CSDS 440: Machine Learning

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Office hours T, Th 11:15-11:45 or by appointment

Zoom Link

Announcements

- Quiz 4 Thursday
  - Up to and including probabilistic machine learning

Recap

- The m____ of the classifier is the distance it can ______. It is important because maximizing this improves the _______ of the classifier.
- The SVM is the l____ d____ with the m____ m____.
- The margin can be computed to be the i____ of the n____ of the w_____. This is another rationale for overfitting control methods such as w___ d____.
- In an SVM, each example in the training set becomes a c____.
- In order to accommodate l_____ i_____ data, we add s______ variables to the SVM program.
- We must also add a term to minimize the s___ o__ s___ to the objective function.
- A tradeoff hyperparameter balances l_______ and g______.
- The entire program is c____.
- The g_____ L_____ lifts the constraints in an optimization program into the objective function. It is equal to the p_____ if the constraints are met.
- To get the dual, we s____ the min and max in the primal formulation.
- At the optimal solution, for each example, either the L______ m______ is zero or the term y(wx+b)-1 is zero. This is called d_____ c_____. If the L____ m____ is NOT zero, the point is a s_____ v_____.

Today

- Support Vector Machines
- Part 2: Ensemble Methods

Linearly-separable SVM, Dual Form

$$\max_{\alpha} D(\boldsymbol{\alpha}) = \sum_{i} \alpha_i - \frac{1}{2}\sum_{i,j} y_i y_j \alpha_i \alpha_j \mathbf{x}_i \bullet \mathbf{x}_j$$

$$\text{so that } \boldsymbol{\alpha} \geq 0, \sum_{i} \alpha_i y_i = 0$$

From derivative w.r.t b

Karush-Kuhn-Tucker conditions

- At the optimal primal/dual solution, the following conditions will hold:

$$\nabla_{\mathbf{w},b}\ell(\mathbf{w}^*, b^*, \boldsymbol{\alpha}^*) = 0$$

Gradient at solution is zero

$$-\left[y_i(\mathbf{w}^* \bullet \mathbf{x}_i + b^*) - 1 \right] \leq 0$$

All constraints satisfied

$$\alpha_i^* \geq 0$$

$$\alpha_i^* \left[y_i(\mathbf{w}^* \bullet \mathbf{x}_i + b^*) - 1 \right] = 0$$

KKT dual complementarity
If i^{th} LM is positive, the i^{th} constraint is "active", i.e. zero
These are the **support vectors**

These conditions are **necessary and sufficient!**

Kernels

- Notice that by using the dual formulation, we could write the formulation and the solution in terms of $\mathbf{x}_i \cdot \mathbf{x}_j$
  - In general, $\boldsymbol{\varphi}(\mathbf{x}_i) \cdot \boldsymbol{\varphi}(\mathbf{x}_j)$
- Define the kernel to be $K(\mathbf{x}_i, \mathbf{x}_j) = \boldsymbol{\varphi}(\mathbf{x}_i) \cdot \boldsymbol{\varphi}(\mathbf{x}_j)$
- For m examples, get an m x m matrix --- the kernel matrix

Nonlinear SVM, kernelized dual form

$$\max_{\alpha} D(\alpha) = \sum_i \alpha_i - \frac{1}{2} \sum_{i,j} y_i y_j \alpha_i \alpha_j K(\mathbf{x}_i, \mathbf{x}_j)$$

$$\text{so that } \alpha \geq 0, \sum_i \alpha_i y_i = 0$$

Why is this useful?

- Given φ, easy to find K
- More interestingly, for certain functions K, can show *there must exist* a φ for which K is a kernel
- This φ could be very high dimensional, but the kernel computation is much more efficient
- This allows us to do classification in very high dimensional spaces, without ever "mapping" the data into those spaces

"Kernel trick"

Example

$$K(\mathbf{a},\mathbf{b}) = (\mathbf{a}\bullet\mathbf{b})^2$$ ← $O(n)$ computation

$$= \left(\sum_i a_i b_i\right)\left(\sum_j a_j b_j\right)$$

$$= \sum_{i,j} (a_i a_j)(b_i b_j)$$

$$= \varphi(\mathbf{a})\bullet\varphi(\mathbf{b}), \text{ where}$$ ← $O(n^2)$ computation!

$$\varphi(\mathbf{x}) = [x_1^2, \sqrt{2}x_1x_2, \ldots, \sqrt{2}x_ix_j, \ldots, x_n^2]$$

Example

$$\mathbf{a} = (1,2), \mathbf{b} = (3,4)$$

$$K(\mathbf{a},\mathbf{b}) = (\mathbf{a} \bullet \mathbf{b})^2 = (1 \times 3 + 2 \times 4)^2 = 121$$

$$\text{If } K(\mathbf{a},\mathbf{b}) = \varphi(\mathbf{a})\varphi(\mathbf{b}) = (\mathbf{a} \bullet \mathbf{b})^2 \text{ then}$$

$$\varphi(\mathbf{a}) = [a_1^2, \sqrt{2}a_1a_2, a_2^2] = [1, 2\sqrt{2}, 4]$$

$$\varphi(\mathbf{b}) = [b_1^2, \sqrt{2}b_1b_2, b_2^2] = [9, 12\sqrt{2}, 16]$$

$$\varphi(\mathbf{a})\varphi(\mathbf{b}) = 9 + 48 + 64 = 121$$

What is a valid kernel?

- Intuitively, the dot product measures the (unnormalized) cosine of the angle between two vectors
  - A measure of similarity
  - “large” $K(\mathbf{x},\mathbf{y}) \rightarrow \mathbf{x}$ and $\mathbf{y}$ are “similar”

- Suppose we choose some other function that measures similarity
  - E.g., $K(\mathbf{x},\mathbf{y}) = \exp\left(\frac{-\|\mathbf{x}-\mathbf{y}\|^2}{2\sigma^2}\right)$
  - Is this a valid kernel?

Yes! Called a Gaussian or RBF Kernel. Corresponds to infinite-dimensional φ!!

Mercer's Conditions

Let $K : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ be a function. K is a valid kernel iff for all finite $\{\mathbf{x}_1, \ldots, \mathbf{x}_m\}$, the kernel matrix is symmetric positive semidefinite.

Symmetry: $K(\mathbf{x}, \mathbf{y}) = K(\mathbf{y}, \mathbf{x})$

PSD ($K \geq 0$): $\forall \mathbf{v} \neq 0, \mathbf{v}^T K \mathbf{v} \geq 0$

Necessary *and* sufficient!

- Given any kernel(s), can compose them in various ways to get other kernels

Classification

$$\max_{\alpha} D(\alpha) = \sum_i \alpha_i - \frac{1}{2}\sum_{i,j} y_i y_j \alpha_i \alpha_j K(\mathbf{x}_i, \mathbf{x}_j)$$

$$\text{so that } \alpha \geq 0, \sum_i \alpha_i y_i = 0$$

- Note that classification also does not require φ:

$$\mathbf{w} \bullet \varphi(\mathbf{x}_{new}) = \sum_{i \in \text{Support Vectors}} \alpha_i y_i \varphi(\mathbf{x}_i) \bullet \varphi(\mathbf{x}_{new})$$

$$= \sum_{i \in \text{Support Vectors}} \alpha_i y_i K(\mathbf{x}_i, \mathbf{x}_{new})$$

Generalizing kernels

- Kernel functions can be used in many other contexts, thanks to the Representer Theorem

Representer Theorem

- *Any* optimization program of the form

$$\min_f \frac{1}{2} g\left(\|f\|\right) + C\sum_i L(y_i, f(\varphi(\mathbf{x}_i)))$$

- With g monotonic has a solution that looks like: $$f(\mathbf{x}) = \sum_i \alpha_i y_i K(\mathbf{x}, \mathbf{x}_i)$$
- (Kimeldorf and Wahba, Scholkopf et al)

SVM

- Standard SVM:

$$\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_i \xi_i$$

$$\text{so that } \forall i, \left[y_i(\mathbf{w}\bullet\mathbf{x}_i + b) + \xi_i \right] \geq 1, \xi_i \geq 0$$

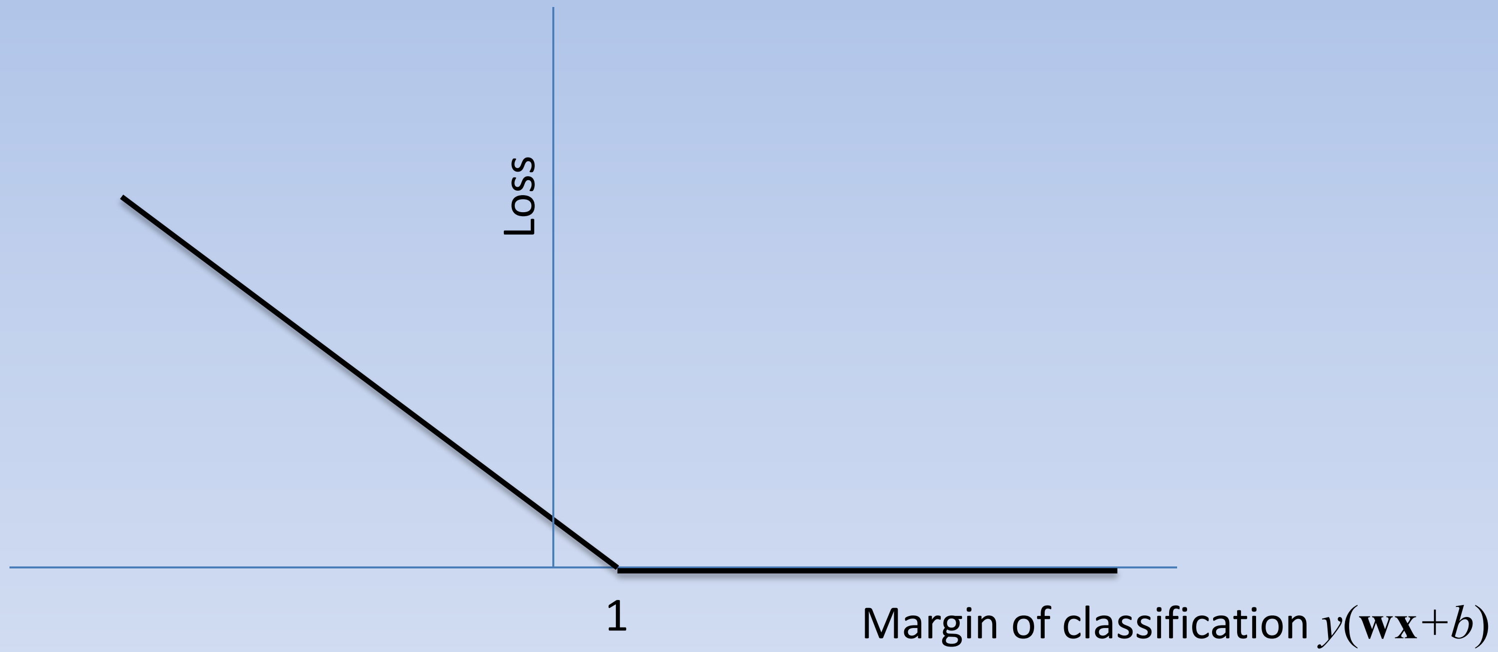
$$\text{So } \xi_i = \left(1 - y_i(\mathbf{w}\bullet\mathbf{x}_i + b)\right)_+$$

Plus function (Also RELU)

$$\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_i \left[\left(1 - y_i(\mathbf{w}\bullet\mathbf{x}_i + b)\right)_+ \right]$$

(Hinge Loss)

"Hinge" Loss



Logistic Regression

- Let us look again at the objective function we optimize to get LR (with overfitting control):

$$\mathbf{w}, b = \arg\min \frac{1}{2}\|\mathbf{w}\|^2 + C\left[\begin{array}{l} \sum_{i \in pos} -\log\left(P(y=1|\mathbf{x}_i)\right) \\ + \sum_{i \in neg} -\log\left(1 - P(y=1|\mathbf{x}_i)\right) \end{array}\right]$$

Rewriting the LR objective

- Note that, if we make the class labels 1 and -1:

$$p(Y=1\,|\,\mathbf{x})=\frac{1}{1+e^{-(\mathbf{w}\bullet\mathbf{x}+b)}}$$

$$p(Y=-1\,|\,\mathbf{x})=1-\frac{1}{1+e^{-(\mathbf{w}\bullet\mathbf{x}+b)}}=\frac{e^{-(\mathbf{w}\bullet\mathbf{x}+b)}}{1+e^{-(\mathbf{w}\bullet\mathbf{x}+b)}}=\frac{1}{1+e^{(\mathbf{w}\bullet\mathbf{x}+b)}}$$

So $p(Y=y\,|\,\mathbf{x})=\dfrac{1}{1+e^{-y(\mathbf{w}\bullet\mathbf{x}+b)}}$, and

$$-\log p(Y=y\,|\,\mathbf{x})=\log\left(1+e^{-y(\mathbf{w}\bullet\mathbf{x}+b)}\right)$$

Rewriting the LR objective

- So we can rewrite the objective:

$$\mathbf{w}, b = \arg\min \frac{1}{2}\|\mathbf{w}\|^2 + C\left[\begin{array}{l} \sum_{i \in pos} -\log\left(P(y=1 \mid \mathbf{x}_i)\right) \\ + \sum_{i \in neg} -\log\left(1 - P(y=1 \mid \mathbf{x}_i)\right) \end{array}\right]$$

$$= \arg\min \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_i \log\left(1 + e^{-y_i(\mathbf{w} \bullet \mathbf{x}_i + b)}\right)$$

SVM and Logistic Regression

- Standard SVM:

Hinge Loss

$$\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_i \left[\left(1 - y_i(\mathbf{w}\bullet\mathbf{x}_i + b)\right)_+\right]$$

Margin

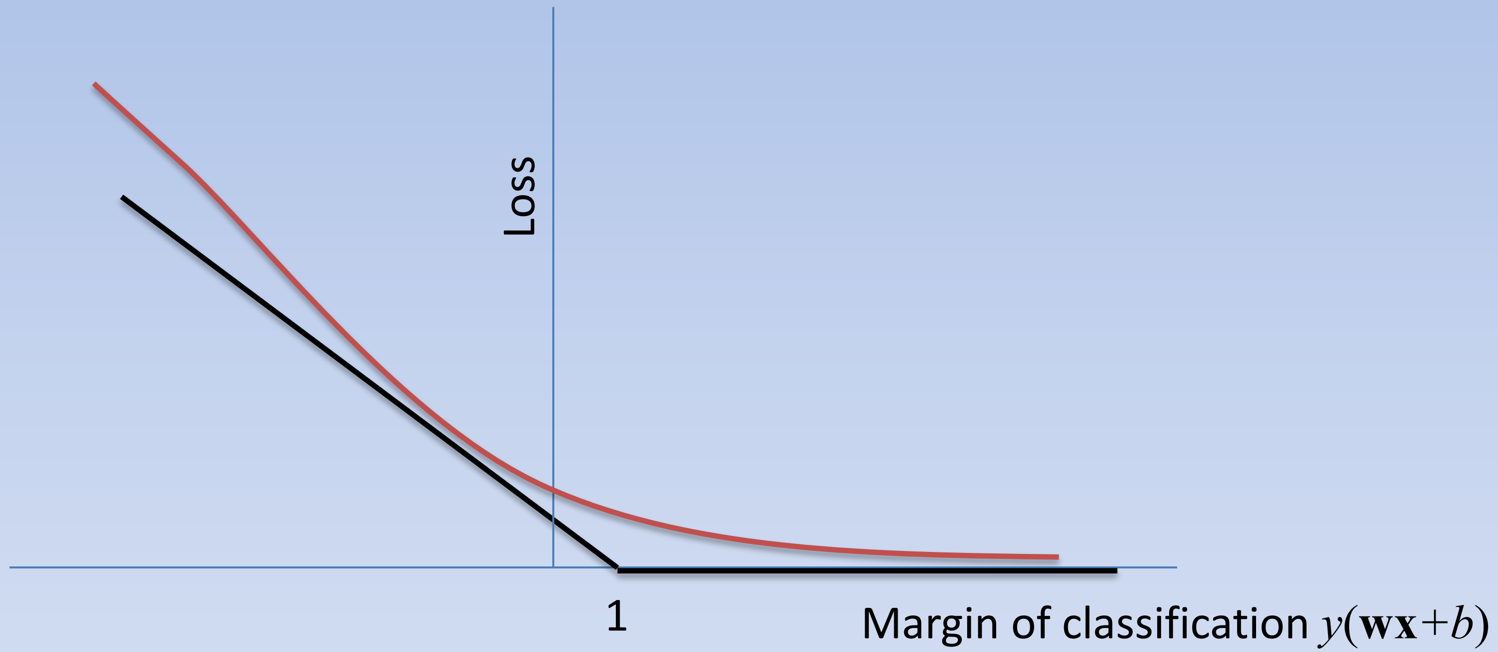
Error on training data

- (Regularized) Logistic Regression:

$$\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_i \log\left(1 + e^{-y_i(\mathbf{w}\bullet\mathbf{x}_i + b)}\right)$$

Logistic Loss

“Hinge” Loss vs Logistic Loss



Kernel Logistic Regression

- The LR objective "looks like" an SVM with an alternative loss function
- By the Representer theorem, the solution to this also must be $\mathbf{w} = \sum_i \alpha_i y_i \mathbf{x}_i$
- And so if we introduce kernels:

$$f(\mathbf{x}) = \sum_i \alpha_i y_i K(\mathbf{x}, \mathbf{x}_i)$$

Zhu and Hastie, "KLR and the Import Vector Machine" (ask for paper)

Pros and Cons of SVMs

+ Well-justified, rigorous theory combines fundamental ideas
+ Can learn very complex hypotheses, but has “built-in” overfitting control
+ Numerous practical applications; often very good performance
+ Kernelizing is a very powerful idea thanks to the representer theorem

− Can be sensitive to noise and outliers with nonlinear kernels
− Requires input scaling
− Not so easy to implement
− Very memory intensive due to large kernel matrices and constraints
− Not easy to parallelize/GPUize

End of Part 1

Part 2: Ensemble Methods

Ensemble Methods: Key Idea

- So far, for each task, we construct a single classifier
- Suppose we had a way of constructing *multiple* classifiers and *combining their output*
  - Would this generalize any better than constructing a single classifier?
  - Why or why not?
  - And how do we construct multiple classifiers in the first place?

Single vs. multiple classifiers

- Suppose for some problem we have k classifiers $h_1, \ldots, h_k$ that:
  - Each has error less than chance: $\varepsilon_i < ½$
  - Make *uncorrelated* errors on new examples
- Suppose we combine their predictions on a new example via majority vote
- What is the error rate of the combined system?