

10-301/601 Introduction to Machine Learning

Machine Learning Department School of Computer Science Carnegie Mellon University

Logistic Regression + Feature Engineering + Regularization

Matt Gormley & Henry Chai Lecture 10 Oct. 1, 2021

Reminders

- **Homework 4: Logistic Regression**
	- **Out: Fri, Oct. 1**
	- **Due: Mon, Oct. 11 at 11:59pm**

MAXIMUM LIKELIHOOD ESTIMATION

MLE

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

Principle of Maximum Likelihood Estimation:

ie parameters t $\frac{1}{N}$ *i*=1 *N* Choose the parameters that maximize the likelihood of the data. $\boldsymbol{\theta}^{\sf MLE} = \operatorname{argmax}$ $\prod p(\mathbf{x}^{(i)}|\boldsymbol{\theta})$ *N*

 $\boldsymbol{\theta}$

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

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/

==

Not legged to Light Charles

 \sim

Book Service

Tel legged in large Chinese

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

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

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 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:

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

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

for:

Background: Hyperplanes

ar
nci *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): $\mathcal{H} = {\mathbf{x} : \mathbf{w}^T\mathbf{x} = b}$ Hyperplane (Definition 2): $\mathcal{H} = \{ \mathbf{x} : \boldsymbol{\theta}^T \mathbf{x} = 0 \}$)
1 1 $\boldsymbol{\theta} = [b, w_1, \dots, w_M]^T$ $\mathbf{x}' = [1, x_1, \ldots, x_M]^T$ Half-spaces: $\mathcal{H}^+=\{\mathbf{x}:\boldsymbol{\theta}^T\mathbf{x}>0\text{ and }x_{1}=1\}$ $\mathcal{H}^- = {\{\mathbf{x}:\boldsymbol{\theta}^T\mathbf{x} < 0 \text{ and } x_{1} = 1\}}$

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

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…

$$
h(\mathbf{x}) = \text{``sign''}(\boldsymbol{\theta}^T \mathbf{x})
$$

 $``sign''(u)$

 \overline{O}

Use a differentiable function instead! $p_{\theta}(y=1|\mathbf{x}) = \frac{1}{1+\exp(\theta)}$ $1 + \exp(-\boldsymbol{\theta}^T \mathbf{x})$

Whiteboard

- Conceptual Change: 2D classification in 3D
- Why is it called Logistic *Regression* and not Logistic *Classification*?

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. $p_{\boldsymbol{\theta}}(y=1|\mathbf{x}) = \frac{1}{1+\alpha \mathbf{x}^2}$ $1 + \exp(-\boldsymbol{\theta}^T \mathbf{x})$

Learning: finds the parameters that minimize some objective function. $\;\;\boldsymbol{\theta}^* = \operatorname{argmin} J(\boldsymbol{\theta})$ $\boldsymbol{\theta}$

Prediction: Output is the most probable class.

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

Whiteboard

- Logistic Regression Model
- Partial derivative for logistic regression
- Gradient for logistic regression
- Decision boundary

LOGISTIC REGRESSION ON GAUSSIAN DATA

Classification with Logistic Regression

LEARNING LOGISTIC REGRESSION

Maximum **Conditional** Likelihood Estimation

Learning: finds the parameters that minimize some objective function**.**

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

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

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

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

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)

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

A when survey is active, respond at polley.com/10301601polls

Lecture 10: In-Class Poll

@ When poll is active, respond at polley.com/10301601polls

Question 1

Gradient Descent

Algorithm 1 Gradient Descent

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

$$
2\colon\qquad \boldsymbol{\theta}\leftarrow \boldsymbol{\theta}^{(0)}
$$

3: while not converged do

4.
$$
\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \gamma \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})
$$

5: return θ

In order to apply GD to Logistic Regression all we need is the **gradient** of the objective function (i.e. vector of partial derivatives). $\nabla_{\bm{\theta}} J({\bm{\theta}})$ =

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

 $L \overline{d\theta_M}$

Stochastic Gradient Descent (SGD) Recall…

Algorithm 1 Stochastic Gradient Descent (SGD)

1: procedure SGD(D,
$$
\theta^{(0)}
$$
)
\n2: $\theta \leftarrow \theta^{(0)}$
\n3: while not converged do
\n4: for *i* ∈ shuffle({{1, 2, ..., N}}**) do**
\n5: $\theta \leftarrow \theta - \gamma \nabla_{\theta} J^{(i)}(\theta)$
\n6: return θ

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

We need a per-example objective:

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

where $J^{(i)}(\boldsymbol{\theta}) = -\log p_{\boldsymbol{\theta}}(y^{i}|\mathbf{x}^{i}).$

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:

@ When poll is active, respond at polley.com/10301601polls

Question 2

OPTIMIZATION METHOD #4: MINI-BATCH SGD

Mini-Batch SGD

• **Gradient Descent**:

Compute true gradient exactly from all N examples

- **Stochastic Gradient Descent (SGD)**: Approximate true gradient by the gradient of one randomly chosen example
- **Mini-Batch SGD**:

Approximate true gradient by the average gradient of K randomly chosen examples

Mini-Batch SGD

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

Three variants of first-order optimization:
Gradient Descent: $\mathbf{g} = \nabla J(\theta) = \frac{1}{N} \sum_{i=1}^{N} \nabla J^{(i)}(\theta)$ 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 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

FEATURE ENGINEERING

Handcrafted Features

Feature Engineering Feature Engineering

Feature Engineering

Feature Engineering

Feature Engineering

Feature Engineering

Feature Engineering

Feature Engineering

Feature Engineering

Feature Engineering

Suppose you build a logistic regression model to predict a part-of-speech (POS) tag for each word in a sentence.

What features should you use?

Per-word Features:

 $...$

1

1

 Ω

 $\overline{0}$

 $\overline{0}$

 $\overline{0}$

…

Context Features:

…

1

 Ω

0

0

 \bigcirc

…

Context Features:

Table 3. Tagging accuracies with different feature templates and other changes on the WSJ 19-21 development set.

Edge detection (Canny)

Corner Detection (Harris)

Scale Invariant Feature Transform (SIFT)

opnow. Recognition results below show model outlines and mage keys used for matching.

Figure 1: For each octave of scale space, the initial image is repeatedly convolved with Gaussians to produce the set of scule space images shown on the left. Adjacent Gaussian images are subtracted to produce the difference-of-Gaussian images on the right. After each octave, the Gaussian image is down-sampled by a factor of 2, and the process repeated.

NON-LINEAR FEATURES

Nonlinear Features

- aka. "nonlinear basis functions"
- So far, input was always $\mathbf{x} = [x_1, \dots, x_M]$
- **Key Idea**: let input be some function of **x**
	- original input:

$$
\text{--}\ \ \mathsf{new}\ \mathsf{input:}\qquad \mathbf{x}'\in\mathbb{R}^M
$$

- define $\mathbf{x}' = b(\mathbf{x}) = [b_1(\mathbf{x}), b_2(\mathbf{x}), \dots, b_{M'}(\mathbf{x})]$

where $b_i : \mathbb{R}^M \to \mathbb{R}$ is any function

• **Examples**: (M = 1) polynomial

$$
b_j(x) = x^j \quad \forall j \in \{1, ..., J\}
$$

$$
b_j(x) = \exp\left(\frac{-(x - \mu_j)^2}{2\sigma_j^2}\right)
$$

$$
b_j(x) = \frac{1}{1 + \exp(-\omega_j x)}
$$

$$
b_j(x) = \log(x)
$$

For a linear model: still a linear function
of $b(x)$ even though a nonlinear function of **x**

Examples:

- Perceptron
- Linear regression
- Logistic regression

radial basis function

sigmoid

log

Goal: Learn $y = w^T f(x) + b$ where f(.) is a polynomial basis function

Goal: Learn $y = w^T f(x) + b$ where f(.) is a polynomial basis function

Goal: Learn $y = w^T f(x) + b$ where f(.) is a polynomial basis function

Goal: Learn $y = w^T f(x) + b$ where f(.) is a polynomial basis function

Goal: Learn $y = w^T f(x) + b$ where f(.) is a polynomial basis function

Goal: Learn $y = w^T f(x) + b$ where f(.) is a polynomial basis function

Goal: Learn $y = w^T f(x) + b$ where f(.) is a polynomial basis function

Over-fitting

 $E_{\rm RMS}=\sqrt{2E({\bf w}^{\star})/N}$ Root-Mean-Square (RMS) Error:

Polynomial Coefficients

Goal: Learn $y = w^T f(x) + b$ points we overfit! where f(.) is a polynomial \cdot But with N = 100 basis function points, the Linear Regression (poly=9) overfitting $2.0 -$ (mostly) **i y x … x9** disappears 1 2.0 1.2 … $(1.2)^9$ • **Takeaway**: more 1.5 data helps 2 1.3 1.7 … $(1.7)^9$ prevent … … … … … 1.0 y overfitting10 1.1 1.9 … (1.9)9 $0.5 0.0 -0.5 1.5$ 2.0 2.5 3.0

• With just $N = 10$

Goal: Learn $y = w^T f(x) + b$ where f(.) is a polynomial basis function

With just $N = 10$

points we overfit!