CPSC 340: Machine Learning and Data Mining

More Linear Classifiers Fall 2020

Last Time: Classification using Regression and SVMs

• Binary classification using sign of linear models:

Fit model
$$y_i = w^T x_i$$
 and predict using sign($w^T x_i$)
+ i^{-1}

- We considered different training "error" functions:
 - Squared error: $(w^T x_i y_i)^2$.
 - If $y_i = +1$ and $w^T x_i = +100$, then squared error $(w^T x_i y_i)^2$ is huge.
 - 0-1 classification error: $(sign(w^Tx_i) = y_i)$?
 - Non-convex and hard to minimize in terms of 'w' (unless optimal error is 0).
 - Degenerate convex approximation to 0-1 error: $max\{0, -y_iw^Tx_i\}$.
 - Has a degenerate solution of 0.
 - Hinge loss: $max\{0, 1-y_iw^Tx_i\}$.
 - Convex upper bound on number of classification errors.
 - With L2-regularization, it's called a support vector machine (SVM).

'λ' vs 'C' as SVM Hyper-Parameter

• We've written SVM in terms of regularization parameter ' λ ':

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

• Some software packages instead have regularization parameter 'C':

$$f(w) = C \sum_{j=1}^{n} \max \{0, 1 - y_i \ w^7 x_i \} + \frac{1}{2} ||w||^2$$

- In our notation, this corresponds to using $\lambda = 1/C$.
 - Equivalent to just multiplying f(w) by constant.
 - Note interpretation of 'C' is different: high regularization for small 'C'.
 - You can think of 'C' as "how much to focus on the classification error".

Logistic Loss

• We can smooth max in degenerate loss with log-sum-exp:

$$\max\{0, -\gamma_i, w^T x_i\} \approx \log(\exp(0) + \exp(-\gamma_i, w^T x_i))$$

• Summing over all examples gives:

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

- This is the "logistic loss" and model is called "logistic regression".
 - It's not degenerate: w=0 now gives an error of log(2) instead of 0.
 - Convex and differentiable: minimize this with gradient descent.
 - You should also add regularization.
 - We'll see later that it has a probabilistic interpretation.



Logistic Regression and SVMs

- Logistic regression and SVMs are used EVERYWHERE!
 - Fast training and testing.
 - Training on huge datasets using "stochastic" gradient descent (next week).
 - Prediction is just computing w^Tx_i.
 - Weights w_i are easy to understand.
 - It's how much w_i changes the prediction and in what direction.
 - We can often get a good test error.
 - With low-dimensional features using RBFs and regularization.
 - With high-dimensional features and regularization.
 - Smoother predictions than random forests.

Comparison of "Black Box" Classifiers

- Fernandez-Delgado et al. [2014]:
 - "Do we Need Hundreds of Classifiers to Solve Real World Classification Problems?"
- Compared 179 classifiers on 121 datasets.
- Random forests are most likely to be the best classifier.
- Next best class of methods was SVMs (L2-regularization, RBFs).
- "Why should I care about logistic regression if I know about deep learning?"

(pause)



- Consider a linearly-separable dataset.
 - Perceptron algorithm finds *some* classifier with zero error.
 - But are all zero-error classifiers equally good?



- Consider a linearly-separable dataset.
 - Maximum-margin classifier: choose the farthest from both classes.



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• Consider a linearly-separable dataset.

- Maximum-margin classifier: choose the farthest from both classes.

Perfect classifier with maximum "margin" Why maximize margin! (largest distance to closest examples) "Imarg" X_{12} If test data is close 000 to training datas 00 6 then max margin 0 000 leques more "room" 00,00 before we make an Perfect classifier with small "margin" × × × × × error. Xil

• For linearly-separable data:



- With small-enough $\lambda > 0$, SVMs find the maximum-margin classifier.
 - Need λ small enough that hinge loss is 0 in solution.
 - Origin of the name: the "support vectors" are the points closest to the line (see bonus).
- Recent result: logistic regression also finds maximum-margin classifier.
 - With λ =0 and if you fit it with gradient descent (not true for many other optimizers).

(pause)

Previously: Identifying Important E-mails

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

COMPOSE Inbox (3) Starred. Important Sent Mail Draffs (1)	🗆 🕁 🕨	Mark Issam, Ricky (10)	Inbox A2, tutorials, marking	O	10:41 am
		Holger, Jim (2)	lists Intro to Computer Science		10:20 am
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	🗆 🏠 💌	sameh, Mark, sameh (3)	Inbox Graduation Project Dema	C	8:01 am
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• We can do binary classification by taking sign of linear model: $\hat{\gamma}_i = sign(w^T x_i)$

- 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.

Predictions vs. Probabilities

• With $z_i = w^T x_i$, linear classifiers make prediction using sign(z_i):



- For predictions, "sign" maps from w^Tx_i to the elements {-1,+1}.
 If w^Tx_i is positive we predict +1, if it's negative we predict -1.
- For probabilities, we want to map from $w^T x_i$ to the range [0,1].
 - If $w^T x_i$ is very positive, we output a value close to +1.
 - If $w^T x_i$ is very negative, we output a value close to 0.
 - If $w^T x_i$ is close to 0, we output a value close to 0.5.

Sigmoid Function

• So we want a transformation of $z_i = w^T x_i$ that looks like this:

The most common choice is the sigmoid function:

$$h(z_i) = \frac{1}{1 + exp(-z_i)}$$

• Values of h(z_i) match what we want:

h(-a) = 0 $h(-1) \simeq 0.27$ h(0) = 0.5 $h(0.5) \simeq 0.62$ $h(+1) \simeq 0.73$ $h(+\infty) = 1$

Probabilities for Linear Classifiers using Sigmoid

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

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

- By rules of probability: $\rho(y_i = -1 \mid w_i, x_i) = 1 \rho(y_i = 1 \mid w_j, x_i)$ $= \frac{1}{1 + e_x p(w^T x_i)} \quad (with some effor 1)$
- We then use these for "probability that e-mail is important".
- This may seem heuristic, but later we'll see that:
 - minimizing logistic loss does "maximum likelihood estimation" in this model.

(pause)

Multi-Class Linear Classification

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



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



https://www.youtube.com/watch?v=tntOCGkgt98

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.

"One vs All" Classification

- Suppose you only know how to do binary classification: ٠
 - "One vs all" is a way to turn a binary classifier into a multi-class method.

Training phase: •

- For each class 'c', train binary classifier to predict whether example is a 'c'.
- For example, train a "cat detector, a use accession.
 If we have 'k' classes, this gives 'k' binary classifiers.
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 - Predict the 'c' with the highest score.

"One vs All" Linear Classification

- "One vs all" logistic regression for classifying as cat/dog/person.
 - Train a separate classifier for each class.
 - Classifier 1 tries to predict +1 for "cat" images and -1 for "dog" and "person" images.
 - Classifier 2 tries to predict +1 for "dog" images and -1 for "cat" and "person" images.
 - Classifier 3 tries to predict +1 for "person" images and -1 for "cat" and "dog" images.
 - This gives us a weight vector w_c for each class 'c':
 - Weights w_c try to predict +1 for class 'c' and -1 for all others.
 - We'll use 'W' as a matrix with the w_c as rows:

"One vs All" Linear Classification

- "One vs all" logistic regression for classifying as cat/dog/person.
 - Prediction on example x_i given parameters 'W' :



- For each class 'c', compute $w_c^T x_i$. $w_1^T x_i = -0.1 \quad ("cat" score)$ $w_2^T x_i = -0.8 \quad ("doy" score)$ $w_3^T x_i = 0.9 \quad ("human" score)$

- Ideally, we'll get sign $(w_c^T x_i) = +1$ for one class and sign $(w_c^T x_i) = -1$ for all others.
- In practice, it might be +1 for multiple classes or no class.
- To predict class, we take maximum value of $w_c^T x_i$ ("highest score").
 - In the example above, predict "human" (0.9 is higher than -0.8 and -0.1).

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.

person dog chair

• But we would take all the sign(w_c^Tx_i)=+1 as the labels. http://image-net.org/challenges/LSVRC/2013/

Multi-Class Linear Classification (MEMORIZE)

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

$$\chi = \begin{bmatrix} 2^{7} \\ 1_{k} \\ \frac{9}{7} \\ 2_{l} \\ 5 \end{bmatrix} \begin{cases} 1_{roin} k^{1} \\ 1_{roin} k^{1} \\ 1_{ssi} \\ 1_{s$$

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

"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.



- 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.

Multi-Class SVMs

- Can we define a loss that encourages largest w_c^Tx_i to be w_{y_i}^Tx_i?
 So when we maximizing over w_c^Tx_i, we choose correct label y_i.
- Recall our derivation of the hinge loss (SVMs):
 - We wanted $y_i w^T x_i > 0$ for all 'i' to classify correctly.
 - We avoided non-degeneracy by aiming for $y_i w^T x_i \ge 1$.
 - We used the constraint violation as our loss: max{0,1- $y_iw^Tx_i$ }.
- We can derive multi-class SVMs using the same steps...

Multi-Class SVMs

- Can we define a loss that encourages largest $w_c^T x_i$ to be $w_{y_i}^T x_i$? We want $w_{y_i}^T x_i \ge w_c^T x_i$ for all 'c' that are not correct label y_i = Tf we penalize violation of this constraint it's degenerate. We use $w_{y_i}^T x_i \ge w_c^T x_i + 1$ for all $c \ne y_i$ to avoid strict in equality Equivalently: $O \ge 1 - w_{y_i}^T x_i + w_c^T x_i$
- For here, there are two ways to measure constraint violation:

$$\sum_{\substack{x \in y_i \\ c \neq y_i}} \sum_{\substack{y_i \in y_i}} \sum_{\substack{y_i \in y_i \\ c \neq y_i}} \sum_{\substack{y_i \in y_i \\ c \neq y_i}} \sum_{\substack{y_i \in y_i}} \sum_{\substack{y_i \in y_i \\ c \neq y_i}} \sum_{\substack{y_i \in y_i \\ c \neq y_i}} \sum_{\substack{y_i \in y_i \\ c \neq y_i}} \sum_{\substack{y_i \in y_i}} \sum_{\substack{y_i \in y_i \\ c \neq y_i}} \sum_{\substack{y_i \in y_i \\ c \neq y_i}} \sum_{\substack{y_i \in y_i}} \sum_{\substack{y_i \in y_i \\ c \neq y_i}} \sum_{\substack{y_i \in y_i \\ c \neq y_i}} \sum_{\substack{y_i \in y_$$

Multi-Class SVMs

- 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.

Summary

- Logistic loss uses a smooth convex approximation to the 0-1 loss.
- SVMs and logistic regression are very widely-used.
 - A lot of ML consulting: "find good features, use L2-regularized logistic/SVM".
 - Under certain conditions, can be viewed as "maximizing the margin".
 - Both are just linear classifiers (a hyperplane dividing into two halfspaces).
- Sigmoid function is a way to turn linear predictions into probabilities.
- One vs all turns a binary classifier into a multi-class classifier.
- Multi-class SVMs measure violation of classification constraints.
- Next time: what makes good features?

Maximum-Margin Classifier

- Consider a linearly-separable dataset.
 - Maximum-margin classifier: choose the farthest from both classes.



Maximum-Margin Classifier

• Consider a linearly-separable dataset.

- Maximum-margin classifier: choose the farthest from both classes.

Perfect classifier with maximum "margin" (largest distance to closest examples) Final classifier only depends on support Xiz Also known as a "Support vector machine" 000 6 Vectors 000 0 0 The examples that are a closest are called 0000 XX "support vectors" χ_{i1}

Maximum-Margin Classifier

• Consider a linearly-separable dataset.

- Maximum-margin classifier: choose the farthest from both classes.

Perfect classifier with maximum "margin" (largest distance to closest examples) Final classifier only X_{i2} Also known as a "Support vector machine" depends on support Vectors You could throw away The examples that are g closest are called the other examples and get the same "support vectors" Classifier. χ_{i1}

Support Vector Machines

For linearly-separable data, SVM minimizes:

$$f(w) = \frac{1}{2} ||w||^2 \quad (equivalent to maximizing margin \frac{1}{1/w})^2$$

$$- \text{Subject to the constraints that:} \quad w^7 x_i \geqslant 1 \quad \text{for } y_i = 1 \quad (c \text{ lassify all } y_i = 1)$$

But most data is not linearly separable.

(see V

• For non-separable data, try to minimize violation of constraints: If $w'x_i \leq -1$ and $y_i = -1$ then "violation" should be zero. If $w'x_i \gg -1$ and $y_i = -1$ then we "violate constraint" by $1 + w'x_i$ -> Constraint violation is the hinge loss.

Support Vector Machines

• Try to maximizing margin and also minimizing constraint violation:

Hinge loss
for example 'i':
if's the amount we violate
$$y_i w^7 x_i \ge 1$$

• We typically control margin/violation trade-off with parameter " λ ":
 $\int (-) = \int \int (-) x_i v^7 x_i \ge 1$

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

- This is the standard SVM formulation (L2-regularized hinge).
 - Some formulations use λ = 1 and multiply hinge by 'C' (equivalent).

• Non-separable case:



• Non-separable case:







Robustness and Convex Approximations

• Because the hinge/logistic grow like absolute value for mistakes, they tend not to be affected by a small number of outliers.



Robustness and Convex Approximations

• Because the hinge/logistic grow like absolute value for mistakes, they tend not to be affected by a small number of outliers.



• But performance degrades if we have many outliers.

Non-Convex 0-1 Approximations

• There exists some smooth non-convex 0-1 approximations.



"Robust" Logistic Regression

• A recent idea: add a "fudge factor" v_i for each example.

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

- If w^Tx_i gets the sign wrong, we can "correct" the mis-classification by modifying v_i.
 - This makes the training error lower but doesn't directly help with test data, because we won't have the v_i for test data.
 - But having the v_i means the 'w' parameters don't need to focus as much on outliers (they can make $|v_i|$ big if sign($w^T x_i$) is very wrong).

"Robust" Logistic Regression

- A recent idea: add a "fudge factor" v_i for each example.
- $f(w_{j}v) = \sum_{i=1}^{n} \log (1 + e_{x_{p}}(-y_{i}v_{j}^{T}x_{i} + v_{i}))$ If w^Tx_i gets the sign wrong, we can "correct" the mis-classification by modifying v_i.
- A problem is that we can ignore the 'w' and get a tiny training error by just updating the v_i variables.
- But we want most v_i to be zero, so "robust logistic regression" puts an L1-regularizer on the v_i values:

$$\hat{f}(w,v) = \sum_{i=1}^{n} \log (1 + exp(-y_i w^T x_i + v_i)) + \lambda \|v\|_1$$

• You would probably also want to regularize the 'w' with different λ .

"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?

– Syberian 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 Syberian husky over bulldog, Chihuahua, etc.
 - Even though we don't know if these are Syberian 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 (c₁,c₂) preferences for each 'i':

- 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:

$$\sum_{i=1}^{n} \sum_{(c_1, c_2)} \max_{i=1}^{n} \sum_{(c_1, c_2)} \sum_{i=1}^{n} \sum_{(c_1, c_2)} \sum_{(c_1, c$$

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"?

https://circle.ubc.ca/bitstream/handle/2429/30519/ubc_2011_spring_brochu_eric.pdf?sequence=3

Learning with Pairwise Preferences (Ranking)

- Pairwise preferences for humour:
 - New Yorker caption contest:



– "Which one is funnier"?

https://homes.cs.washington.edu/~jamieson/resources/next.pdf