CPSC 340: Machine Learning and Data Mining

Multi-Class Linear Classifiers Summer 2021

Admin



- Canvas grades released. Good job!
- Assignment 4 due Monday.
 GO TO TUTORIALS. THEY'RE VERY HELPFUL.
- Assignment 5 out Friday.
- Final exam is Wednesday, June 23, 2021
 Probably similar format as midterm.

Last Time: SVM and Logistic Regression

$$f(w) = \sum_{j=1}^{2} \max \{0, 1-y_i, w^T x_i\} + \frac{1}{2} ||w||^2$$

Hinge loss for support vector machine

$$f(w) = \sum_{i=1}^{n} log(1 + exp(-y_iw^7x_i))$$

Logistic loss for logistic regression

- We derived these losses step-by-step.
- We will do similar stuff today.

Last Time: SVM and Logistic Regression



In This Lecture

- 1. Linear Probabilistic Classifiers (10 minutes)
- 2. Multi-Class Classification Intro (10 minutes)
- 3. Multi-Class SVM (20 minutes)
- 4. Multi-Class Logistic Regression (15 minutes)

Coming Up Next
LINEAR PROBABILISTIC CLASSIFIERS

Previously: Identifying Important E-mails

• Recall problem of identifying 'important' e-mails:



• We can do binary classification by taking sign of linear model:

 $\hat{y}_i = sign(w^7 x_i)$

- Convex loss functions (hinge/logistic loss) let us find an appropriate 'w'.
- But what if we want a probabilistic classifier?
 - Want a model of $p(y_i = "important" | x_i)$ for use in decision theory.



Linear Prediction of "+1-ness"



Q: How should $p(y_i=+1 | x_i)$ behave?

Sigmoid Function





+1-ness with Sigmoid -10 -5 0 0 5 10 f(x) = sigmoid(wx)

- Idea: let's compute +1-ness with sigmoid.
- Given parameters w:
 - 1. Compute $z_i = w^T x_i$
 - 2. Compute $p(y_i = +1 | w, x_i) = sigmoid(z_i)$

$$P(y_{i}=+1 | W, \cdot): | \mathbb{R}^{d} \longrightarrow (0, 1)$$

$$P(y_{i}=+1 | W, X_{i}) = \text{Sigmoid}(W^{T}X_{i})$$

Probabilities for Linear Classifiers using Sigmoid

• Using sigmoid function, we output probabilities for linear models using:

$$p(y_i = +| | w_i, x_i) = \frac{1}{|texp(-w^T x_i)|}$$



• Visualization for 2 features:

What About "-1-ness"?

• Using sigmoid function, we output probabilities for linear models using:

$$P(y_i = +| | w_i, x_i) = \frac{1}{| + e_{x_i}(-w_i^T x_i)}$$

• By rules of probability:

$$p(y_{i} = -1 | w_{i} x_{i}) = 1 - p(y_{i} = 1 | w_{i} x_{i})$$
$$= \frac{1}{1 + ex_{p}(w^{2} x_{i})} \quad (with some effor 1)$$

- We then use these for "probability that an email x_i is important".
- This may seem heuristic, but later we'll see that:
 - minimizing logistic loss does "maximum likelihood estimation" in this model.

MULTI-CLASS CLASSIFICATION INTRO

Coming Up Next



People with no idea about AI, telling me my AI will destroy the world Me wondering why my neural network is classifying a cat as a dog..

Multi-Class Linear Classification

• We've been considering linear models for binary classification:



• E.g., is there a cat in this image or not?



Multi-Class Linear Classification

• Today we'll discuss linear models for multi-class classification:



- For example, classify image as "cat", "dog", or "person".
 - This was natural for methods of Part 1 (decision trees, naïve Bayes, KNN).
 - For linear models, we need some new notation.

Q: Can we use binary classifiers for multi-class?

"One vs All" Classification

- Training phase:
 - For each class 'c', train binary classifier to predict whether example is a 'c'.
 - For example, train a "cat detector", a "dog detector", and a "human detector".
 - If we have 'k' classes, this gives 'k' binary classifiers .



"One vs All" Classification $W = \begin{bmatrix} -W_{cat} \\ -W_{dog} \\ -W_{dog} \end{bmatrix}$ # choses

- Prediction phase:
 - Apply the 'k' binary classifiers to get a "score" for each class 'c'.
 - Predict the 'c' with the highest score.

$$W_{cat} X_{i} = -0.1$$

$$W_{log} X_{i} = -0.8$$

$$y_{i} = human$$

$$W_{log} X_{i} = 0.9$$

$$W_{human} X_{i} = 0.9$$
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Multi-Class Linear Classification (MEMORIZE)

• Back to multi-class classification where we have 1 "correct" label:



We'll use ' W_{y'} as classifier where c=y_i (row of correct class label).
 So if y_i=2 then W_{yi} = w₂.

Shape of Decision Boundaries

• Recall that a binary linear classifier splits space using a hyper-plane:



• Divides x_i space into 2 "half-spaces".

Shape of Decision Boundaries

- Multi-class linear classifier is intersection of these "half-spaces":
 - This divides the space into convex regions (like k-means):



Could be non-convex with change of basis.

Digression: Multi-Label Classification

• A related problem is multi-label classification:



- Which of the 'k' objects are in this image?
 - There may be more than one "correct" class label.
 - Here we can also fit 'k' binary classifiers.
 - But we would take all the sign($w_c^T x_i$)=+1 as the labels.



"One vs All" Multi-Class Linear Classification

- Problem: We didn't train the w_c so that the largest $w_c^T x_i$ would be $W_{y_i^T} x_i$.
 - Each classifier is just trying to get the sign right.

$$\int \frac{w_1^{T}x_i}{features x_i} = -0.1 \quad ("cat" \ score)$$

- Here the classifier incorrectly predicts "dog".
 - "One vs All" doesn't try to put $w_2^T x_i$ and $w_3^T x_i$ on same scale for decisions like this.
 - We should try to make $w_3^T x_i$ positive and $w_2^T x_i$ negative relative to each other.
 - The multi-class hinge losses and the multi-class logistic loss do this.

Coming Up Next MULTI-CLASS SVM

Binary Classifiers are "Under-constrained"



Binary Classifiers are "Under-constrained"



What Do We Want for Multi-Class Classifiers?

- Idea: additional constraints on slopes
 - Will "force" classifier to find better boundaries

- Think of W_{cat}^TX_i, W_{dog}^TX_i, W_{human}^TX_i as scores.
 - Previously, we only wanted $w_{cat}^T x_i > 0$ (underconstrained!)
 - New constraint: "cat" example x_i should have higher $w_{cat}^T x_i$ than $w_{dog}^T x_i$, $w_{human}^T x_i$
 - Now, we want: $W_{cat}^T X_i > W_{dog}^T X_i$ and $W_{cat}^T X_i > W_{human}^T X_i$

Q: How should we design the error here?

Multi-Class Loss Function

Now, we want: $W_{cat}^T X_i > W_{dog}^T X_i$ and $W_{cat}^T X_i > W_{human}^T X_i$

Let's count # times
$$W_{cat}X_i \leq W_{dog}X_i + W_{cat}X_i \leq W_{human}X_i$$

$$\begin{bmatrix} I \end{bmatrix} = \int_{Cot} \left[(W_{cat}X_i \leq W_{dog}X_i) + I(W_{cat}X_i \leq W_{human}X_i) + I(W_{cat}X_i \leq W_{human}X_i) + I(W_{cat}X_i \leq W_{human}X_i) + I(W_{cat}X_i \leq W_{human}X_i) + I(W_{cat}X_i + W_{cat}X_i + W_{human}X_i) + I(W_{cat}X_i + W_{cat}X_i + W_{ca$$

 $[3] \approx \sum_{i \in Cat} \max\{0, -W_{Cat}X_i + W_{dag}X_i\} + \max\{0, -W_{Cat}X_i + W_{human}X_i\}$

Multi-Class Loss Function

• Let's generalize this!



$$\begin{aligned} \text{Multi-Class Hinge Loss} \\ f(W) &= \sum_{i=1}^{n} \sum_{c' \neq y_i} \max \{ o_i - W_{y_i}^T X_i + W_{c'} X_i \} \end{aligned}$$

- This function is degenerate: $f(0) = ___$.
- As with binary SVM, we introduce an offset

$$f(W) = \sum_{i=1}^{n} \sum_{c' \neq y_i} \max \{0, 1 - W_{y_i}^T X_i + W_{c'} X_i\}$$

'sum"-rule multi-class hinge loss

$$f(W) = \sum_{i=1}^{n} \max_{c' \neq y_i} \{0, 1 - W_{y_i}^T X_i + W_{c'} X_i \}$$

"max"-rule multi-class hinge loss

Multi-Class SVMs

- Idea: for a cat example, we want: $W_{cat}^{T}X_{i} > W_{dog}^{T}X_{i}$ and $W_{cat}^{T}X_{i} > W_{human}^{T}X_{i}$ $f(W) = \sum_{i=1}^{n} \sum_{c' \neq y_{i}} \max \{0, 1 - W_{y_{i}}^{T}X_{i} + W_{c'}X_{i}\}$ $f(W) = \sum_{i=1}^{n} \max \{\max \{0, 1 - W_{y_{i}}^{T}X_{i} + W_{c'}X_{i}\}\}$
- For each training example 'i':
 - "Sum" rule penalizes for each 'c' that violates the constraint.
 - "Max" rule penalizes for one 'c' that violates the constraint the most.
 - "Sum" gives a penalty of 'k-1' for W=0, "max" gives a penalty of '1'.
- If we add L2-regularization, both are called multi-class SVMs:
 - "Max" rule is more popular, "sum" rule usually works better.
 - Both are convex upper bounds on the 0-1 loss.

Coming Up Next MULTI-CLASS LOGISTIC REGRESSION

Multi-Class Logistic Regression

• Idea: for a cat example, we want: $W_{cat}^T X_i > W_{dog}^T X_i$ and $W_{cat}^T X_i > W_{human}^T X_i$ - In other words: we want $W_{cat}^T X_i$ to be max $W_c^T X_i$

$$\begin{array}{c} c > \alpha \ c > b \ c \\ w_{cat} T_{X_{i}} > W_{dog} T_{X_{i}} \\ w_{cat} T_{X_{i}} > W_{dog} T_{X_{i}} \\ w_{cat} T_{X_{i}} > W_{human} T_{X_{i}} \end{array} \right\} \Leftrightarrow \begin{array}{c} W_{cat} T_{X_{i}} = \max \left\{ \begin{array}{c} W_{at} T_{X_{i}} \\ W_{dog} T_{X_{i}} \\ W_{human} T_{X_{i}} \end{array} \right\} \\ \begin{array}{c} w_{cat} T_{X_{i}} > W_{human} T_{X_{i}} \end{array} \right\} \\ \begin{array}{c} w_{cat} T_{X_{i}} \\ w_{dog} T_{X_{i}} \\ W_{human} T_{X_{i}} \end{array} \right\} \\ \begin{array}{c} w_{cat} T_{X_{i}} \\ w_{dog} T_{X_{i}} \\ W_{human} T_{X_{i}} \end{array} \right\} \\ \begin{array}{c} w_{cat} T_{X_{i}} \\ w_{dog} T_{X_{i}} \\ W_{human} T_{X_{i}} \end{array} \right\} \\ \begin{array}{c} w_{cat} T_{X_{i}} \\ w_{dog} T_{X_{i}} \\ w_{human} T_{X_{i}} \end{array} \right\} \\ \begin{array}{c} w_{cat} T_{X_{i}} \\ w_{dog} T_{X_{i}} \\ w_{human} T_{X_{i}} \end{array} \right\} \\ \end{array}$$

Q: What happens when W=0?



- 1. use log-sum-exp to approximate max
- 2. instead of counting number of times this quantity is positive, use this quantity as objective function

Q: What happens when W=0?

Multi-Class Logistic Regression

$$f(W) = \sum_{i=1}^{n} -W_{y_i}^{T} X_i + \log \left(\sum_{c=1}^{k} e^{x_i} p(w_c^{T} x_i) \right)$$

$$(Softmax loss)'' = \sum_{i=1}^{n} -W_{y_i}^{T} X_i + \log \left(\sum_{c=1}^{k} e^{x_i} p(w_c^{T} x_i) \right) + \frac{\lambda}{2} \sum_{c=1}^{k} \sum_{j=1}^{k} w_{cj}^{T}$$

$$L2-regularized softmax loss$$

 Multi-class (multinomial) logistic regression: optimize W with L2-regularized softmax loss

Multi-Class Logistic Regression

$$f(W) = \sum_{i=1}^{k} (W_{y_i}^{T} x_i + \log(\sum_{i=1}^{k} exp(w_c^{T} x_i))) + \frac{1}{2} \sum_{i=1}^{k} \frac{d}{w_{c_j}} W_{c_j}^{2}$$

Tries to Approximates max $\frac{1}{2} w_c^{T} x_i^{2}$
Make $w_c^{T} x_i = \frac{1}{2} \log for$ so tries to make $w_c^{T} x_i^{2} \sum_{i=1}^{k} \frac{1}{2} \log \frac{1}{2} \log$

- This objective is convex (should be clear for 1st and 3rd terms).
 It's differentiable so you can use gradient descent.
- When k=2, equivalent to using binary logistic loss.
 - Not obvious at the moment.



- Evaluates "max-ness" of z compared to group
 - if z is big compared to every other z_c , softmax is close to 1

"Max-ness" to Find "Cat-ness"

$$P(y_{i} = \operatorname{``Cat"} | W, \cdot) : | R^{d} \longrightarrow (0, 1)$$

$$P(y_{i} = \operatorname{``Cat"} | W, X_{i}) = \operatorname{Softmax} \left(\bigcup_{cat}^{T} X_{i} \right) \left(\bigcup_{dag}^{T} X_{i} \right)$$

$$W_{core}^{T}X_{i} = 1.83$$

 $W_{dog}^{T}X_{i} = -1.17$
 $W_{human}^{T}X_{i} = -2.20$
 $Cot-ness = ~93.6'/.
 $dog-ness = ~0.04'/$
human-ness = ~0.02'/.$



Multi-Class Linear Prediction in Matrix Notation

• In multi-class linear classifiers our weights are:



- To predict on all training examples, we first compute all $w_c^T x_i$.
 - Or in matrix notation:



– So predictions are maximum column indices of XW^T (which is 'n' by 'k').

How Do I Regularize W?

• The Frobenius norm of a ('k' by 'd') matrix 'W' is defined by:

• We can use this to write regularizer in matrix notation:

$$\begin{aligned} \frac{1}{2} \sum_{c=1}^{k} \sum_{j=1}^{d} w_{cj}^{2} &= \frac{1}{2} \sum_{c=1}^{k} ||w_{c}||^{2} \quad ("L_{2} \operatorname{regularizer} on each vector") \\ &= \frac{1}{2} ||W||_{F}^{2} \quad ("frobenius \operatorname{regularizer} on matrix") \end{aligned}$$

Summary

- Sigmoid function: turn linear predictions into probabilities.
- One vs all: turn binary classifiers into a multi-class classifier.
- Multi-class SVM: measure violation of classification constraints.
- Multi-class logistic regression: log-sum-exp approximation of "correct=max" constraint violations
- Next time: feature engineering and how to represent text data

Review Questions

• Q1: How does the sigmoid function satisfy the definition of probability?

• Q2: What makes the one-vs-all classifier under-constrained?

• Q3: Mathematically, what leads to the "sum"-rule and "max"-rule variants of multi-class SVM?

• Q4: How do we know that the objective functions for multi-class SVM and multi-class logistic regression are convex?

"All-Pairs" and ECOC Classification

- Alternative to "one vs. all" to convert binary classifier to multi-class is "all pairs".
 - For each pair of labels 'c' and 'd', fit a classifier that predicts +1 for examples of class 'c' and -1 for examples of class 'd' (so each classifier only trains on examples from two classes).
 - To make prediction, take a vote of how many of the (k-1) classifiers for class 'c' predict +1.
 - Often works better than "one vs. all", but not so fun for large 'k'.
- A variation on this is using "error correcting output codes" from information theory (see Math 342).
 - Each classifier trains to predict +1 for some of the classes and -1 for others.
 - You setup the +1/-1 code so that it has an "error correcting" property.
 - It will make the right decision even if some of the classifiers are wrong.

Motivation: Dog Image Classification

• Suppose we're classifying images of dogs into breeds:



- What if we have images where class label isn't obvious?
 - Siberian husky vs. Inuit dog?



https://www.slideshare.net/angjoo/dog-breed-classification-using-part-localization https://ischlag.github.io/2016/04/05/important-ILSVRC-achievements

Learning with Preferences

- Do we need to throw out images where label is ambiguous?
 - We don't have the y_i.



- We want classifier to prefer Siberian husky over bulldog, Chihuahua, etc.
 - Even though we don't know if these are Siberian huskies or Inuit dogs.
- Can we design a loss that enforces preferences rather than "true" labels?

Learning with Pairwise Preferences (Ranking)

• Instead of y_i , we're given list of (c_1, c_2) preferences for each 'i':

We want
$$W_{c_1}^T x_i > W_{c_2}^T x_i$$
 for these particular (c_{1}, c_2) values

- Multi-class classification is special case of choosing (y_i,c) for all 'c'.
- By following the earlier steps, we can get objectives for this setting:

$$\sum_{i=1}^{n} \sum_{(c_{i},c_{2})} \max_{z} \{0, 1-w_{c_{i}}^{T}x_{i}+w_{c_{2}}^{T}x_{i}\} + \frac{1}{2} ||W||_{F}^{2}$$

Learning with Pairwise Preferences (Ranking)

- Pairwise preferences for computer graphics:
 - We have a smoke simulator, with several parameters:



- Don't know what the optimal parameters are, but we can ask the artist:
 - "Which one looks more like smoke"?

Learning with Pairwise Preferences (Ranking)

• Pairwise preferences for humour:

- New Yorker caption contest:



– "Which one is funnier"?

Risk Scores

• In medicine/law/finance, risk scores are sometimes used to give probabilities:

1.	Congestive Heart Failure	1 point		
2.	H ypertension	1 point	+	
3.	Age \geq 75	1 point	+	
4.	Diabetes Mellitus	1 point	+	
5.	Prior Stroke or Transient Ischemic Attack	2 points	+	
		SCORE	=	

SCORE	0	1	2	3	4	5	6
RISK	1.9%	2.8%	4.0%	5.9%	8.5%	12.5%	18.2%

Figure 1: CHADS₂ risk score of Gage et al. (2001) to assess stroke risk (see www.mdcalc.com for other medical scoring systems). The variables and points of this model were determined by a panel of experts, and the risk estimates were computed empirically from data.

- Get integer-valued "points" for each "risk factor", and probability is computed from data based on people with same number of points.
- Less accurate than fancy models, but interpretable and can be done by hand.
 - Some work on trying to "learn" the whole thing (like doing feature selection then rounding).

Support Vector Regression

• Support vector regression objective (with hyper-parameter ϵ):

$$f(w) = \sum_{i=1}^{n} \max\{0, |w'x_i - y_i| - \varepsilon\} + \frac{1}{2} ||w||^2$$

- Looks like L2-regularized robust regression with the L1-loss.
- But have loss of 0 if \hat{y}_i within ϵ of \tilde{y}_i .
 - So doesn't try to fit data exactly.
 - This can help fight overfitting.
- Support vectors are points with loss>0.
 - Points outside the "epsilon-tube".
- Example with Gaussian-RBFs as features:



1-Class SVMs

• 1-class SVMs for outlier detection.

$$f(w, w_0) = \sum_{i=1}^{N} \left[\max\{0, w_0 - w^T x_i\} - w_0 \right] + \frac{\lambda}{2} \|w\|_2^2$$

- Variables are 'w' (vector) and 'w₀' (scalar).
- Only trains on "inliers".
 - Tries to make $w^T x_i$ bigger than w_0 for inliers.
 - At test time: says "outlier" if $w^T x_i < w_0$.
 - Usually used with RBFs.

