Slides adapted from Prof Carpuat and Duraiswami

CMSC 422 Introduction to Machine Learning

Lecture 24 Support Vector Machines II

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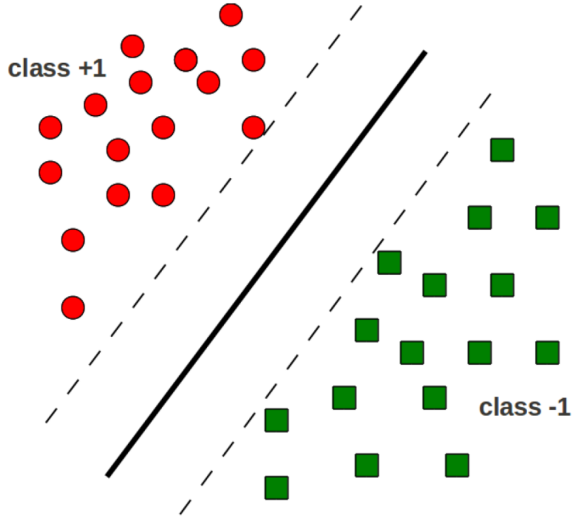
What we know about SVM so far

REVIEW

The Maximum Margin Principle

Find the hyperplane with maximum separation margin on the training data



Support Vector Machine (SVM)

A hyperplane based linear classifier defined by $\mathbf{w}$ and b

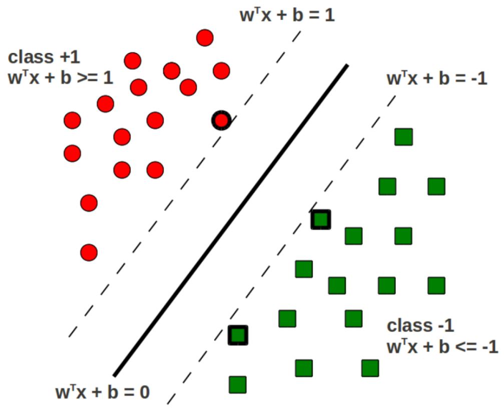
Prediction rule: $y = sign(\mathbf{w}^T\mathbf{x} + b)$

Given: Training data $\{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\}$

Goal: Learn $\mathbf{w}$ and b that achieve the maximum margin

Characterizing the margin

Let's assume the entire training data is correctly classified by ($\mathbf{w}$,b) that achieve the maximum margin



- Assume the hyperplane is such that
  - $\mathbf{w}^T\mathbf{x}_n + b \geq 1$ for $y_n = +1$
  - $\mathbf{w}^T\mathbf{x}_n + b \leq -1$ for $y_n = -1$
  - Equivalently, $y_n(\mathbf{w}^T\mathbf{x}_n + b) \geq 1$
    $\Rightarrow \min_{1\leq n\leq N} |\mathbf{w}^T\mathbf{x}_n + b| = 1$
  - The hyperplane's margin:

$$\gamma = \min_{1\leq n\leq N} \frac{|\mathbf{w}^T\mathbf{x}_n + b|}{||\mathbf{w}||} = \frac{1}{||\mathbf{w}||}$$

Solving the SVM Optimization Problem (assuming linearly separable data)

Our optimization problem is:

$$\boxed{\begin{array}{l} \text{Minimize} \quad f(\mathbf{w}, b) = \dfrac{||\mathbf{w}||^2}{2} \\ \text{subject to} \quad 1 \leq y_n(\mathbf{w}^T \mathbf{x}_n + b), \qquad n = 1, \ldots, N \end{array}}$$

Introducing Lagrange Multipliers α_n $(n = \{1, \ldots, N\})$, one for each constraint, leads to the **Lagrangian**:

$$\boxed{\begin{array}{l} \text{Minimize} \quad L(\mathbf{w}, b, \alpha) = \dfrac{||\mathbf{w}||^2}{2} + \displaystyle\sum_{n=1}^{N} \alpha_n \{1 - y_n(\mathbf{w}^T \mathbf{x}_n + b)\} \\ \text{subject to} \quad \alpha_n \geq 0; \quad n = 1, \ldots, N \end{array}}$$

Solving the SVM Optimization Problem (assuming linearly separable data)

Take (partial) derivatives of L_P w.r.t. $\mathbf{w}$, b and set them to zero

$$\frac{\partial L_P}{\partial \mathbf{w}} = 0 \Rightarrow \mathbf{w} = \sum_{n=1}^{N} \alpha_n y_n \mathbf{x}_n, \qquad \frac{\partial L_P}{\partial b} = 0 \Rightarrow \sum_{n=1}^{N} \alpha_n y_n = 0$$

Substituting these in the Primal Lagrangian L_P gives the Dual Lagrangian

$$\boxed{\begin{aligned} &\text{Maximize} \quad L_D(\mathbf{w}, b, \alpha) = \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{m,n=1}^{N} \alpha_m \alpha_n y_m y_n (\mathbf{x}_m^T \mathbf{x}_n) \\ &\text{subject to} \quad \sum_{n=1}^{N} \alpha_n y_n = 0, \quad \alpha_n \geq 0; \quad n = 1, \ldots, N \end{aligned}}$$

Solving the SVM Optimization Problem (assuming linearly separable data)

Take (partial) derivatives of L_P w.r.t. $\mathbf{w}$, b and set them to zero

A Quadratic Program for which many off-the-shelf solvers exist

$$= \sum_{n=1}^{N} \alpha_n y_n \mathbf{x}_n, \qquad \frac{\partial L_P}{\partial b} = 0 \Rightarrow \sum_{n=1}^{N} \alpha_n y_n = 0$$

Substituting thes the Primal Lagrangian L_P gives the Dual Lagrangian

$$\text{Maximize} \quad L_D(\mathbf{w}, b, \alpha) = \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{m,n=1}^{N} \alpha_m \alpha_n y_m y_n (\mathbf{x}_m^T \mathbf{x}_n)$$

$$\text{subject to} \quad \sum_{n=1}^{N} \alpha_n y_n = 0, \quad \alpha_n \geq 0; \quad n = 1, \ldots, N$$

SVM: the solution!
(assuming linearly separable data)

Once we have the α_n's, $\mathbf{w}$ and b can be computed as:

$$\mathbf{w} = \sum_{n=1}^{N} \alpha_n y_n \mathbf{x}_n$$

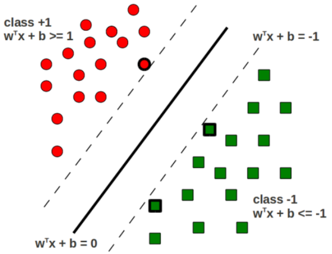
$$b = -\frac{1}{2}\left(\min_{n:y_n=+1} \mathbf{w}^T\mathbf{x}_n + \max_{n:y_n=-1} \mathbf{w}^T\mathbf{x}_n\right)$$

Note: Most α_n's in the solution are zero (sparse solution)

- Reason: Karush-Kuhn-Tucker (KKT) conditions
- For the optimal α_n's

$$\alpha_n\{1 - y_n(\mathbf{w}^T\mathbf{x}_n + b)\} = 0$$

- α_n is non-zero only if $\mathbf{x}_n$ lies on one of the two margin boundaries, i.e., for which $y_n(\mathbf{w}^T\mathbf{x}_n + b) = 1$
- These examples are called support vectors
- Support vectors "support" the margin boundaries



What if the data is not separable?

GENERAL CASE SVM SOLUTION

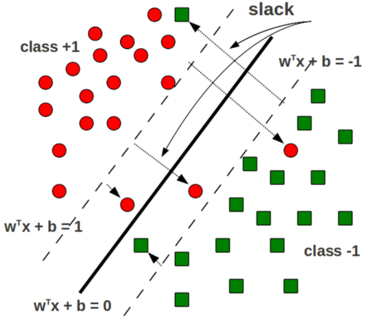
SVM in the non-separable case

no hyperplane can separate the classes perfectly

We still want to find the max margin hyperplane, but

- We will allow some training examples to be **misclassified**
- We will allow some training examples to fall **within** the margin region

SVM in the non-separable case



Recall: For the separable case (training loss $= 0$), the constraints were:

$$y_n(\mathbf{w}^T\mathbf{x}_n + b) \geq 1 \quad \forall n$$

For the non-separable case, we relax the above constraints as:

$$\boxed{y_n(\mathbf{w}^T\mathbf{x}_n + b) \geq 1 - \xi_n \quad \forall n}$$

ξ_n is called slack variable (distance $\mathbf{x}_n$ goes past the margin boundary)

$\xi_n \geq 0, \forall n$, misclassification when $\xi_n > 1$

SVM Optimization Problem

Non-separable case: We will allow misclassified training examples

- .. but we want their number to be minimized

  $\Rightarrow$ by *minimizing* the sum of slack variables $(\sum_{n=1}^{N} \xi_n)$

The optimization problem for the non-separable case

$$\text{Minimize} \quad f(\mathbf{w}, b) = \frac{||\mathbf{w}||^2}{2} + C \sum_{n=1}^{N} \xi_n$$

$$\text{subject to} \quad y_n(\mathbf{w}^T \mathbf{x}_n + b) \geq 1 - \xi_n, \quad \xi_n \geq 0 \qquad n = 1, \ldots, N$$

C hyperparameter dictates which term dominates the minimization

- Small C => prefer large margins and allows more misclassified examples
- Large C => prefer small number of misclassified examples, but at the expense of a small margin

Introducing Lagrange Multipliers…

Our optimization problem is:

$$\text{Minimize} \quad f(\mathbf{w}, b, \xi) = \frac{||\mathbf{w}||^2}{2} + C\sum_{n=1}^{N} \xi_n$$

$$\text{subject to} \quad 1 \leq y_n(\mathbf{w}^T\mathbf{x}_n + b) + \xi_n, \quad 0 \leq \xi_n \qquad n = 1, \ldots, N$$

Introducing Lagrange Multipliers α_n, β_n $(n = \{1, \ldots, N\})$, for the constraints, leads to the Primal Lagrangian:

$$\text{Minimize} \quad L_P(\mathbf{w}, b, \xi, \alpha, \beta) = \frac{||\mathbf{w}||^2}{2} + C\sum_{n=1}^{N} \xi_n + \sum_{n=1}^{N} \alpha_n\{1 - y_n(\mathbf{w}^T\mathbf{x}_n + b) - \xi_n\} - \sum_{n=1}^{N} \beta_n \xi_n$$

$$\text{subject to} \quad \alpha_n, \beta_n \geq 0; \quad n = 1, \ldots, N$$

Terms in red are those that were not there in the separable case!

Formulating the dual objective

Take (partial) derivatives of L_P w.r.t. $\mathbf{w}$, b, ξ_n and set them to zero

$$\frac{\partial L_P}{\partial \mathbf{w}} = 0 \Rightarrow \mathbf{w} = \sum_{n=1}^{N} \alpha_n y_n \mathbf{x}_n, \quad \frac{\partial L_P}{\partial b} = 0 \Rightarrow \sum_{n=1}^{N} \alpha_n y_n = 0, \quad \frac{\partial L_P}{\partial \xi_n} = 0 \Rightarrow C - \alpha_n - \beta_n = 0$$

Using $C - \alpha_n - \beta_n = 0$ and $\beta_n \geq 0 \Rightarrow \alpha_n \leq C$

Substituting these in the Primal Lagrangian L_P gives the Dual Lagrangian

Maximize $L_D(\mathbf{w}, b, \xi, \alpha, \beta) = \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{m,n=1}^{N} \alpha_m \alpha_n y_m y_n (\mathbf{x}_m^T \mathbf{x}_n)$

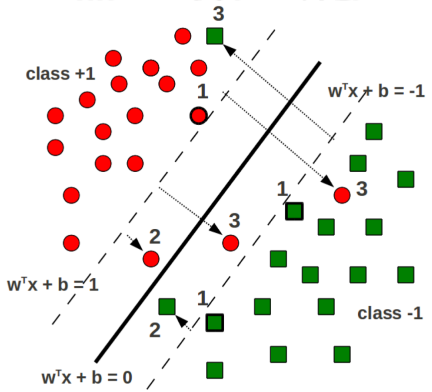
subject to $\sum_{n=1}^{N} \alpha_n y_n = 0, \quad 0 \leq \alpha_n \leq C; \quad n = 1, \ldots, N$

Note

- Given α the solution for w, b has the same form as in the separable case
- α is again sparse, nonzero α_n's correspond to support vectors

Support Vectors in the Non-Separable Case

We now have 3 types of support vectors!



(1) Lying on the margin boundaries $\mathbf{w}^T\mathbf{x} + b = -1$ and $\mathbf{w}^T\mathbf{x} + b = +1$ ($\xi_n = 0$)

(2) Lying within the margin region ($0 < \xi_n < 1$) but still on the correct side

(3) Lying on the wrong side of the hyperplane ($\xi_n \geq 1$)

Notes on training

Solving the quadratic problem is O(N^3)

- Can be prohibitive for large datasets

But many options to speed up training

- Approximate solvers
- Learn from what we know about training linear models

Recall: Learning a Linear Classifier as an Optimization Problem

Objective function

Loss function measures how well classifier fits training data

Regularizer prefers solutions that generalize well

$$\min_{\mathbf{w},b} L(\mathbf{w},b) = \min_{\mathbf{w},b} \sum_{n=1}^{N} \mathbb{I}(y_n(\mathbf{w}^T\mathbf{x}_n + b) < 0) + \lambda R(\mathbf{w},b)$$

$$\mathbb{I}(.)$$

Indicator function: 1 if (.) is true, 0 otherwise

The loss function above is called the 0-1 loss

Recall: Learning a Linear Classifier as an Optimization Problem

$$\min_{\mathbf{w},b} L(\mathbf{w}, b) = \min_{\mathbf{w},b} \sum_{n=1}^{N} \mathbb{I}(y_n(\mathbf{w}^T\mathbf{x}_n + b) < 0) + \lambda R(\mathbf{w}, b)$$

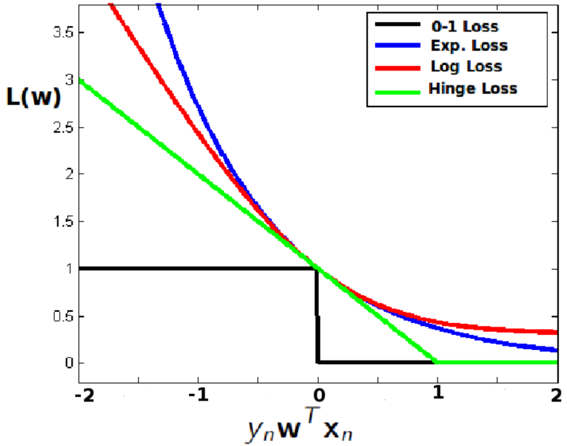
- **Problem:** The 0-1 loss above is NP-hard to optimize exactly/approximately in general
- **Solution:** Different loss function approximations and regularizers lead to specific algorithms
  (e.g., perceptron, support vector machines, etc.)

Recall: Approximating the 0-1 loss with surrogate loss functions

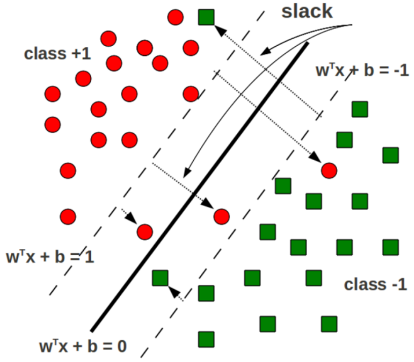
Examples (with b = 0)

- Hinge loss $[1 - y_n \mathbf{w}^T \mathbf{x}_n]_+ = \max\{0, 1 - y_n \mathbf{w}^T \mathbf{x}_n\}$
- Log loss $\log[1 + \exp(-y_n \mathbf{w}^T \mathbf{x}_n)]$
- Exponential loss $\exp(-y_n \mathbf{w}^T \mathbf{x}_n)$

All are convex upper-bounds on the 0-1 loss



What is the SVM loss function?



No penalty ($\xi_n = 0$) if $y_n(\mathbf{w}^T\mathbf{x}_n + b) \geq 1$

Linear penalty ($\xi_n = 1 - y_n(\mathbf{w}^T\mathbf{x}_n + b)$) if $y_n(\mathbf{w}^T\mathbf{x}_n + b) < 1$

It's precisely the hinge loss $\max\{0, 1 - y_n(\mathbf{w}^T\mathbf{x}_n + b)\}$

Recall: What is the perceptron optimizing?

Algorithm 5 $\textsc{PerceptronTrain}(\mathbf{D}, \mathit{MaxIter})$

```
w_d ← 0, for all d = 1 ... D                         // initialize weights
b ← 0                                                 // initialize bias
for iter = 1 ... MaxIter do
    for all (x,y) ∈ D do
        a ← Σ_{d=1}^{D} w_d x_d + b                   // compute activation for this example
        if ya ≤ 0 then
            w_d ← w_d + y x_d, for all d = 1 ... D    // update weights
            b ← b + y                                 // update bias
        end if
    end for
end for
return w_0, w_1, ..., w_D, b
```

Loss function is a variant of the hinge loss

$$\max\{0, -y_n(\mathbf{w}^T\mathbf{x}_n + b)\}$$

SVM + KERNELS

Kernelized SVM training

Recall the SVM dual Lagrangian:

$$\text{Maximize} \quad L_D(\mathbf{w}, b, \xi, \alpha, \beta) = \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{m,n=1}^{N} \alpha_m \alpha_n y_m y_n (\mathbf{x}_m^T \mathbf{x}_n)$$

$$\text{subject to} \quad \sum_{n=1}^{N} \alpha_n y_n = 0, \quad 0 \leq \alpha_n \leq C; \quad n = 1, \ldots, N$$

Replacing $\mathbf{x}_m^T \mathbf{x}_n$ by $\phi(\mathbf{x}_m)^\top \phi(\mathbf{x}_n) = k(\mathbf{x}_m, \mathbf{x}_n) = K_{mn}$, where $k(.,.)$ is some suitable kernel function

$$\text{Maximize} \quad L_D(\mathbf{w}, b, \xi, \alpha, \beta) = \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{m,n=1}^{N} \alpha_m \alpha_n y_m y_n K_{mn}$$

$$\text{subject to} \quad \sum_{n=1}^{N} \alpha_n y_n = 0, \quad 0 \leq \alpha_n \leq C; \quad n = 1, \ldots, N$$

SVM now learns a linear separator in the kernel defined feature space $\mathcal{F}$

Kernelized SVM prediction

Prediction for a test example $\mathbf{x}$ (assume $b = 0$)

$$y = sign(\mathbf{w}^\top \mathbf{x}) = sign(\sum_{n \in SV} \alpha_n y_n \mathbf{x}_n{}^\top \mathbf{x})$$

SV is the set of support vectors (i.e., examples for which $\alpha_n > 0$)

Replacing each example with its feature mapped representation ($\mathbf{x} \rightarrow \phi(\mathbf{x})$)

$$y = sign(\sum_{n \in SV} \alpha_n y_n \phi(\mathbf{x}_n)^\top \phi(\mathbf{x})) = sign(\sum_{n \in SV} \alpha_n y_n k(\mathbf{x}_n, \mathbf{x}))$$

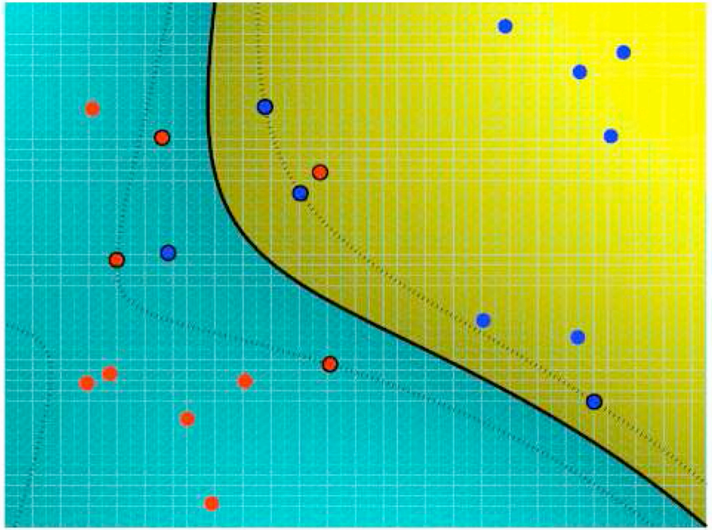
The weight vector for the kernelized case can be expressed as:

$$\mathbf{w} = \sum_{n \in SV} \alpha_n y_n \phi(\mathbf{x}_n) = \sum_{n \in SV} \alpha_n y_n k(\mathbf{x}_n, .)$$

Note

- Kernelized SVM needs the support vectors at test time!
- While unkernelized SVM can just store w

Example: decision boundary of an SVM with an RBF Kernel



What you should know

What are Support Vector Machines

How to train SVMs

    Which optimization problem we need to solve

Geometric interpretation

    - What are support vectors and what is their relationship with parameters **w**,b?

How do SVM relate to the general formulation of linear classifiers

Why/how can SVMs be kernelized

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