## 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

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

Hinge loss for support vector machine

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

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)

#### **LINEAR PROBABILISTIC CLASSIFIERS** Coming Up Next

## Previously: Identifying Important E-mails

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



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

 $y_i =$  sign(w<sup>7</sup> $x_i$ )

- 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

![](_page_9_Figure_1.jpeg)

x

 $f(x) = wx$ 

 $f(x) =$  sigmoid(wx)

#### +1-ness with Sigmoid  $f(x) =$  sigmoid(wx)  $-10$  $-5$ 5  $10<sup>°</sup>$

- 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<sub>i</sub>)

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

$$
P(y_i = +1 | w, x_i) = Sigmoid(wTx_i)
$$

#### Probabilities for Linear Classifiers using Sigmoid

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

$$
\rho(y_i = +1 \mid w_j x_i) = \frac{1}{1 + exp(-w^T x_i)}
$$

![](_page_11_Figure_3.jpeg)

• Visualization for 2 features:

## What About "-1-ness"?

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

$$
\rho(y_i = ||\mid w_j x_j) = \frac{1}{|+e_{\text{p}}(-w'x_j)|}
$$

• By rules of probability:

$$
\rho(y_i = -1 | w_j x_i) = 1 - \rho(y_i = 1 | w_j x_i)
$$
  
= 
$$
\frac{1}{1 + \rho_{x}(\sqrt{x} x_i)} \quad (with some \text{erf}(\sqrt{x} t_i))
$$

- 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.

# TH <del>- MULTIN</del><br>INITR∩ **INTRO**

Coming Up Next

![](_page_13_Picture_2.jpeg)

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:

![](_page_14_Figure_2.jpeg)

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

![](_page_14_Picture_4.jpeg)

## Multi-Class Linear Classification

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

![](_page_15_Figure_2.jpeg)

- 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 .

![](_page_16_Figure_5.jpeg)

# "One vs All" Classification

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

$$
W_{cat}^T x_i = -0.1
$$
  
 
$$
W_{tan}^T x_i = -0.8
$$
  
 
$$
W_{intra}^T x_i = 0.9
$$
  
 
$$
W_{intra}^T x_i = 0.9
$$

## Multi-Class Linear Classification (MEMORIZE)

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

![](_page_18_Figure_2.jpeg)

 $-$  So if y $_{\textrm{i}}$ =2 then  $\text{ W}_{\textrm{y}_{\textrm{i}}}$  = w $_{\textrm{2}}$ .

## Shape of Decision Boundaries

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

![](_page_19_Figure_2.jpeg)

• 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):

![](_page_20_Figure_3.jpeg)

– Could be non-convex with change of basis. The could be non-convex with change of basis.

## Digression: Multi-Label Classification

• A related problem is multi-label classification:

![](_page_21_Figure_2.jpeg)

- 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  $\mathsf{sign}(\mathsf{w}_\mathsf{c}^\mathsf{T} \mathsf{x}_\mathsf{i}) {\,=\,} {\,+\,} 1$  as the labels.

![](_page_21_Picture_7.jpeg)

#### "One vs All" Multi-Class Linear Classification

- Problem: We didn't train the w $_{\rm c}$  so that the largest w $_{\rm c}$ T $_{\rm X_i}$  would be  $\rm\,W\!_{\rm yi}^{T}x_{i}$ .
	- Each classifier is just trying to get the sign right.

$$
w_{1}^{T}x_{i} = -5
$$
 ("cal" score)  
\n $w_{2}^{T}x_{i} = -0.1$  ("dog" score)  
\n $w_{3}^{T}x_{i} = -0.1$  ("dog" score)  
\n $w_{3}^{T}x_{i} = -0.2$  ("humani" score)

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

### **MULTI-CLASS SVM** Coming Up Next

## Binary Classifiers are "Under-constrained"

![](_page_24_Figure_1.jpeg)

## Binary Classifiers are "Under-constrained"

![](_page_25_Figure_1.jpeg)

#### What Do We Want for Multi-Class Classifiers?

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

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

#### 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 
$$
W_{cat}^T x_i \le W_{dog}^T x_i + W_{cat}^T x_i \le W_{ham}^T x_i
$$
  
\n
$$
F_{cat}(W) = \sum_{i \in cat \text{ examples}} I(w_{cat}^T x_i \le W_{dog}^T x_i) + I(w_{cat}^T x_i \le W_{human}^T x_i)
$$
\n
$$
F_{cat}^T x_i = \sum_{i \in cat \text{ examples}} I(\omega \le -W_{cat}^T x_i + W_{bg}^T x_i) + I(\omega \le -W_{cat}^T x_i + W_{human}^T x_i)
$$

$$
[3] \approx \sum_{i \in \text{Cat} \text{ examples}} \text{max} \Big\{ O, -W_{\text{Cat}}X_i + W_{\text{diag}}X_i \Big\} + \text{max} \Big\{ O, -W_{\text{Cat}}^{\top}X_i + W_{\text{human}}^{\top}X_i \Big\}
$$

## Multi-Class Loss Function

• Let's generalize this!

[*i*] 
$$
f_{\text{cat}}(W) = \sum_{i \in \text{cat example}} \text{max} \{ o, -W_{\text{cat}}X_i + W_{\text{diag}}X_i \} + \text{max} \{ o, -W_{\text{cat}}X_i + W_{\text{limman}}X_i \}
$$
\n[*i*] 
$$
f_{\text{cat example}}(W) = \sum_{i \in \text{``example}} \sum_{c' \neq c} \text{max} \{ o, -W_{\text{cat }X_i}^T + W_{\text{cat }X_i} \}
$$
\n[*i*] 
$$
f_{\text{cat }i} = \sum_{c=1}^K f_c(W) = \sum_{c=1}^K \sum_{i \in \text{``example of example}} \sum_{c' \neq c} \text{max} \{ o, -W_{\text{cat }X_i}^T + W_{\text{cat }X_i} \}
$$
\n[*i*] 
$$
= \sum_{i=1}^K \sum_{c' \neq y_i} \text{max} \{ o, -W_{\text{cat }X_i}^T + W_{\text{cat }X_i} \}
$$

![](_page_29_Figure_0.jpeg)

Multi-Class Hinge Loss  

$$
f(w) = \sum_{i=1}^{n} \sum_{c' \neq y_i} max\{o, -wy_i'X_i + w_c'X_i\}
$$

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

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

"sum"-rule multi-class hinge loss

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

"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  $w_{cat}^T x_i$  ,  $w_{human}^T x_i$  $f(W) = \sum_{i=1}^{n} \frac{max}{c' \neq y_i} \text{max} \{0, 1 - W_y^T X_i + W_c X_i\}$
- 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.  $32$

#### **MULTI-CLASS LOGISTIC REGRESSION** Coming Up Next

## Multi-Class Logistic Regression

• Idea: for a cat example, we want:  $w_{cat}^T x_i$  ,  $w_{dog}^T x_i$  and  $w_{cat}^T x_i$  ,  $w_{human}^T x_i$  $-$  ln other words: we want  $w_{\text{cat}}^{\top}x_i$  to be max  $w_{\text{c}}^{\top}x_i$ 

$$
W_{cat}X_i > W_{dog}^{\top}X_i
$$
\n
$$
W_{cat}X_i > W_{human}X_i
$$
\n
$$
W_{cat}X_i < max \left\{\begin{array}{c} W_{cat}X_i \\ W_{dog}^{\top}X_i \\ W_{bag}^{\top}X_i \\ \end{array}\right\}
$$
\n
$$
W_{cat}X_i > W_{human}X_i
$$
\n
$$
W_{dog}^{\top}X_i
$$
\n
$$
W_{com}X_i
$$
\n
$$
W_{com}X_i
$$
\n
$$
W_{com}X_i
$$
\n
$$
W_{homon}X_i
$$
\n
$$
W_{human}X_i
$$
\n
$$
W_{human}X_i
$$

Q: What happens when W=0?

![](_page_34_Figure_0.jpeg)

- 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  
\n
$$
f(w) = \sum_{i=1}^{n} -w_{y_i}^T x_i + \log \left( \sum_{c=1}^{k} exp(w_c^T x_i) \right)
$$
\n
$$
f(w) = \sum_{i=1}^{n} -w_{y_i}^T x_i + \log \left( \sum_{c=1}^{k} exp(w_c^T x_i) \right) + \frac{\lambda}{2} \sum_{c=1}^{k} w_{y_i}^2
$$
\n
$$
L2\text{-regularized softmax loss}
$$

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

## Multi-Class Logistic Regression

$$
f(W) = \sum_{i=1}^{n} [-w_{y_i}^T x_i + \log(\sum_{c=1}^{K} exp(w_c^T x_i))] + \frac{1}{2} \sum_{c=1}^{K} \sum_{j=1}^{d} w_c^2
$$
\n
$$
T_{rles} + 0
$$
\n
$$
W_c^T x_i
$$
\n
$$
V_s u dL_z^{\text{-regularized}}
$$

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

![](_page_37_Figure_0.jpeg)

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

\n
$$
\text{Max-ness}^{\prime\prime} \text{ to Find } \text{``Cat-ness''}
$$
\n

\n\n $P(y_i = \text{`Cat'}^{\prime} | W, \cdot) : \mathbb{R}^d \rightarrow (0, 1)$ \n

\n\n $P(y_i = \text{``cat''} | W, X_i) = \text{Softmax} \left( \mathbb{W}_{cat}^T X_i \right) \mathbb{W}_{dog}^T X_i$ \n

\n\n $\text{W}_{cat}^T X_i$ \n

\n\n $\text{W}_{cat}^T X_i$ \n

\n\n $\text{W}_{cont}^T X_i$ \n

\n\n $\text{W}_{cont}^T X_i$ \n

$$
M_{cat}X_i = 1.83
$$
  
\n $W_{dog}X_i = -1.17$   
\n $W_{bound}X_i = -2.20$   
\n $M_{human}X_i = -2.20$   
\n $M_{human}X_i = -2.20$   
\n $M_{human}X_i = -2.20$   
\n $M_{human}X_i = -2.20$   
\n $M_{normal}X_i = -2.20$ 

![](_page_38_Picture_2.jpeg)

#### Multi-Class Linear Prediction in Matrix Notation

• In multi-class linear classifiers our weights are:

![](_page_39_Figure_2.jpeg)

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

![](_page_39_Figure_5.jpeg)

– So predictions are maximum column indices of  $XW<sup>T</sup>$  (which is 'n' by 'k').

# How Do I Regularize W?

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

$$
||W||_F = \int_{c=1}^{k} \sum_{j=1}^{d} w_{jc}^2
$$
  
(L<sub>2</sub>-norm if you "stack" elements  
into one big vector)

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

$$
\frac{1}{2}\sum_{c=1}^{k}\sum_{j=1}^{d}w_{cj}^{2} = \frac{1}{2}\sum_{c=1}^{k}||w_{c}||^{2} \quad (\text{``}l_{2} \text{``regularlyarizer on each vector")}
$$
\n
$$
= \frac{1}{2}||W||_{F}^{2} \quad (\text{``frobvrius "regularlyarizer on matrix")}
$$

## 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:

![](_page_44_Picture_2.jpeg)

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

![](_page_44_Picture_5.jpeg)

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<sub>i</sub>.

![](_page_45_Picture_3.jpeg)

- 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 
$$
w_{c_i}^T x_i > w_{c_j}^T x_i
$$
 for these particular  $(c_{12}, c_{2})$  values

- Multi-class classification is special case of choosing  $({\sf y}_{\sf i},$ c) for all 'c'.
- By following the earlier steps, we can get objectives for this setting:

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

#### Learning with Pairwise Preferences (Ranking)

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

![](_page_47_Picture_3.jpeg)

- 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:

![](_page_48_Picture_3.jpeg)

#### – "Which one is funnier"?

## Risk Scores

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

![](_page_49_Picture_53.jpeg)

![](_page_49_Picture_54.jpeg)

**Figure 1:** CHADS<sub>2</sub> 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  $\epsilon$ ):

$$
f(w)=\sum_{i=1}^{n}max\{0, |w'x_i-y_i|-\epsilon\} + \frac{\sqrt{3}}{2}||w||^2
$$

- Looks like L2-regularized robust regression with the L1-loss.
- But have loss of 0 if  $\hat{y}_i$  within  $\epsilon$  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:

![](_page_50_Figure_10.jpeg)

## 1-Class SVMs

• 1-class SVMs for outlier detection.

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

- Variables are 'w' (vector) and 'w<sub>0</sub>' (scalar).
- Only trains on "inliers".
	- Tries to make  $w^Tx_i$  bigger than  $w_0$  for inliers.
	- At test time: says "outlier" if  $w^Tx_i < w_0$ .
	- Usually used with RBFs.

![](_page_51_Figure_8.jpeg)