10-301/601: Introduction to Machine Learning Lecture 9 – Logistic Regression

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2/14/24

Front Matter

- Announcements:
  - Exam 1 on 2/19 from 7 PM – 9 PM
    - Exam 1 practice problems released on the course website, under Coursework

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*, $y \sim p^*(Y|\boldsymbol{x})$
  - Distribution, $p(Y|\boldsymbol{x})$
  - Goal: find a distribution, p, that best approximates p^*

Likelihood

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

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

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

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

Log-Likelihood

- Given N independent, identically distribution (iid) samples $\mathcal{D} = \{x^{(1)}, \ldots, x^{(N)}\}$ 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

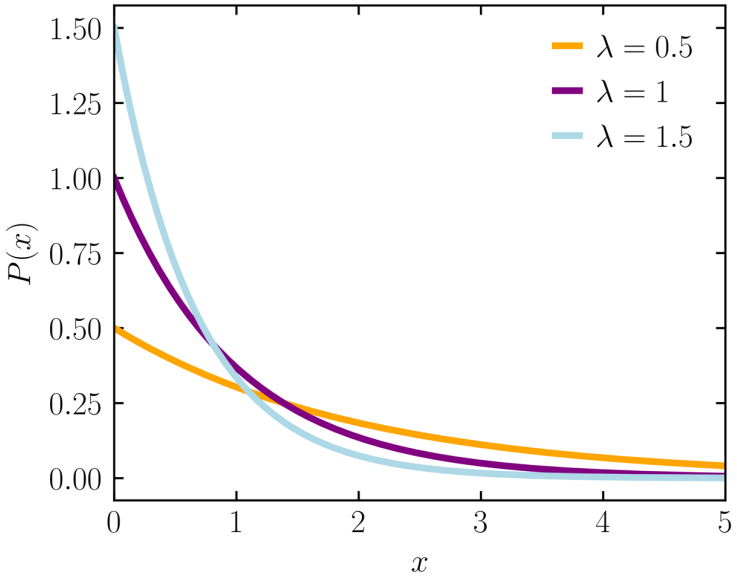
$$\ell(\theta) = \log \prod_{n=1}^{N} p\left(x^{(n)}|\theta\right) = \sum_{n=1}^{N} \log p\left(x^{(n)}|\theta\right)$$

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

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

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



Source: https://en.wikipedia.org/wiki/Exponential_distribution#/media/File:Exponential_probability_density.svg

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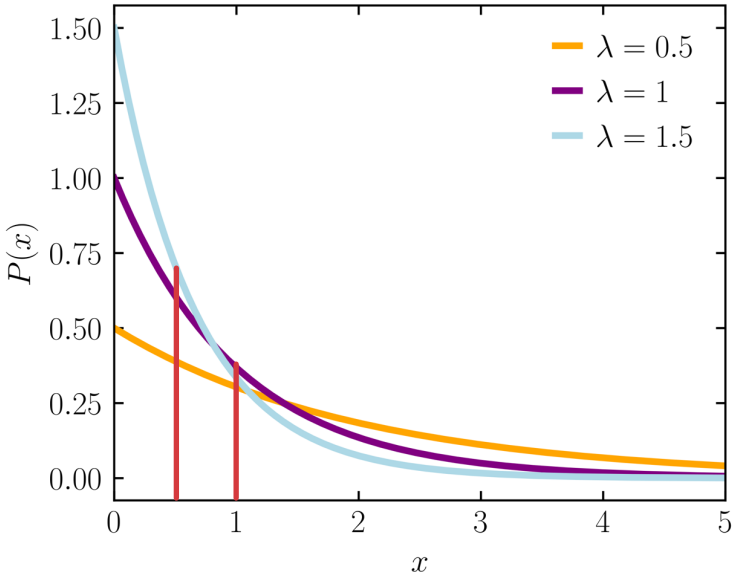

$\{x^{(1)} = 0.5, x^{(2)} = 1\}$

Source: https://en.wikipedia.org/wiki/Exponential_distribution#/media/File:Exponential_probability_density.svg

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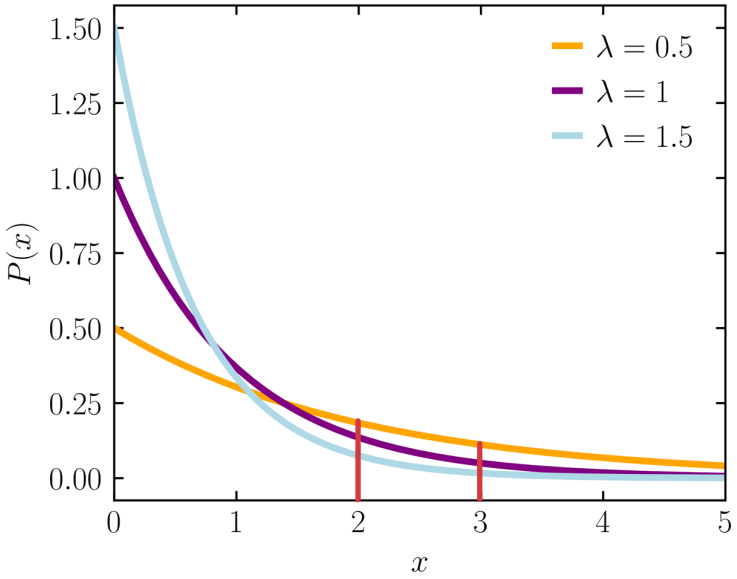


$\{x^{(1)} = 2, x^{(2)} = 3\}$

Source: https://en.wikipedia.org/wiki/Exponential_distribution#/media/File:Exponential_probability_density.svg

Exponential Distribution MLE

- The pdf of the exponential distribution is

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

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

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

Exponential Distribution MLE

- The pdf of the exponential distribution is

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

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

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

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

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

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

Exponential Distribution MLE

- The pdf of the exponential distribution is

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

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

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

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

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

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

Building a Probabilistic Classifier

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

Modelling the Posterior

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

  1 prepended to $\boldsymbol{x}$

- **Assume**

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

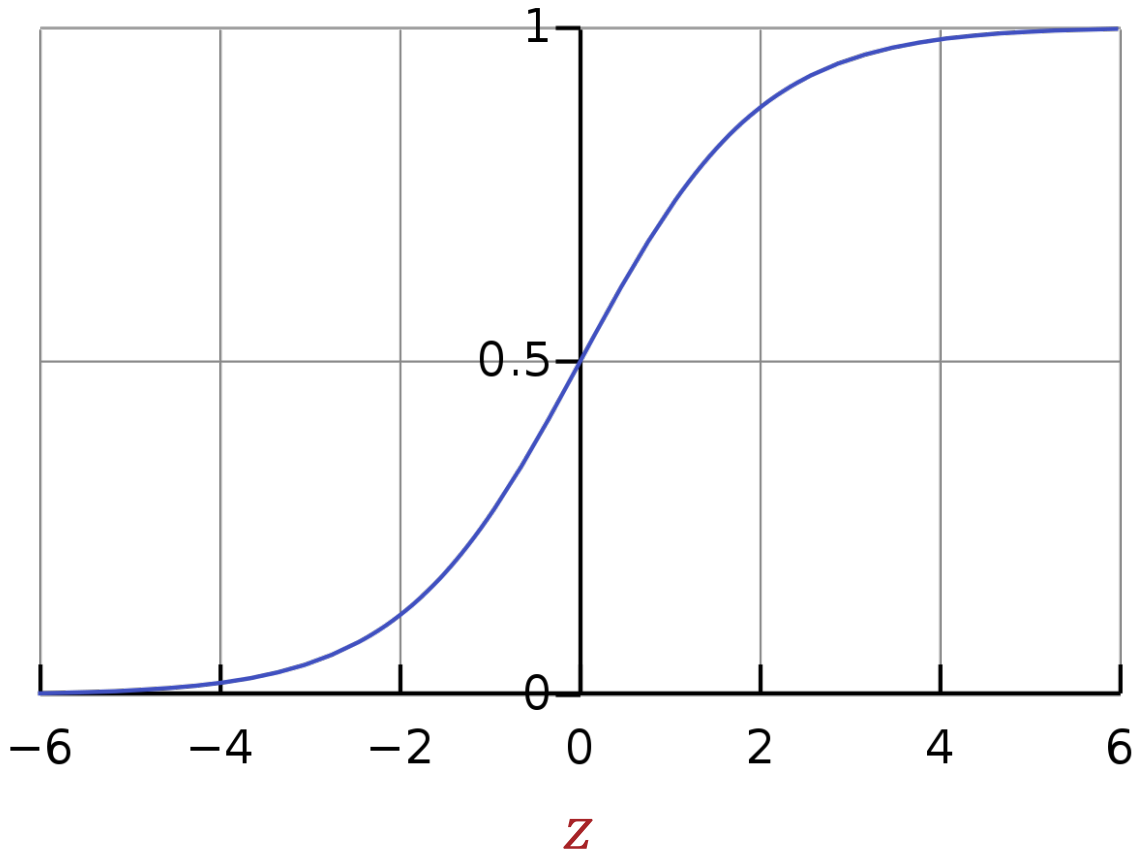
- This implies two useful facts:

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

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

Logistic Function

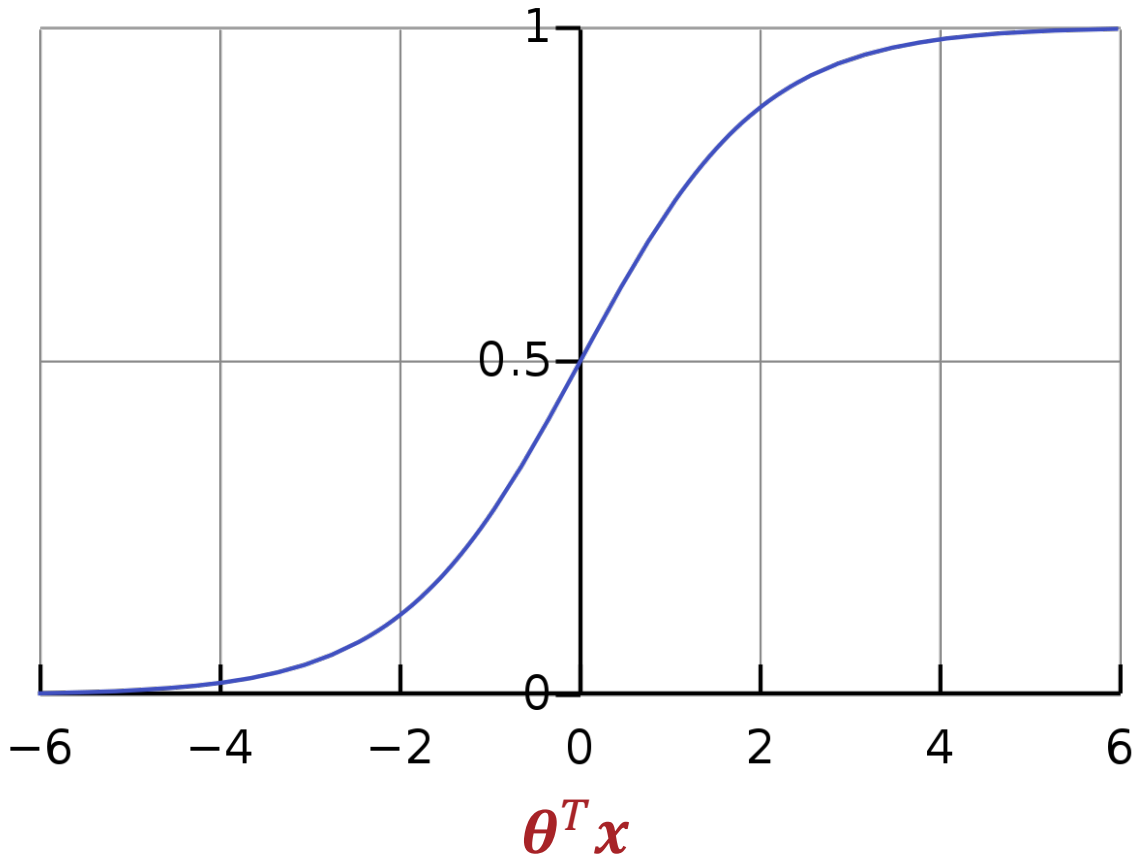
$$\sigma(z) = \frac{1}{1+e^{-z}}$$



Source: https://en.wikipedia.org/wiki/Logistic_function#/media/File:Logistic-curve.svg

Why use the Logistic Function?

$$\sigma(\boldsymbol{\theta}^T \boldsymbol{x}) = \frac{1}{1 + e^{-\boldsymbol{\theta}^T \boldsymbol{x}}}$$



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Logistic Regression Decision Boundary

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

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

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

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

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

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

Logistic Regression Decision Boundary

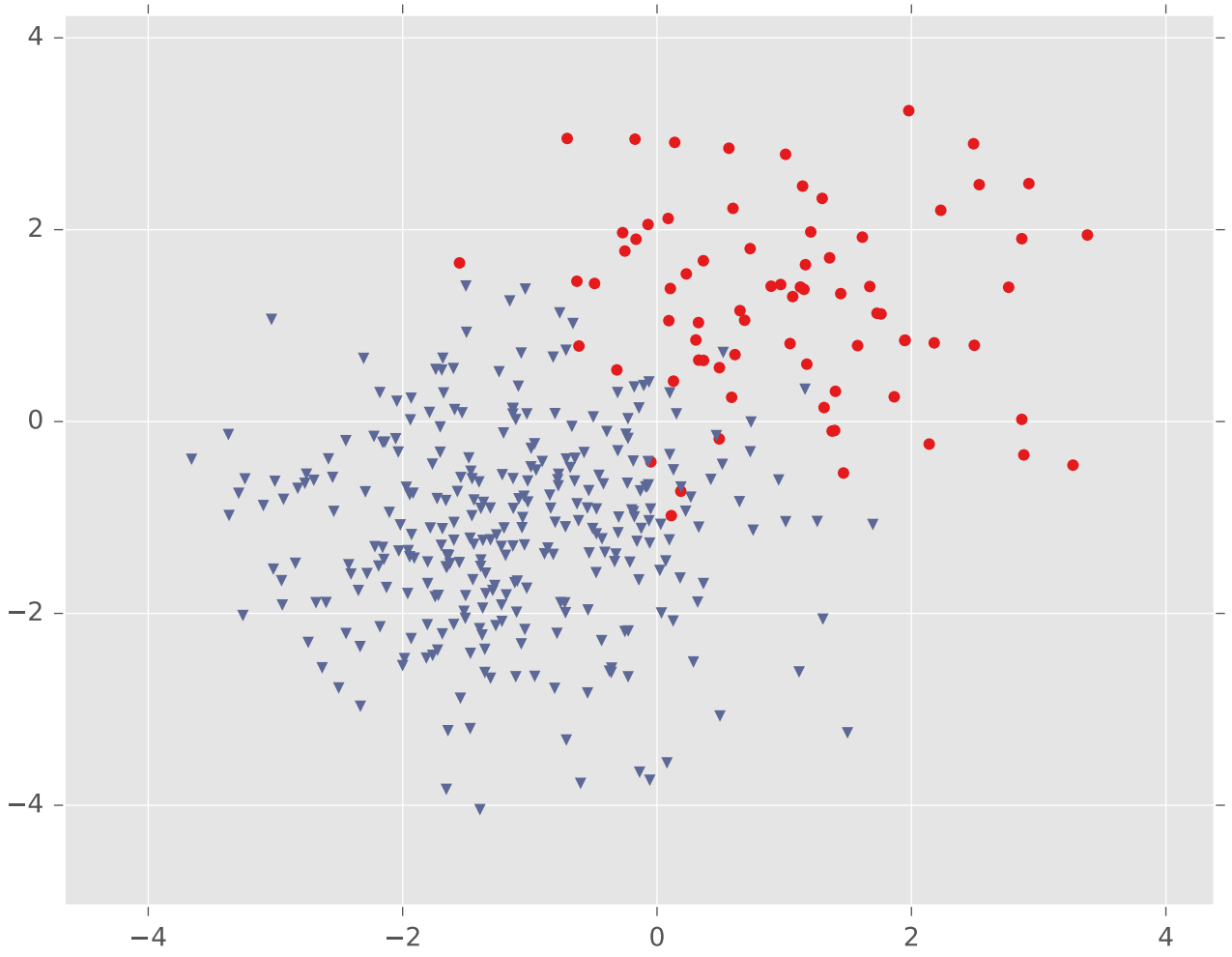
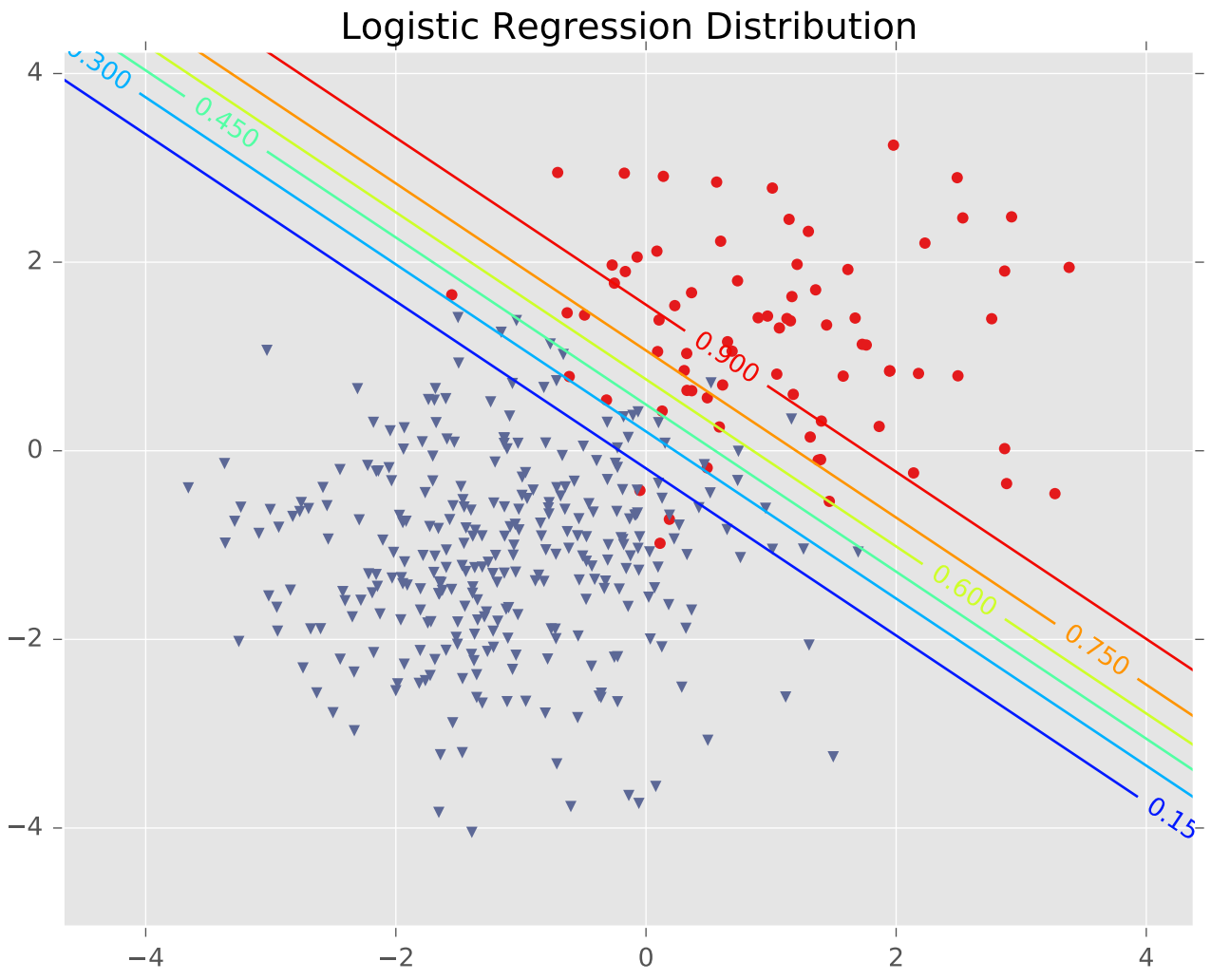


Figure courtesy of Matt Gormley

Logistic Regression Decision Boundary



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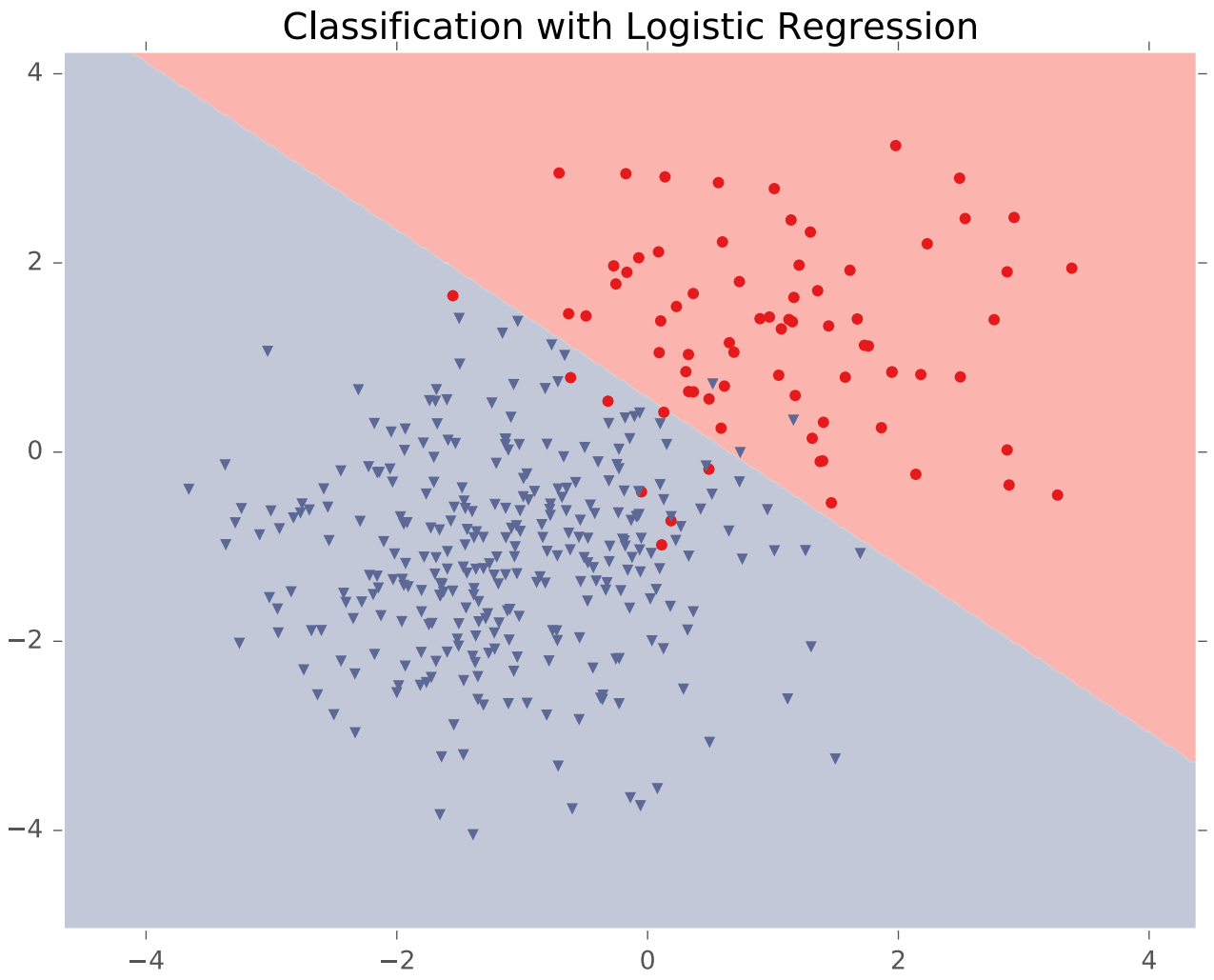


Figure courtesy of Matt Gormley

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

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

$$\ell(\boldsymbol{\theta}) = -\log P\left(y^{(1)}, \ldots, y^{(N)} \middle| \boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(N)}, \boldsymbol{\theta}\right) = -\log \prod_{n=1}^{N} P\left(y^{(n)} \middle| \boldsymbol{x}^{(n)}, \boldsymbol{\theta}\right)$$

$$= -\log \prod_{n=1}^{N} P\left(Y = 1 \middle| \boldsymbol{x}^{(n)}, \boldsymbol{\theta}\right)^{y^{(n)}} \left(P\left(Y = 0 \middle| \boldsymbol{x}^{(n)}, \boldsymbol{\theta}\right)\right)^{1-y^{(n)}}$$

$$= -\sum_{n=1}^{N} y^{(n)} \log P\left(Y = 1 \middle| \boldsymbol{x}^{(n)}, \boldsymbol{\theta}\right) + \left(1 - y^{(n)}\right) \log P\left(Y = 0 \middle| \boldsymbol{x}^{(n)}, \boldsymbol{\theta}\right)$$

$$= -\sum_{n=1}^{N} y^{(n)} \log \frac{P\left(Y = 1 \middle| \boldsymbol{x}^{(n)}, \boldsymbol{\theta}\right)}{P\left(Y = 0 \middle| \boldsymbol{x}^{(n)}, \boldsymbol{\theta}\right)} + \log P\left(Y = 0 \middle| \boldsymbol{x}^{(n)}, \boldsymbol{\theta}\right)$$

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

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

Minimizing the Negative Conditional (log-)Likelihood

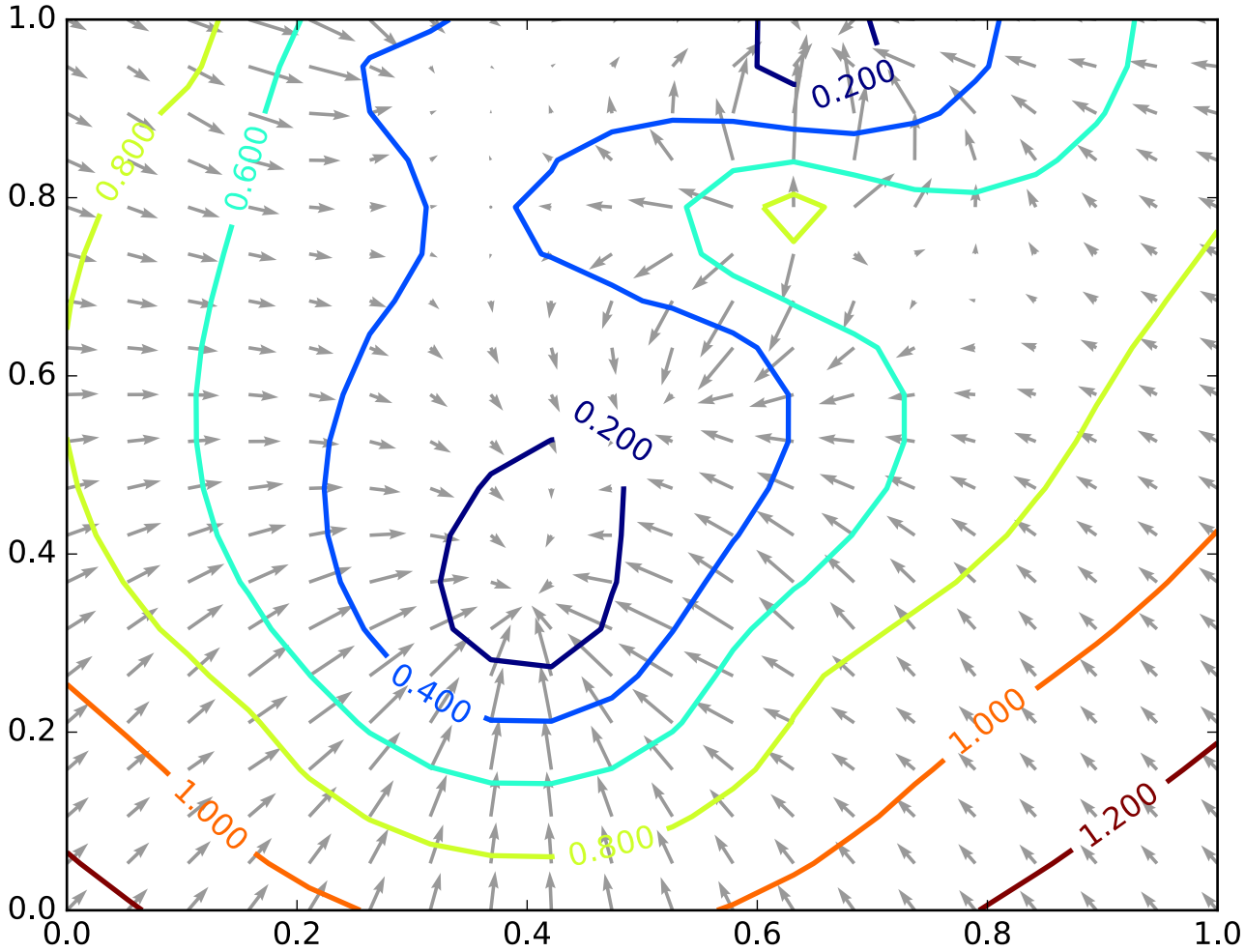
$$J(\boldsymbol{\theta}) = -\frac{1}{N}\sum_{n=1}^{N} y^{(n)}\boldsymbol{\theta}^T\boldsymbol{x}^{(n)} - \log\left(1+\exp\left(\boldsymbol{\theta}^T\boldsymbol{x}^{(n)}\right)\right)$$

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

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

$$= \frac{1}{N}\sum_{n=1}^{N} \boldsymbol{x}^{(n)}\left(P\left(Y=1\middle|\boldsymbol{x}^{(n)},\boldsymbol{\theta}\right) - y^{(n)}\right)$$

Recall: Gradient Descent



Gradient Descent

- Input: training dataset $\mathcal{D} = \{(\boldsymbol{x}^{(i)}, y^{(i)})\}_{i=1}^{N}$ 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:

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

   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: $\boldsymbol{\theta}^{(t)}$

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 $\mathcal{D} = \{(\boldsymbol{x}^{(i)}, y^{(i)})\}_{i=1}^{N}$ and step size γ

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

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

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   c. Increment t: $t \leftarrow t + 1$

- Output: $\boldsymbol{\theta}^{(t)}$

Stochastic Gradient Descent (SGD)

- Input: training dataset $\mathcal{D} = \left\{\left(\boldsymbol{x}^{(i)}, y^{(i)}\right)\right\}_{i=1}^{N}$ 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 $\mathcal{D}$, $\left(\boldsymbol{x}^{(i)}, y^{(i)}\right)$
   b. Compute the pointwise gradient:

$$\nabla_{\boldsymbol{\theta}} J^{(i)}\left(\boldsymbol{\theta}^{(t)}\right) = \boldsymbol{x}^{(i)}\left(P\left(Y = 1 \middle| \boldsymbol{x}^{(i)}, \boldsymbol{\theta}^{(t)}\right) - y^{(i)}\right)$$

   c. Update $\boldsymbol{\theta}$: $\boldsymbol{\theta}^{(t+1)} \leftarrow \boldsymbol{\theta}^{(t)} - \gamma \nabla_{\boldsymbol{\theta}} J^{(i)}\left(\boldsymbol{\theta}^{(t)}\right)$
   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!

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

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

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

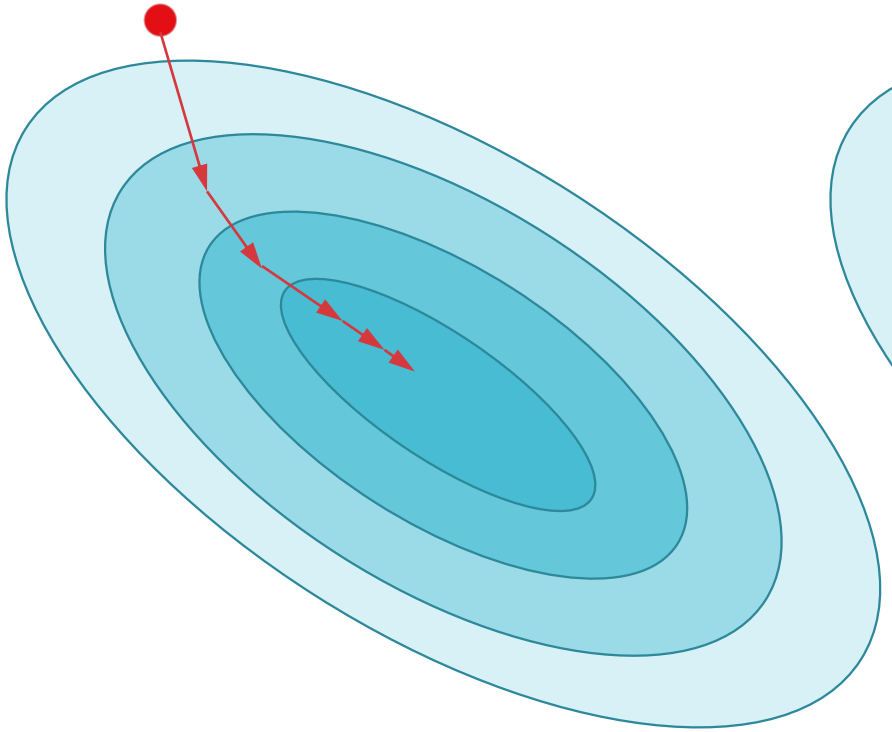
Stochastic Gradient Descent (SGD)

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

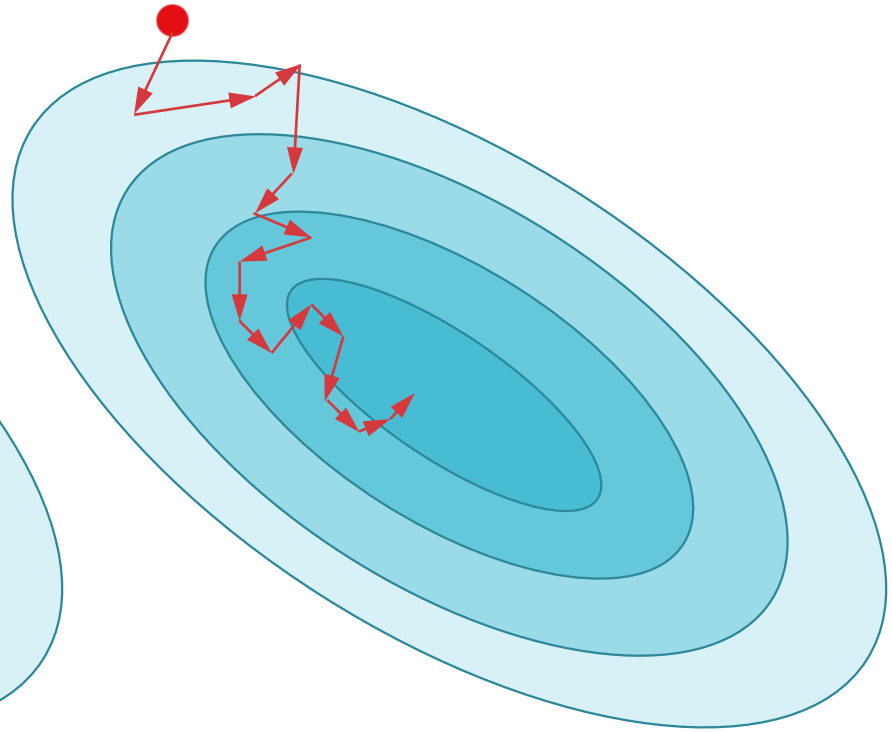
1. Initialize $\boldsymbol{\theta}^{(0)}$ to all zeros and set $t = 0$
2. While TERMINATION CRITERION is not satisfied
   a. For $i \in \text{shuffle}(\{1, \ldots, N\})$
      i. Compute the pointwise gradient:
      $$\nabla_{\boldsymbol{\theta}} J^{(i)}(\boldsymbol{\theta}^{(t)}) = \boldsymbol{x}^{(i)}\left(P\left(Y = 1 \middle| \boldsymbol{x}^{(i)}, \boldsymbol{\theta}^{(t)}\right) - y^{(i)}\right)$$
      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: $\boldsymbol{\theta}^{(t)}$

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

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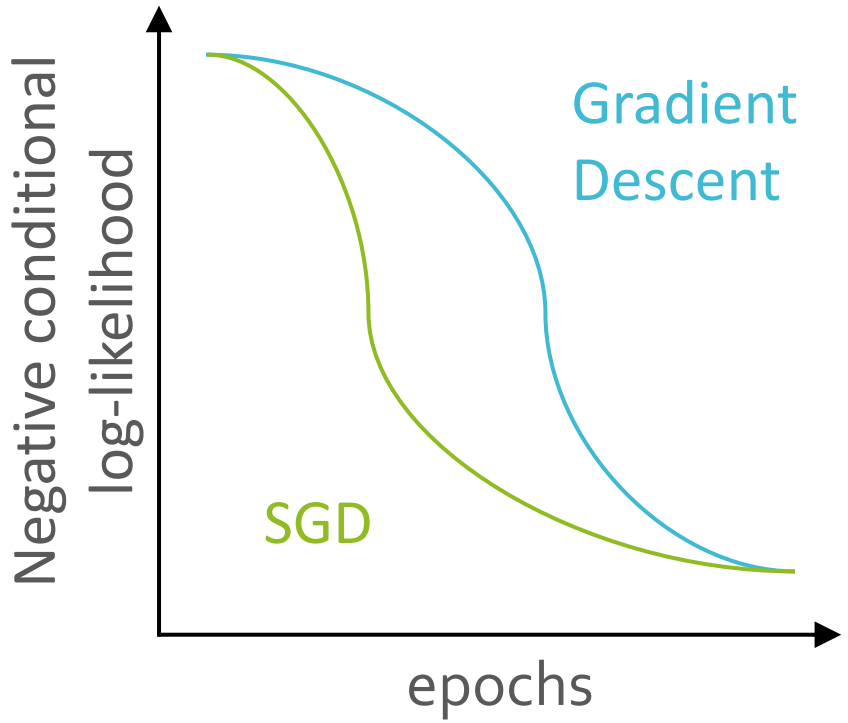

Empirically, SGD reduces the negative conditional log-likelihood much faster than gradient descent

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