Support Vector Machines (II)

CMSC 422

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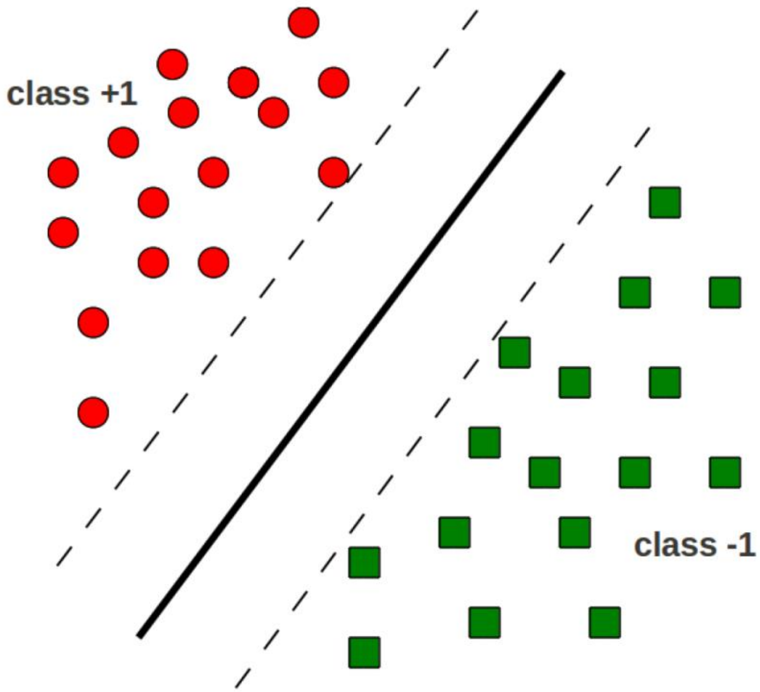
What we know about SVM so far

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

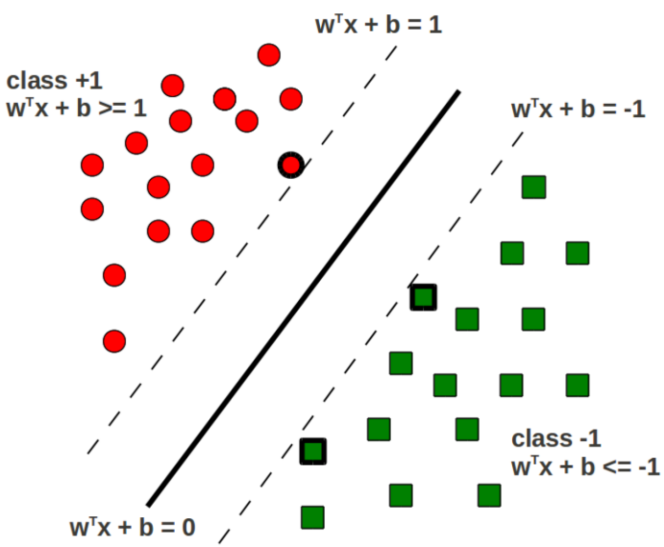
Prediction rule: $y = sign(\mathbf{w}^T\mathbf{x} + b)$

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:

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

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

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

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

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

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

SVM: the solution!
(assuming linearly separable data)

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

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

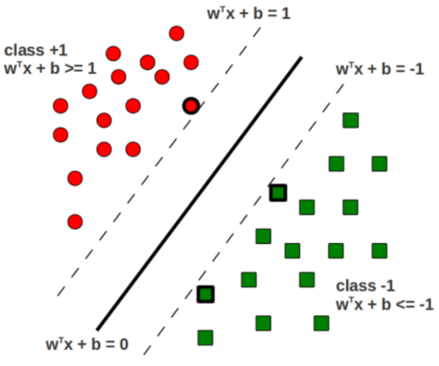
$$b = -\frac{1}{2}\left(\min_{n:y_n=+1} \mathbf{w}^T\mathbf{x}_n + \max_{n:y_n=-1} \mathbf{w}^T\mathbf{x}_n\right)$$

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?

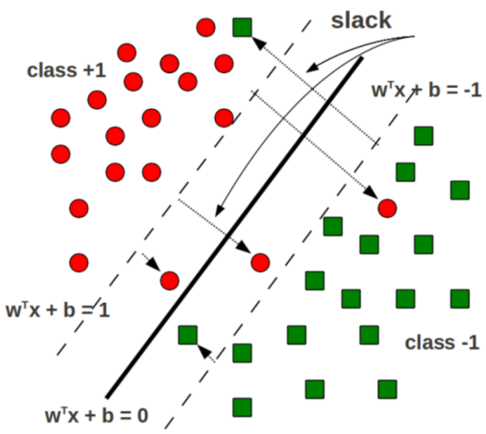
GENERAL CASE SVM SOLUTION

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

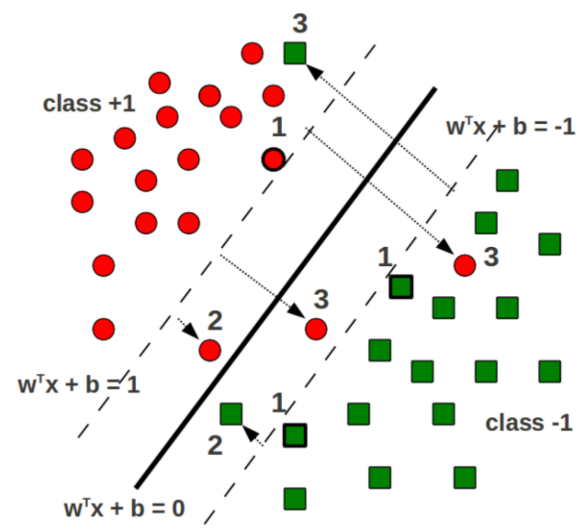
subject to $\quad \sum_{n=1}^{N} \alpha_n y_n = 0, \quad 0 \leq \alpha_n \leq C; \quad n = 1, \ldots, N$

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

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

Recall: Learning a Linear Classifier as an Optimization Problem

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

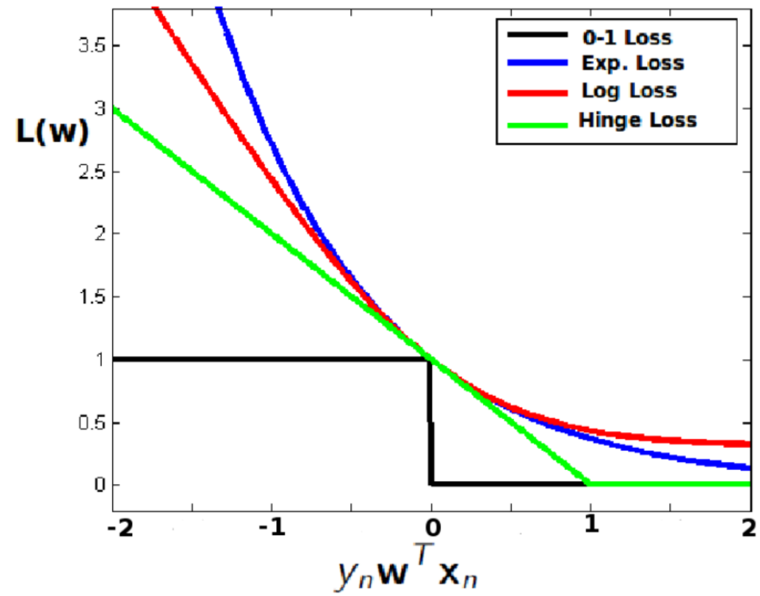
- **Problem:** The 0-1 loss above is NP-hard to optimize exactly/approximately in general
- **Solution:** Different loss function approximations and regularizers lead to specific algorithms

  (e.g., perceptron, support vector machines, etc.)

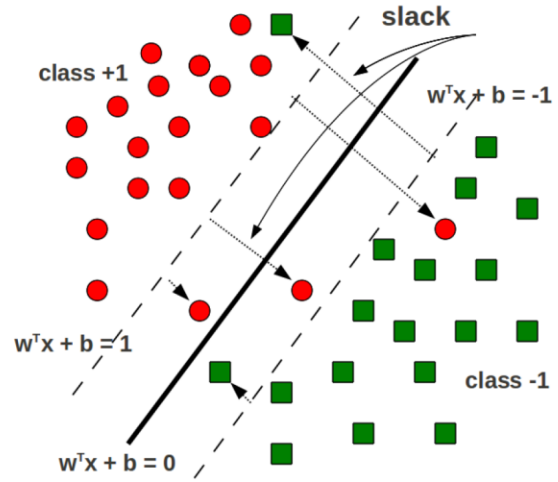
Recall: Approximating the 0-1 loss with surrogate loss functions

- 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 PerceptronTrain($\mathbf{D}$, *MaxIter*)

$w_d \leftarrow 0$, for all $d = 1 \ldots D$ // initialize weights
$b \leftarrow 0$ // initialize bias
for $iter = 1 \ldots MaxIter$ **do**
  for all $(x,y) \in \mathbf{D}$ **do**
    $a \leftarrow \sum_{d=1}^{D} w_d \, x_d + b$ // compute activation for this example
    if $ya \leq 0$ **then**
      $w_d \leftarrow w_d + y x_d$, for all $d = 1 \ldots D$ // update weights
      $b \leftarrow b + y$ // update bias
    end if
  end for
end for
return $w_0, w_1, \ldots, w_D, b$

- 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 ($\mathbf{x} \rightarrow \phi(\mathbf{x})$)

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

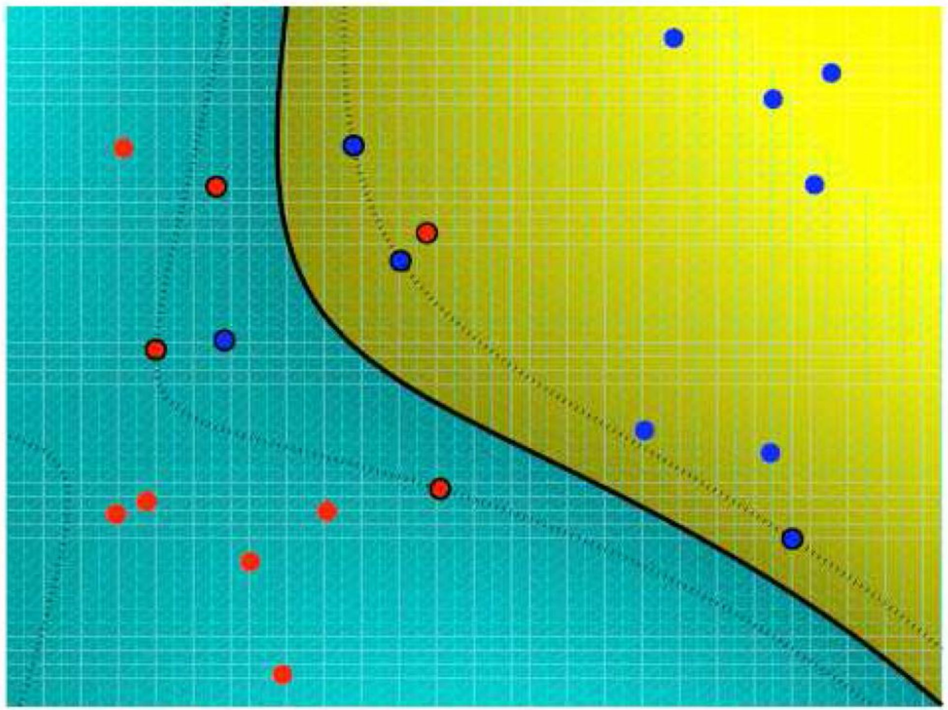
The weight vector for the kernelized case can be expressed as:

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

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