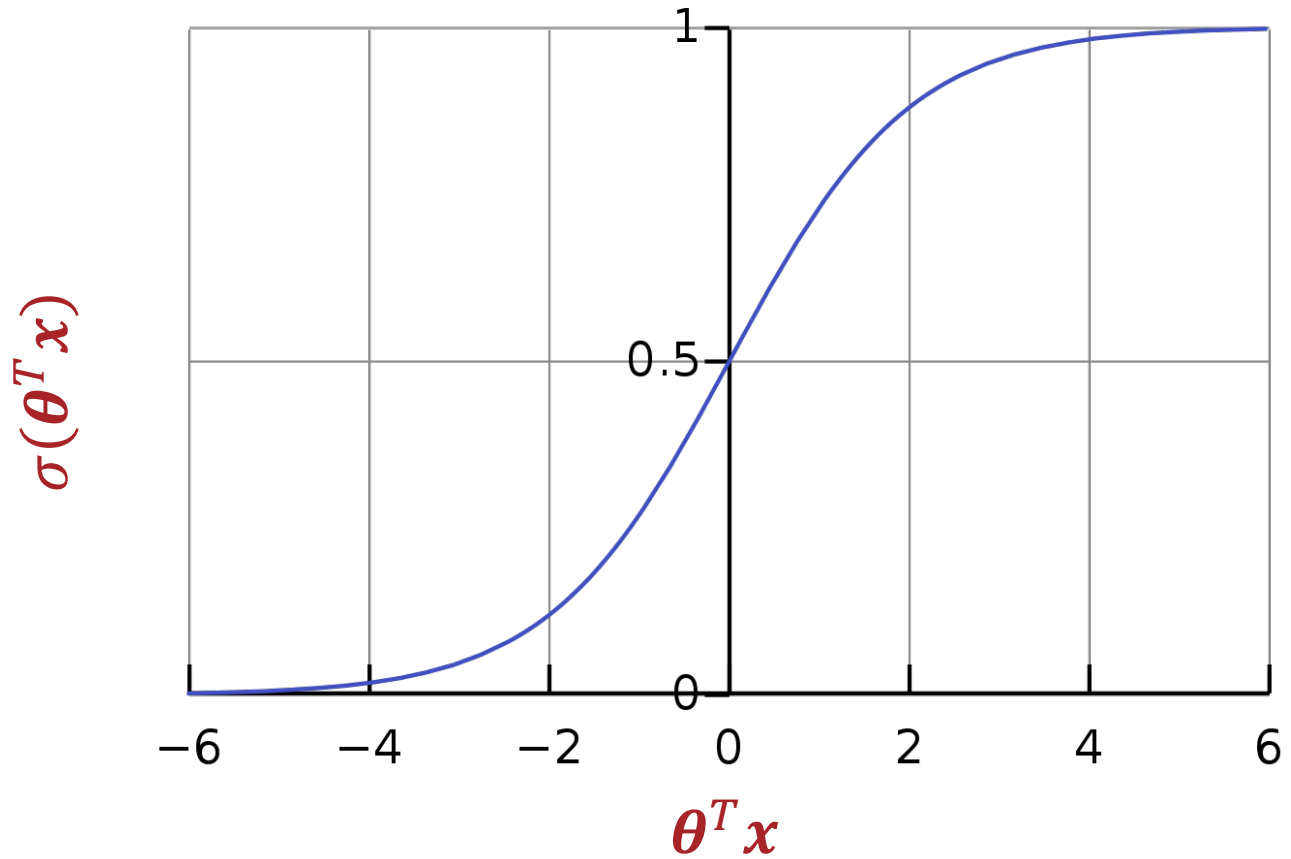
- This implies two useful facts:

1. $P(Y = 0|\mathbf{x}, \boldsymbol{\theta}) = 1 - P(Y = 1|\mathbf{x}, \boldsymbol{\theta}) = \frac{1}{\exp(\boldsymbol{\theta}^T \mathbf{x}) + 1}$
2. $\frac{P(Y = 1|\mathbf{x}, \boldsymbol{\theta})}{P(Y = 0|\mathbf{x}, \boldsymbol{\theta})} = \exp(\boldsymbol{\theta}^T \mathbf{x}) \rightarrow \log \frac{P(Y = 1|\mathbf{x}, \boldsymbol{\theta})}{P(Y = 0|\mathbf{x}, \boldsymbol{\theta})} = \boldsymbol{\theta}^T \mathbf{x}$

Logistic Function



Why use the Logistic Function?



- Differentiable everywhere
- $\sigma: \mathbb{R} \rightarrow [0, 1]$
- The decision boundary is linear in x !

Logistic Regression Decision Boundary

$$\hat{y} = \begin{cases} 1 & \text{if } P(Y = 1|\mathbf{x}, \boldsymbol{\theta}) \geq \frac{1}{2} \\ 0 & \text{otherwise.} \end{cases}$$

$$P(Y = 1|\mathbf{x}) = \sigma(\boldsymbol{\theta}^T \mathbf{x}) = \frac{1}{1 + \exp(-\boldsymbol{\theta}^T \mathbf{x})} \geq \frac{1}{2}$$

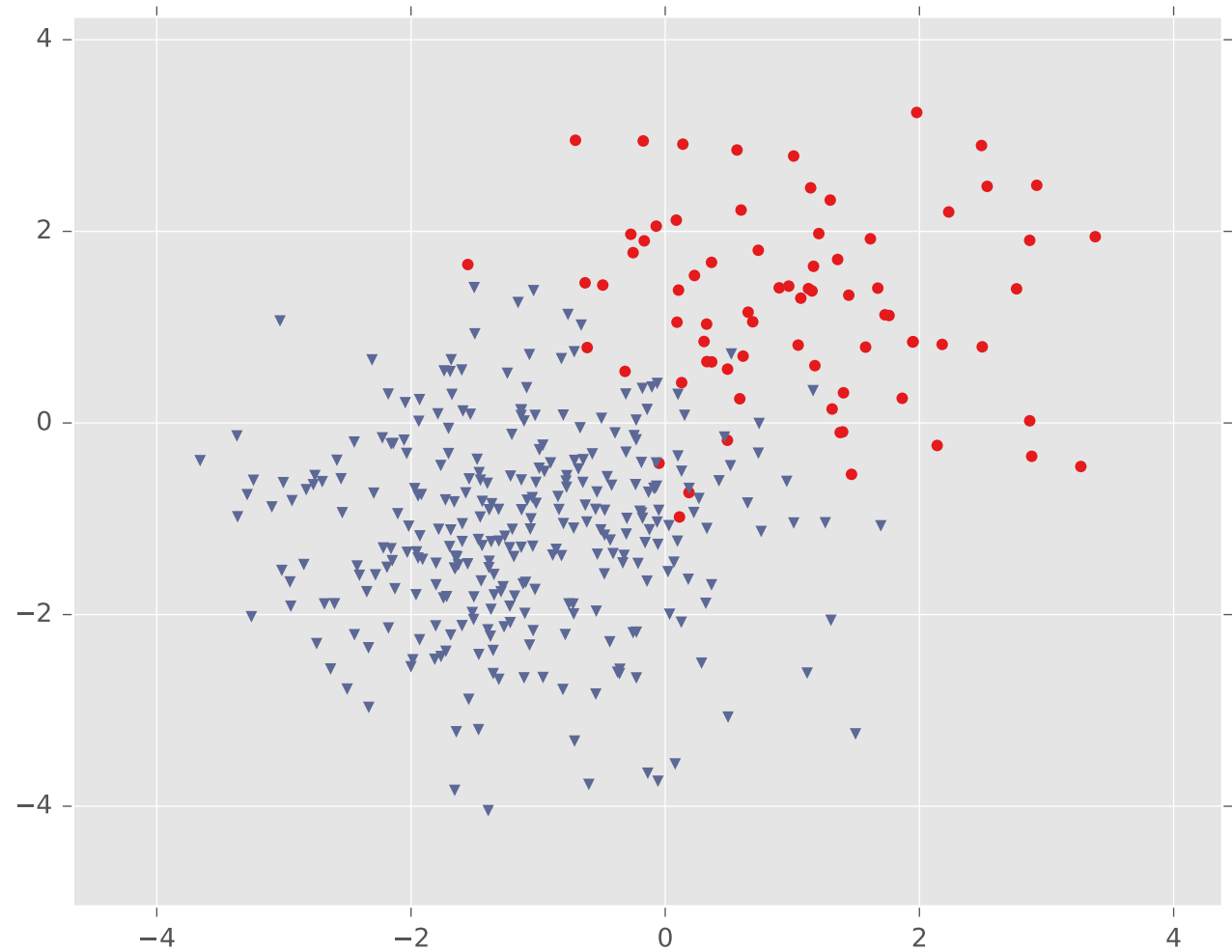
$$2 \geq 1 + \exp(-\boldsymbol{\theta}^T \mathbf{x})$$

$$1 \geq \exp(-\boldsymbol{\theta}^T \mathbf{x})$$

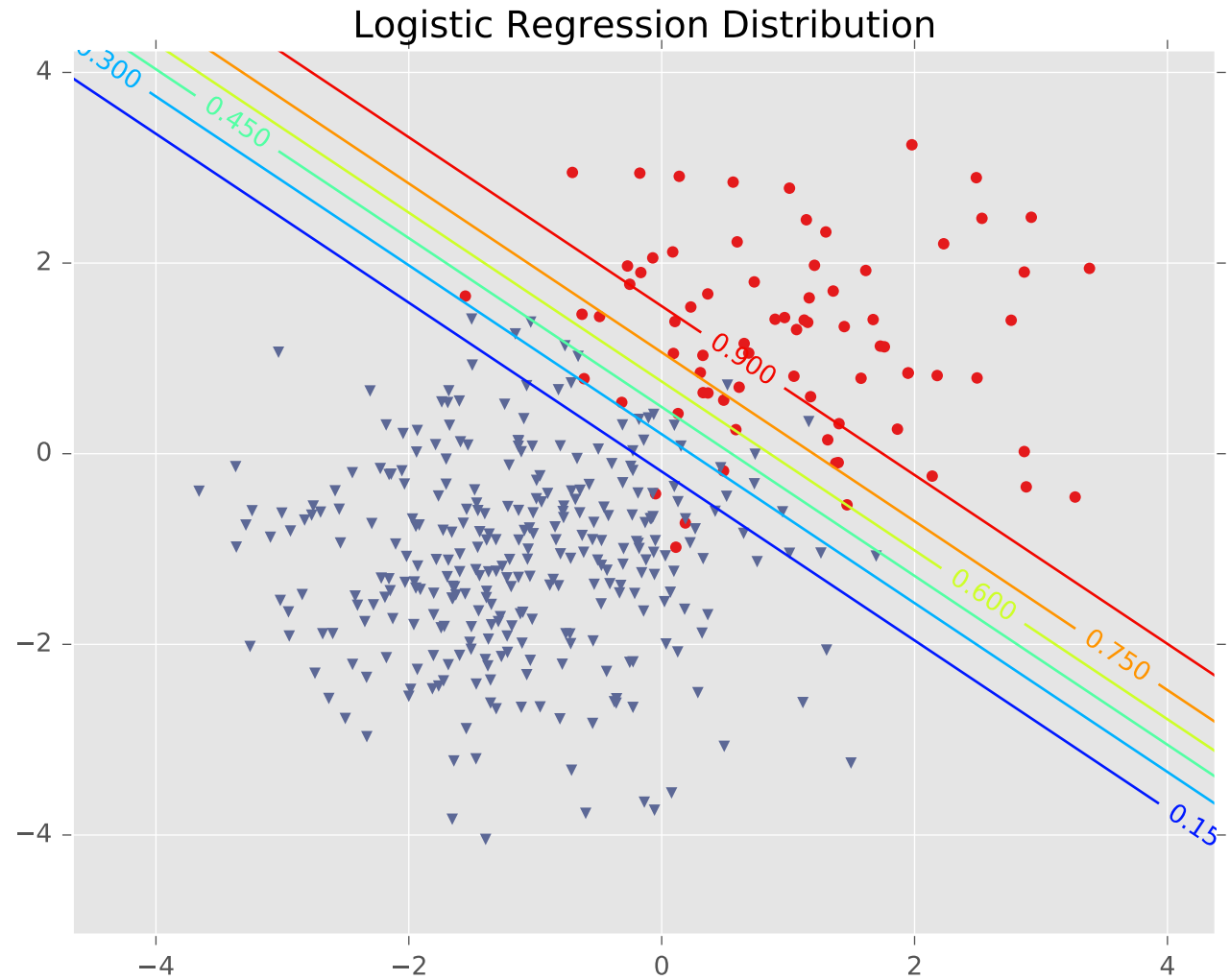
$$\log(1) \geq -\boldsymbol{\theta}^T \mathbf{x}$$

$$0 \leq \boldsymbol{\theta}^T \mathbf{x}$$

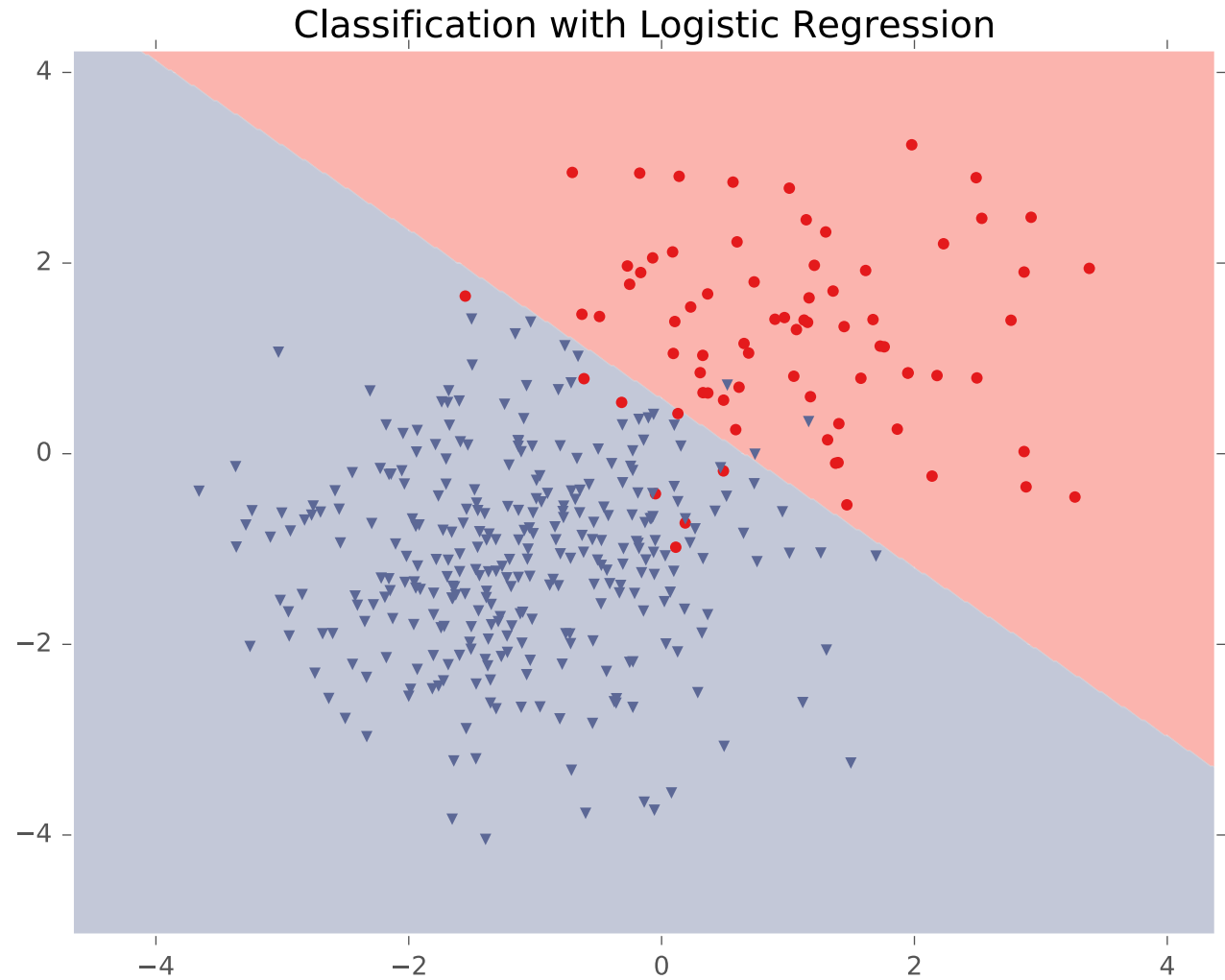
Logistic Regression Decision Boundary



Logistic Regression Decision Boundary



Logistic Regression Decision Boundary



Setting the Parameters via Minimum Negative Conditional (log-)Likelihood Estimation (MCLE)

- Find $\boldsymbol{\theta}$ that minimizes

$$\begin{aligned}\ell(\boldsymbol{\theta}) &= -\log P(y^{(1)}, \dots, y^{(N)} | \mathbf{x}^{(1)}, \dots, \mathbf{x}^{(N)}, \boldsymbol{\theta}) = -\log \prod_{i=1}^N P(y^{(i)} | \mathbf{x}^{(i)}, \boldsymbol{\theta}) \\ &= -\log \prod_{i=1}^N P(Y = 1 | \mathbf{x}^{(i)}, \boldsymbol{\theta})^{y^{(i)}} \left(P(Y = 0 | \mathbf{x}^{(i)}, \boldsymbol{\theta}) \right)^{1-y^{(i)}} \\ &= -\sum_{i=1}^N y^{(i)} \log P(Y = 1 | \mathbf{x}^{(i)}, \boldsymbol{\theta}) + (1 - y^{(i)}) \log P(Y = 0 | \mathbf{x}^{(i)}, \boldsymbol{\theta}) \\ &= -\sum_{i=1}^N y^{(i)} \log \frac{P(Y = 1 | \mathbf{x}^{(i)}, \boldsymbol{\theta})}{P(Y = 0 | \mathbf{x}^{(i)}, \boldsymbol{\theta})} + \log P(Y = 0 | \mathbf{x}^{(i)}, \boldsymbol{\theta}) \\ &= -\sum_{i=1}^N y^{(i)} \boldsymbol{\theta}^T \mathbf{x}^{(i)} - \log \left(1 + \exp(\boldsymbol{\theta}^T \mathbf{x}^{(i)}) \right) \\ J(\boldsymbol{\theta}) &= \frac{1}{N} \ell(\boldsymbol{\theta}) = -\frac{1}{N} \sum_{i=1}^N y^{(i)} \boldsymbol{\theta}^T \mathbf{x}^{(i)} - \log \left(1 + \exp(\boldsymbol{\theta}^T \mathbf{x}^{(i)}) \right)\end{aligned}$$

Minimizing the Negative Conditional (log-)Likelihood

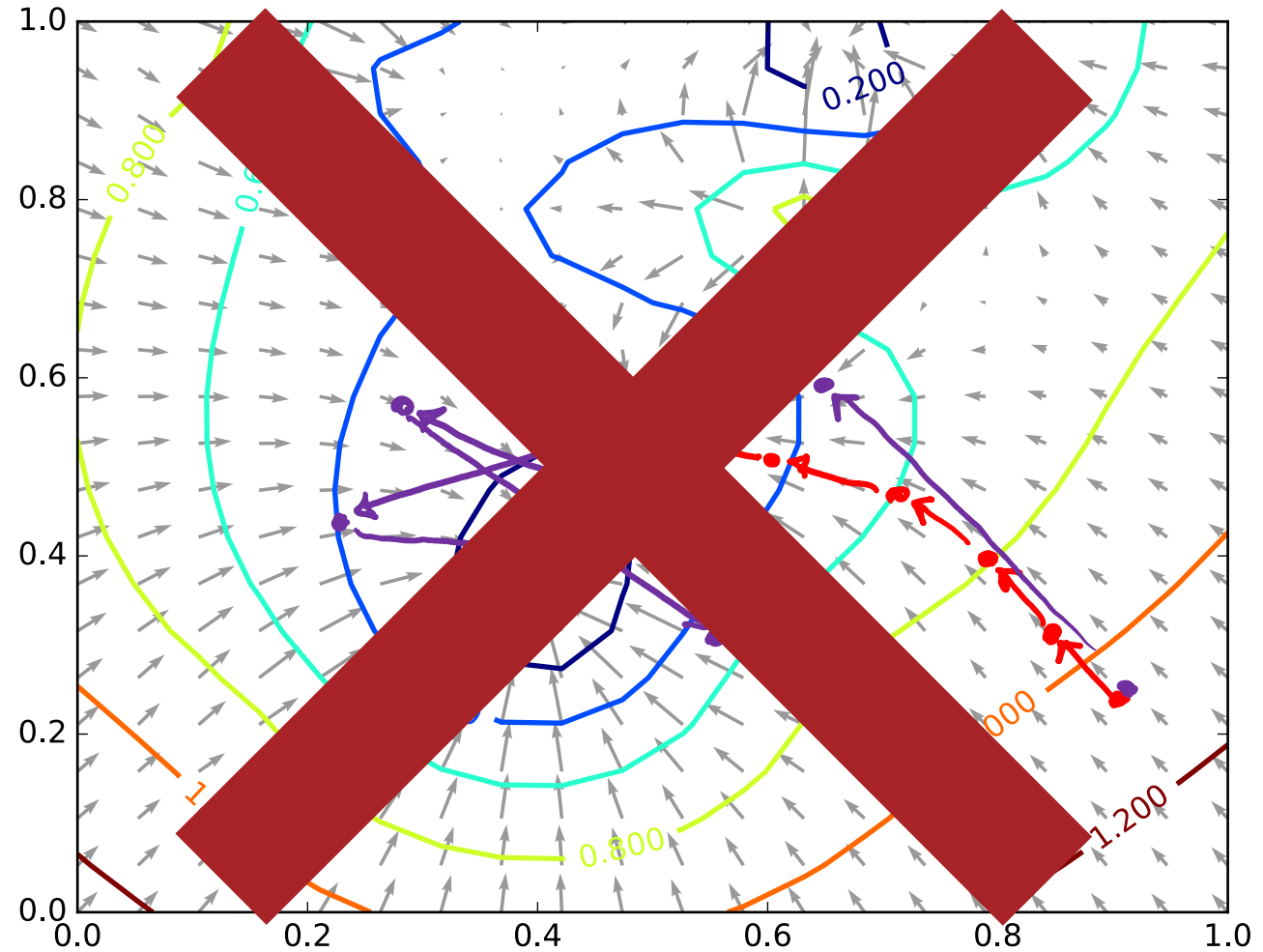
$$J(\boldsymbol{\theta}) = -\frac{1}{N} \sum_{i=1}^N y^{(i)} \boldsymbol{\theta}^T \mathbf{x}^{(i)} - \log \left(1 + \exp(\boldsymbol{\theta}^T \mathbf{x}^{(i)}) \right)$$

$$\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) = -\frac{1}{N} \sum_{i=1}^N y^{(i)} \nabla_{\boldsymbol{\theta}} (\boldsymbol{\theta}^T \mathbf{x}^{(i)}) - \nabla_{\boldsymbol{\theta}} \log \left(1 + \exp(\boldsymbol{\theta}^T \mathbf{x}^{(i)}) \right)$$

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

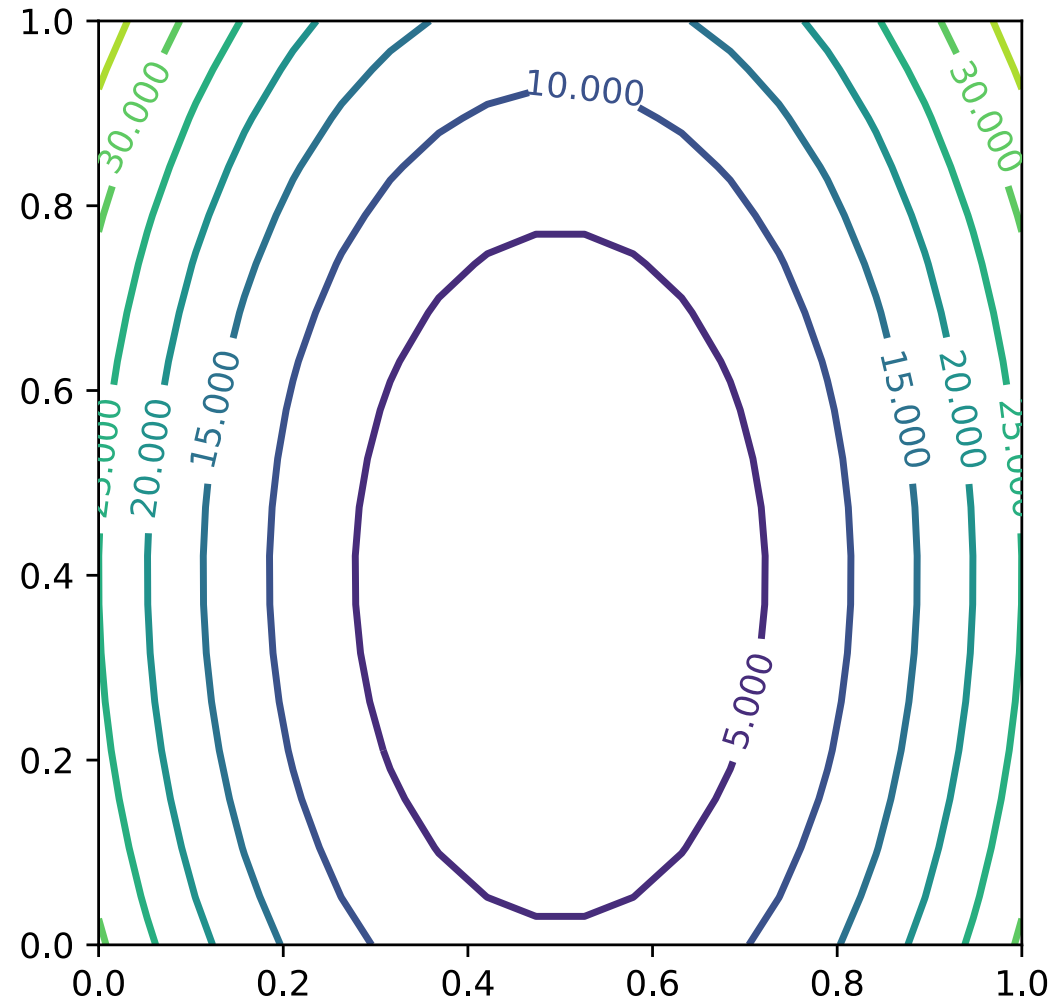
$$= \frac{1}{N} \sum_{i=1}^N \mathbf{x}^{(i)} (P(Y = 1 | \mathbf{x}^{(i)}, \boldsymbol{\theta}) - y^{(i)})$$

Recall: Gradient Descent



Good news: the negative conditional log-likelihood is convex!
(See HW/recitation)

Recall: Gradient Descent



Good news: the negative conditional log-likelihood is convex!
(See HW/recitation)

Gradient Descent

- Input: training dataset $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$ and step size γ
 1. Initialize $\boldsymbol{\theta}^{(0)}$ to all zeros and set $t = 0$
 2. While TERMINATION CRITERION is not satisfied
 - a. Compute the gradient:
$$\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}^{(t)}) = \frac{1}{N} \sum_{i=1}^N \mathbf{x}^{(i)} (P(Y = 1 | \mathbf{x}^{(i)}, \boldsymbol{\theta}^{(t)}) - y^{(i)})$$
 - b. Update $\boldsymbol{\theta}$: $\boldsymbol{\theta}^{(t+1)} \leftarrow \boldsymbol{\theta}^{(t)} - \gamma \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}^{(t)})$
 - c. Increment t : $t \leftarrow t + 1$
- Output: $\boldsymbol{\theta}^{(t)}$

Poll Question 1:

What is the computational cost of one iteration of gradient descent for logistic regression?

A. $O(1)$ (TOXIC)

B. $O(N)$

C. $O(D)$

D. $O(ND)$

- Input: training dataset $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$ and step size γ

1. Initialize $\boldsymbol{\theta}^{(0)}$ to all zeros and set $t = 0$
2. While TERMINATION CRITERION is not satisfied
 - a. Compute the gradient:

$$\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}^{(t)}) = \frac{1}{N} \sum_{i=1}^N \mathbf{x}^{(i)} (P(Y = 1 | \mathbf{x}^{(i)}, \boldsymbol{\theta}^{(t)}) - y^{(i)})$$

- b. Update $\boldsymbol{\theta}$: $\boldsymbol{\theta}^{(t+1)} \leftarrow \boldsymbol{\theta}^{(t)} - \gamma \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}^{(t)})$
 - c. Increment t : $t \leftarrow t + 1$
- Output: $\boldsymbol{\theta}^{(t)}$

Gradient Descent

- Input: training dataset $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$ and step size γ

1. Initialize $\boldsymbol{\theta}^{(0)}$ to all zeros and set $t = 0$
2. While TERMINATION CRITERION is not satisfied
 - a. Compute the gradient:

$$O(ND) \left\{ \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}^{(t)}) = \frac{1}{N} \sum_{i=1}^N \mathbf{x}^{(i)} (P(Y = 1 | \mathbf{x}^{(i)}, \boldsymbol{\theta}^{(t)}) - y^{(i)}) \right.$$

- b. Update $\boldsymbol{\theta}$: $\boldsymbol{\theta}^{(t+1)} \leftarrow \boldsymbol{\theta}^{(t)} - \gamma \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}^{(t)})$
 - c. Increment t : $t \leftarrow t + 1$
- Output: $\boldsymbol{\theta}^{(t)}$

Stochastic Gradient Descent (SGD)

- Input: training dataset $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$ and step size γ
 1. Initialize $\boldsymbol{\theta}^{(0)}$ to all zeros and set $t = 0$
 2. While TERMINATION CRITERION is not satisfied
 - a. Randomly sample a data point from $\mathcal{D}$, $(\mathbf{x}^{(i)}, y^{(i)})$
 - b. Compute the pointwise gradient:
$$\nabla_{\boldsymbol{\theta}} J^{(i)}(\boldsymbol{\theta}^{(t)}) = \mathbf{x}^{(i)} (P(Y = 1 | \mathbf{x}^{(i)}, \boldsymbol{\theta}^{(t)}) - y^{(i)})$$
 - c. Update $\boldsymbol{\theta}$: $\boldsymbol{\theta}^{(t+1)} \leftarrow \boldsymbol{\theta}^{(t)} - \gamma \nabla_{\boldsymbol{\theta}} J^{(i)}(\boldsymbol{\theta}^{(t)})$
 - d. Increment t : $t \leftarrow t + 1$
- Output: $\boldsymbol{\theta}^{(t)}$

Stochastic Gradient Descent (SGD)

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

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

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

Stochastic Gradient Descent (SGD)

- Input: training dataset $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$ and step size γ
 1. Initialize $\boldsymbol{\theta}^{(0)}$ to all zeros and set $t = 0$
 2. While TERMINATION CRITERION is not satisfied
 - a. For $i \in \text{shuffle}(\{1, \dots, N\})$
 - i. Compute the pointwise gradient:
$$\nabla_{\boldsymbol{\theta}} J^{(i)}(\boldsymbol{\theta}^{(t)}) = \mathbf{x}^{(i)} (P(Y = 1 | \mathbf{x}^{(i)}, \boldsymbol{\theta}^{(t)}) - y^{(i)})$$
 - ii. Update $\boldsymbol{\theta}$: $\boldsymbol{\theta}^{(t+1)} \leftarrow \boldsymbol{\theta}^{(t)} - \gamma \nabla_{\boldsymbol{\theta}} J^{(i)}(\boldsymbol{\theta}^{(t)})$
 - iii. Increment t : $t \leftarrow t + 1$
- Output: $\boldsymbol{\theta}^{(t)}$

Wait, have we seen something like this before?



- Input: training dataset $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$ and step size γ
 1. Initialize $\boldsymbol{\theta}^{(0)}$ to all zeros and set $t = 0$
 2. While TERMINATION CRITERION is not satisfied
 - a. For $i \in \text{shuffle}(\{1, \dots, N\})$
 - i. Compute the pointwise gradient:
$$\nabla_{\boldsymbol{\theta}} J^{(i)}(\boldsymbol{\theta}^{(t)}) = \mathbf{x}^{(i)} (P(Y = 1 | \mathbf{x}^{(i)}, \boldsymbol{\theta}^{(t)}) - y^{(i)})$$
 - ii. Update $\boldsymbol{\theta}$: $\boldsymbol{\theta}^{(t+1)} \leftarrow \boldsymbol{\theta}^{(t)} - \gamma \nabla_{\boldsymbol{\theta}} J^{(i)}(\boldsymbol{\theta}^{(t)})$
 - iii. Increment t : $t \leftarrow t + 1$
- Output: $\boldsymbol{\theta}^{(t)}$

Recall: Perceptron Learning Algorithm

- Input: training dataset $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$
- 1. Initialize $\boldsymbol{\theta}^{(0)}$ to all zeros and set $t = 0$
- 2. While NOT CONVERGED
 - a. For $t \in \text{shuffle}(\{1, \dots, N\})$
 - i. Predict the label of $\mathbf{x}^{(t)}$, $\hat{y} = \text{sign}(\boldsymbol{\theta}^T \mathbf{x}^{(t)})$
 - ii. Observe its true label, $y^{(t)}$
 - iii. If we misclassified $\mathbf{x}^{(t)}$ ($y^{(t)} \neq \hat{y}$):

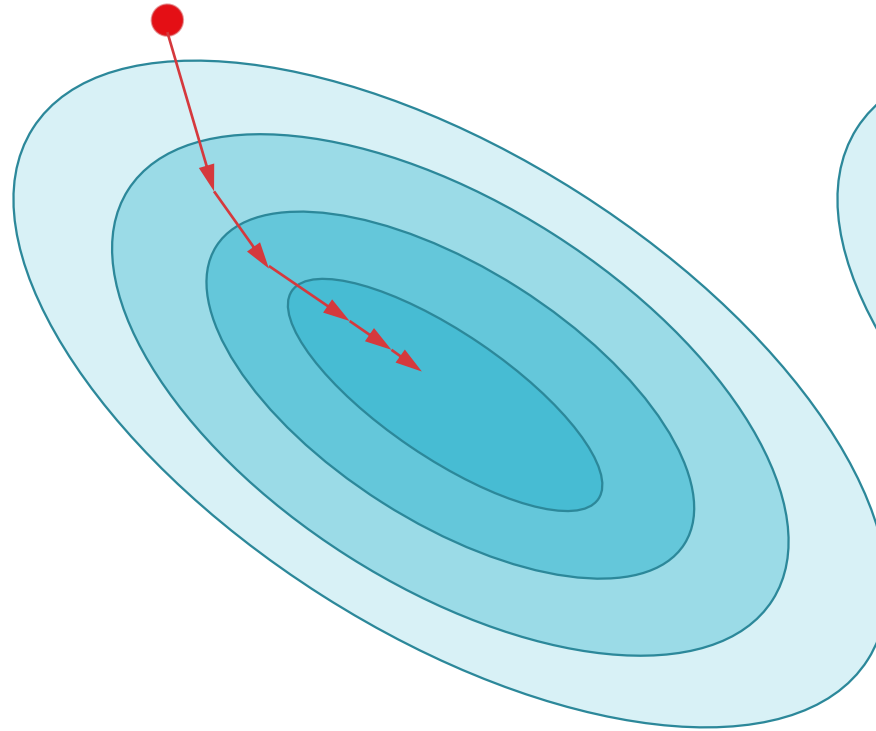
$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + y^{(t)} \mathbf{x}^{(t)}$$

↑
|

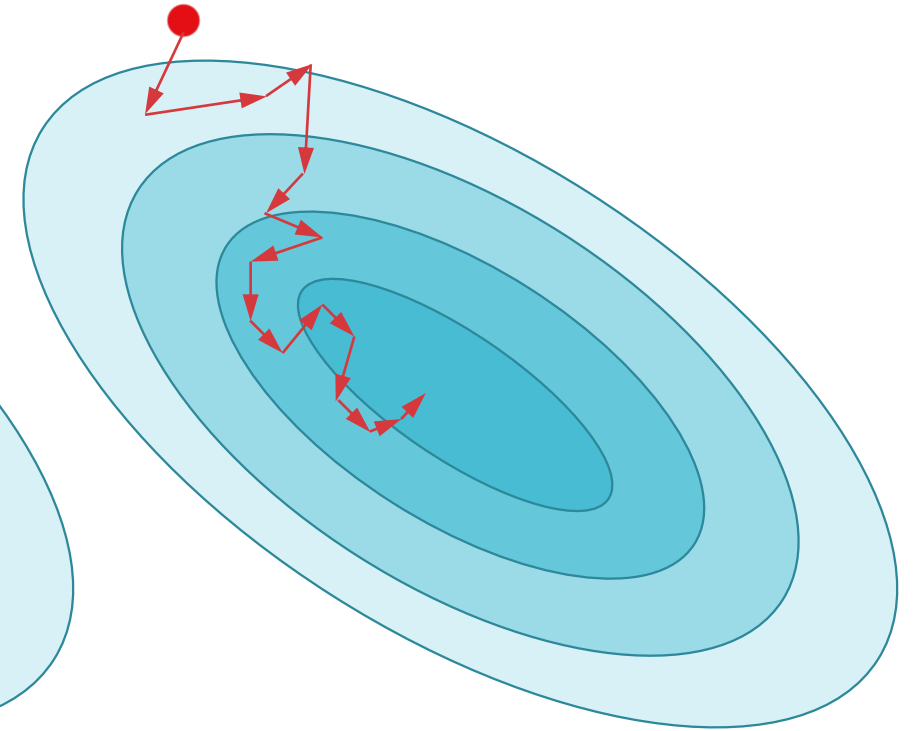
This is the negative gradient of the *hinge loss*

$$J^{(i)}(\boldsymbol{\theta}) = \max(0, 1 - y^{(i)} \boldsymbol{\theta}^T \mathbf{x}^{(i)})$$

Stochastic Gradient Descent vs. Gradient Descent



Gradient Descent



Stochastic Gradient Descent

Stochastic Gradient Descent vs. Gradient Descent

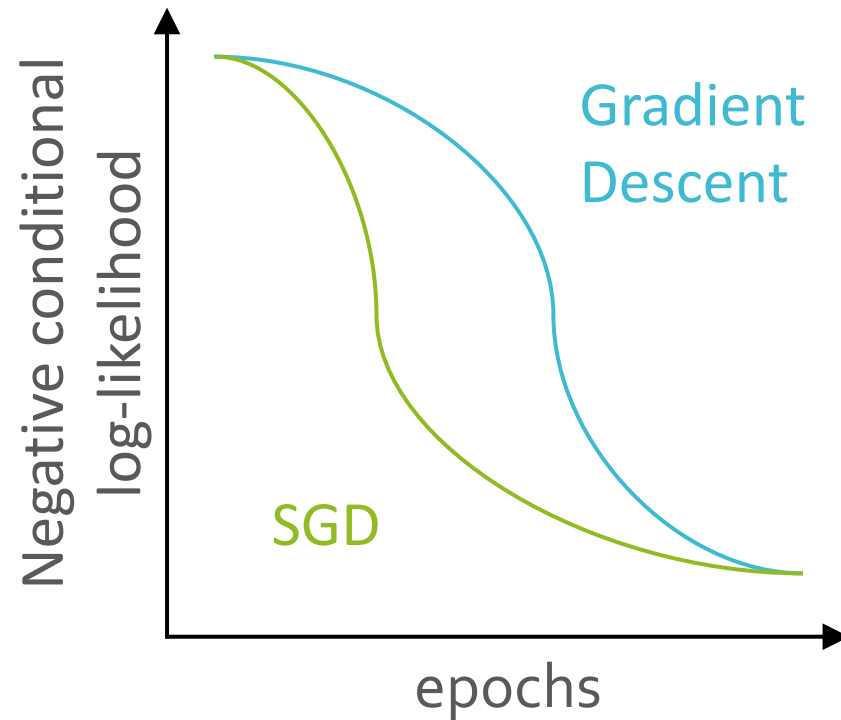
- An *epoch* is a single pass through the entire training dataset
 - Gradient descent updates the parameters once per epoch
 - SGD updates the parameters N times per epoch
- Theoretical comparison:
 - Define convergence to be when $J(\boldsymbol{\theta}^{(t)}) - J(\boldsymbol{\theta}^*) < \epsilon$

Method	Steps to Convergence	Computation per Step
Gradient descent	$O(\log 1/\epsilon)$	$O(ND)$
SGD	$O(1/\epsilon)$	$O(D)$

(with high probability under certain assumptions)

Stochastic Gradient Descent vs. Gradient Descent

- An *epoch* is a single pass through the entire training dataset
 - Gradient descent updates the parameters once per epoch
 - SGD updates the parameters N times per epoch



Empirically, SGD reduces the negative conditional log-likelihood much faster than gradient descent

Optimization for ML Learning 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

Logistic Regression Learning 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 (and multiclass) classification
- Prove that the decision boundary of binary logistic regression is linear