

10-301/601 Introduction to Machine Learning

Machine Learning Department School of Computer Science Carnegie Mellon University

(Logistic Regression) + Feature Engineering + Regularization

Matt Gormley Lecture 10 Feb. 21, 2022

Q&A

- **Q:** How do I avoid submitting a misaligned written homework on Gradescope?
- A: Great question, since this will help avoid AI-assisted grading incorrectly grading your submission. Here are some tips:
 - 1. Check that your PDF has the same number of pages as our PDF.
 - Check that your submission boxes match on Gradescope. Be sure to check at least one box on each page.
 - 3. Attend our special OH on how to use LaTeX!

Q&A

- **Q:** I think you graded seven different questions incorrectly. Should I put them all in on Gradescope regrade request and submit that?
- A: Please, no. I'd encourage you to watch this tutorial video from Gradescope so you know how to use this important tool.

https://help.gradescope.com/article/8hchz9h8wh-studentregrade-request

Reminders

- Homework 4: Logistic Regression
 - Out: Fri, Feb 18
 - Due: Sun, Feb. 27 at 11:59pm

LOGISTIC REGRESSION REMARKS

Why is it not "Logistic Classification"?

Whiteboard

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

LOGISTIC REGRESSION ON GAUSSIAN DATA

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 actually MCLE! more on this later...)

Maximum **Conditional** Likelihood Estimation

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

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 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 loglikelihood 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

Algorithm 1 Gradient Descent

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

- 2: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta}^{(0)}$
- 3: while not converged do 4: $\theta \leftarrow \theta - \gamma \nabla_{\theta} J(\theta)$

5: return θ



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

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

Stochastic Gradient Descent (SGD)

Algorithm 1 Stochastic Gradient Descent (SGD)

1: procedure SGD(
$$\mathcal{D}, \boldsymbol{\theta}^{(0)}$$
)

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta}^{(0)}$$

while not converged do 3: for $i \in \mathsf{shuffle}(\{1, 2, \dots, N\})$ do 4: $oldsymbol{ heta} \leftarrow oldsymbol{ heta} - \gamma
abla_{oldsymbol{ heta}} J^{(i)}(oldsymbol{ heta})$



return θ 6:

5:

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.





BAYES OPTIMAL CLASSIFIER

Bayes Optimal Classifier

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Suppose you knew the distribution p*(y | x) or had a good approximation to it.

Question:

How would you design a function y = h(x) to predict a single label?

Answer:

You'd use the Bayes optimal classifier!

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 $p(y|\mathbf{x})$ that best approximates $p^*(y|\mathbf{x})$

Bayes Optimal Classifier Uscally Def: an oracle knows everythy (e.g. p*(y|x)) Q: What is the optimal classifier in this setting? YE 20, 13 A: $\hat{y} = h(\vec{x}) = \begin{cases} 1 & \text{if } p(y=1|x) \ge p(y=0|x) \\ 0 & \text{otherwise} \end{cases}$ 1 p (y=1 |x) *(y=0 ×) = argmax p(y|x)ye {0,13 p(y|x)reducible error Bayes Optimul Classifier Х for % loss further

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

while not converged:
$$oldsymbol{ heta} \leftarrow oldsymbol{ heta} - \gamma \mathbf{g}$$

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 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 for NLP

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?



Feature Engineering for NLP

Per-word Features:

```
is-capital(w<sub>i</sub>)
endswith(w<sub>i</sub>, "e")
endswith(w<sub>i</sub>, "d")
endswith(w<sub>i</sub>, "ed")
w<sub>i</sub> == "aardvark"
w<sub>i</sub> == "hope"
```

...





Feature Engineering for NLP

Context Features:









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...




Feature Engineering for NLP

Context Features:





Feature Engineering for NLP

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

Model	Feature Templates	#	Sent.	Token	Unk.
		Feats	Acc.	Acc.	Acc.
3gramMemm	See text	248,798	52.07%	96.92%	88.99%
NAACL 2003	See text and $[1]$	$460,\!552$	55.31%	97.15%	88.61%
Replication	See text and [1]	$460,\!551$	55.62%	97.18%	88.92%
$\operatorname{Replication}'$	+rareFeatureThresh $= 5$	$482,\!364$	55.67%	97.19%	88.96%
$5 \mathrm{W}$	$+\langle t_0,w_{-2} angle,\langle t_0,w_2 angle$	$730,\!178$	56.23%	97.20%	89.03%
5wShapes	$+\langle t_0,s_{-1} angle,\langle t_0,s_0 angle,\langle t_0,s_{+1} angle$	$731,\!661$	56.52%	97.25%	89.81%
5wShapesDS	+ distributional similarity	$737,\!955$	56.79%	97.28%	90.46%



Feature Engineering for CV

Edge detection (Canny)



Corner Detection (Harris)



Feature Engineering for CV

Scale Invariant Feature Transform (SIFT)



Figure 3: Model images of planar objects are shown in the op row. 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 scale 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" ۲
- So far, input was always $\mathbf{x} = [x_1, \dots, x_M]$ ullet
- Key Idea: let input be some function of x
 - original input: $\mathbf{x} \in \mathbb{R}^{M}$ where M' > M (usually)

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

- 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)ulletpolynomial

radial basis function

 $b_i(x) = x^j \quad \forall j \in \{1, \dots, J\}$ $b_j(x) = \exp\left(\frac{-(x-\mu_j)^2}{2\sigma_i^2}\right)$ $b_j(x) = \frac{1}{1 + \exp(-\omega_j x)}$ $b_i(x) = \log(x)$

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

Examples:

- Perceptron
- Linear regression
- Logistic regression

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

i	у	x	X ²
1	2.0	1.2	(1.2)2
2	1.3	1.7	(1.7) ²
10	1.1	1.9	(1.9)2

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

i	у	х	X ²	X ³
1	2.0	1.2	(1.2)2	(1.2) ³
2	1.3	1.7	(1.7)2	(1.7) ³
•••				
10	1.1	1.9	(1.9) ²	(1 . 9) ³

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

i	у	x	•••	x ⁵
1	2.0	1.2		(1.2)5
2	1.3	1.7		(1.7)5
10	1.1	1.9		(1.9) ⁵

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

i	у	х	•••	x ⁸
1	2.0	1.2		(1.2)8
2	1.3	1.7		(1.7) ⁸
10	1.1	1.9		(1.9) ⁸

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

i	у	х	•••	x ⁹
1	2.0	1.2		(1.2) ⁹
2	1.3	1.7		(1.7) ⁹
10	1.1	1.9		(1.9) ⁹

Over-fitting

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

Polynomial Coefficients

	M = 0	M = 1	M=3	M = 9
θ_0	0.19	0.82	0.31	0.35
${ heta}_1$		-1.27	7.99	232.37
$ heta_2$			-25.43	-5321.83
$ heta_3$			17.37	48568.31
$ heta_4$				-231639.30
$ heta_5$				640042.26
$ heta_6$				-1061800.52
$ heta_7$				1042400.18
θ_8				-557682.99
$ heta_9$				125201.43

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Goal: Learn $y = w^T f(x) + b$ points we overfit! where f(.) is a polynomial But with N = 100basis function points, the Linear Regression (poly=9) overfitting 2.5 (mostly) **X**⁹ X ••• disappears 2.0 1.2 ... (1.2)9 2.0 1 Takeaway: more data helps ... (1.7)9 1.7 1.3 2 1,5 prevent ... (2.7)⁹ V 2.7 3 0.1 overfitting 1.0 ... (1.9)9 1.9 4 1.1 0.5 • • • 0.0 -... 98 -0.5... . . . • • • ... 99 ... • • • 1.5 2.0 2.5 1.0 3.0 ... (1.5)9 100 0.9 1.5

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With just N = 10

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REGULARIZATION

Overfitting

Definition: The problem of **overfitting** is when the model captures the noise in the training data instead of the underlying structure

Overfitting can occur in all the models we've seen so far:

- Decision Trees (e.g. when tree is too deep)
- KNN (e.g. when k is small)
- Perceptron (e.g. when sample isn't representative)
- Linear Regression (e.g. with nonlinear features)
- Logistic Regression (e.g. with many rare features)

Motivation: Regularization

- Occam's Razor: prefer the simplest hypothesis
- What does it mean for a hypothesis (or model) to be simple?
 - 1. small number of features (model selection)
 - small number of "important" features (shrinkage)

- **Given** objective function: $J(\theta)$
- **Goal** is to find: $\hat{\theta} = \underset{\theta}{\operatorname{argmin}} J(\theta) + \lambda r(\theta)$
- Key idea: Define regularizer r(θ) s.t. we tradeoff between fitting the data and keeping the model simple
- Choose form of r(θ):

– Example: q-norm (usually p-norm): $\|\boldsymbol{\theta}\|_q =$

		$\left \begin{array}{c} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 $
=	$\sum_{m=1}$	$ \theta_m ^q$

q	$r(oldsymbol{ heta})$	yields parame- ters that are	name	optimization notes
0	$ \boldsymbol{\theta} _0 = \sum \mathbb{1}(\theta_m \neq 0)$	zero values	Lo reg.	no good computa- tional solutions
$rac{1}{2}$	$egin{aligned} oldsymbol{ heta} _1 &= \sum heta_m \ (oldsymbol{ heta} _2)^2 &= \sum heta_m^2 \end{aligned}$	zero values small values	L1 reg. L2 reg.	subdifferentiable differentiable

Regularization Examples

Add an L2 regularizer to Linear Regression (aka. Ridge Regression)

$$J_{\mathsf{R}\mathsf{R}}(\boldsymbol{\theta}) = J(\boldsymbol{\theta}) + \lambda ||\boldsymbol{\theta}||_2^2$$
$$= \frac{1}{N} \sum_{i=1}^N \frac{1}{2} (\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)})^2 + \lambda \sum_{m=1}^M \theta_m^2$$

Add an L1 regularizer to Linear Regression (aka. LASSO)

$$J_{\text{LASSO}}(\boldsymbol{\theta}) = J(\boldsymbol{\theta}) + \lambda ||\boldsymbol{\theta}||_{1}$$
$$= \frac{1}{N} \sum_{i=1}^{N} \frac{1}{2} (\boldsymbol{\theta}^{T} \mathbf{x}^{(i)} - y^{(i)})^{2} + \lambda \sum_{m=1}^{M} |\boldsymbol{\theta}_{m}|$$

Regularization Examples

Add an L2 regularizer to Logistic Regression

$$J'(\boldsymbol{\theta}) = J(\boldsymbol{\theta}) + \lambda ||\boldsymbol{\theta}||_2^2$$
$$= \frac{1}{N} \sum_{i=1}^N -\log p(y^{(i)} \mid \mathbf{x}^{(i)}, \boldsymbol{\theta}) + \lambda \sum_{m=1}^M \theta_m^2$$

Add an L1 regularizer to Logistic Regression

$$J'(\boldsymbol{\theta}) = J(\boldsymbol{\theta}) + \lambda ||\boldsymbol{\theta}||_1$$
$$= \frac{1}{N} \sum_{i=1}^N -\log p(y^{(i)} \mid \mathbf{x}^{(i)}, \boldsymbol{\theta}) + \lambda \sum_{m=1}^M |\boldsymbol{\theta}_m|$$

Question:

Suppose we are minimizing $J'(\theta)$ where

 $J'(\boldsymbol{\theta}) = J(\boldsymbol{\theta}) + \lambda r(\boldsymbol{\theta})$

As λ increases, the minimum of J'(θ) will...

- A. ... move towards the midpoint between $J(\theta)$ and $r(\theta)$
- B. ... move towards the minimum of $J(\theta)$
- C. ... move towards the minimum of $r(\theta)$
- D. ... move towards a theta vector of positive infinities
- E. ... move towards a theta vector of negative infinities
- F. ... stay the same

Whiteboard

– Why does L2 regularization lead to small numbers and L1 regularization lead to zeros?

Don't Regularize the Bias (Intercept) Parameter!

- In our models so far, the bias / intercept parameter is usually denoted by θ_0 -- that is, the parameter for which we fixed $x_0 = 1$
- Regularizers always avoid penalizing this bias / intercept parameter
- Why? Because otherwise the learning algorithms wouldn't be invariant to a shift in the y-values

Whitening Data

- It's common to whiten each feature by subtracting its mean and dividing by its variance
- For regularization, this helps all the features be penalized in the same units (e.g. convert both centimeters and kilometers to z-scores)

Regularization Exercise

In-class Exercise

- 1. Plot train error vs. regularization weight (cartoon)
- 2. Plot validation error vs. regularization weight (cartoon)

REGULARIZATION EXAMPLE: LOGISTIC REGRESSION

- For this example, we construct nonlinear features (i.e. feature engineering)
- Specifically, we add polynomials up to order 9 of the two original features x₁ and x₂
- Thus our classifier is linear in the high-dimensional feature space, but the decision boundary is nonlinear when visualized in low-dimensions (i.e. the original two dimensions)

Classification with Logistic Regression (lambda=1e-05)

Classification with Logistic Regression (lambda=0.0001)

Classification with Logistic Regression (lambda=0.001)

Classification with Logistic Regression (lambda=0.01)

Classification with Logistic Regression (lambda=0.1)

Classification with Logistic Regression (lambda=1)

Classification with Logistic Regression (lambda=10)

Classification with Logistic Regression (lambda=100)



Classification with Logistic Regression (lambda=1000)



Classification with Logistic Regression (lambda=10000)



Classification with Logistic Regression (lambda=100000)



Classification with Logistic Regression (lambda=1e+06)



Classification with Logistic Regression (lambda=1e+07)





Regularization as MAP

- L1 and L2 regularization can be interpreted as maximum a-posteriori (MAP) estimation of the parameters
- To be discussed later in the course...

Takeaways

- Nonlinear basis functions allow linear models (e.g. Linear Regression, Logistic Regression) to capture nonlinear aspects of the original input
- Nonlinear features are require no changes to the model (i.e. just preprocessing)
- 3. Regularization helps to avoid overfitting
- **4. Regularization** and **MAP estimation** are equivalent for appropriately chosen priors

Feature Engineering / Regularization Objectives

You should be able to...

- Engineer appropriate features for a new task
- Use feature selection techniques to identify and remove irrelevant features
- Identify when a model is overfitting
- Add a regularizer to an existing objective in order to combat overfitting
- Explain why we should **not** regularize the bias term
- Convert linearly inseparable dataset to a linearly separable dataset in higher dimensions
- Describe feature engineering in common application areas