Kernels, SVMs

CMSC 422

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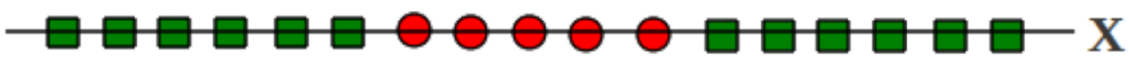
Slides adapted from MARINE CARPUAT

Today’s topics

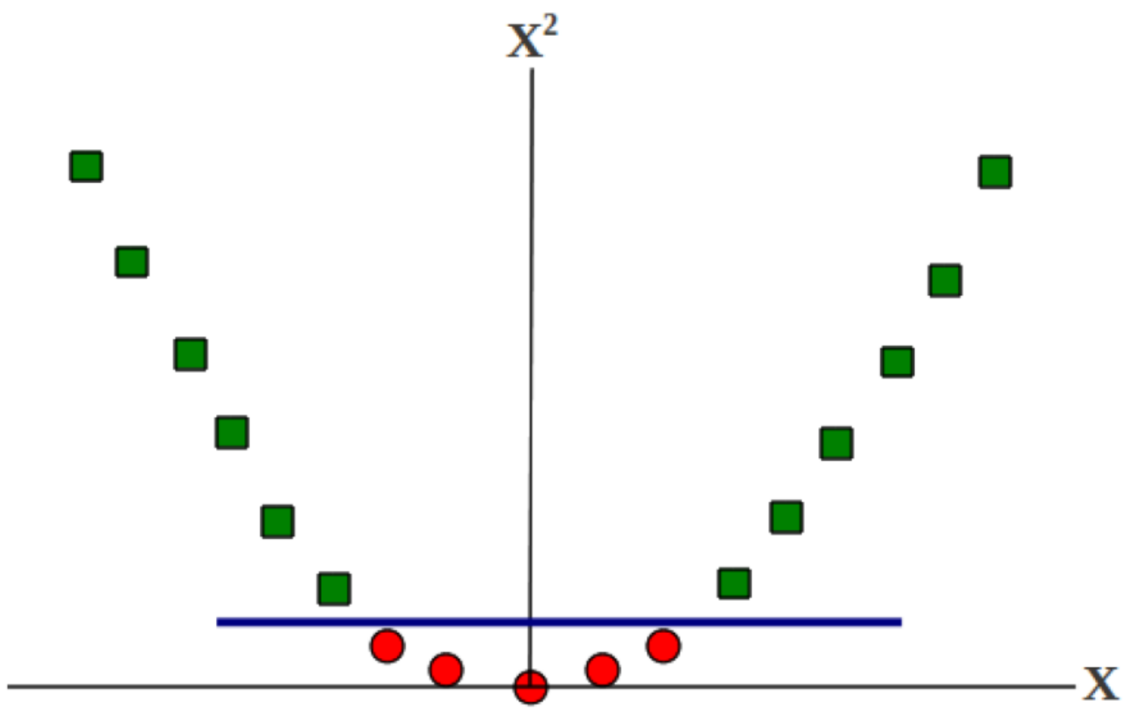
- Continue Kernel methods

- SVMs

Classifying non-linearly separable data with a linear classifier: examples



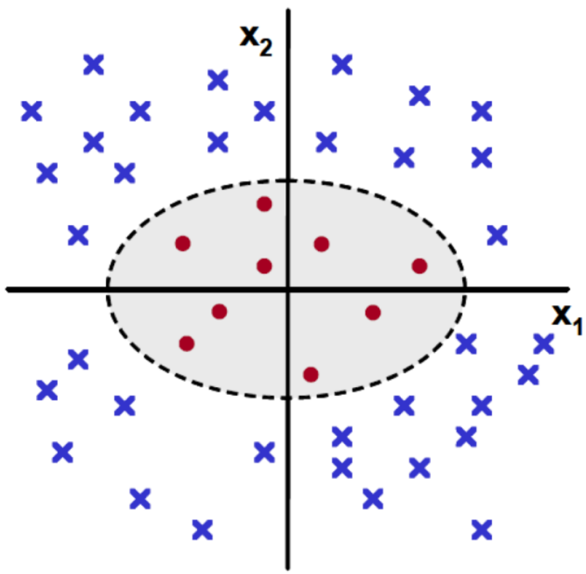
Non-linearly separable data in 1D



Becomes linearly separable in new 2D space
defined by the following mapping:

$$x \rightarrow \{x, x^2\}$$

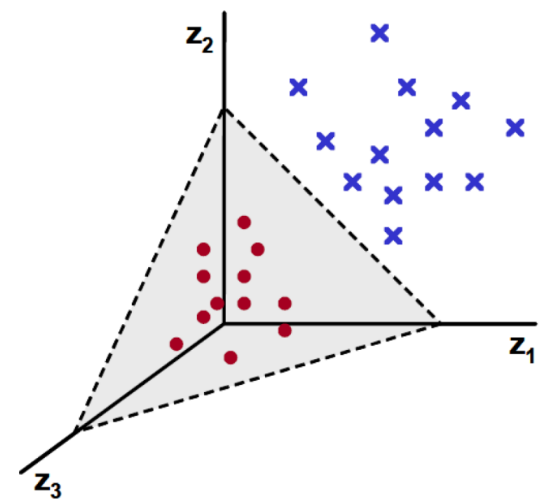
Classifying non-linearly separable data with a linear classifier: examples



Non-linearly separable data in 2D

Becomes linearly separable in the 3D space defined by the following transformation:

$$\mathbf{x} = \{x_1, x_2\} \rightarrow \mathbf{z} = \{x_1^2, \sqrt{2}x_1x_2, x_2^2\}$$



The Kernel Trick

- Rewrite learning algorithms so they only depend on **dot products between two examples**

- Replace dot product $\phi(\mathbf{x})^\top \phi(\mathbf{z})$
  by **kernel function** $k(\mathbf{x}, \mathbf{z})$
  which computes the dot product **implicitly**

Example of Kernel function

Consider two examples $\mathbf{x} = \{x_1, x_2\}$ and $\mathbf{z} = \{z_1, z_2\}$

Let's assume we are given a function k (kernel) that takes as inputs $\mathbf{x}$ and $\mathbf{z}$

$$
\begin{aligned}
k(\mathbf{x}, \mathbf{z}) &= (\mathbf{x}^\top \mathbf{z})^2 \\
&= (x_1 z_1 + x_2 z_2)^2 \\
&= x_1^2 z_1^2 + x_2^2 z_2^2 + 2 x_1 x_2 z_1 z_2 \\
&= (x_1^2, \sqrt{2} x_1 x_2, x_2^2)^\top (z_1^2, \sqrt{2} z_1 z_2, z_2^2) \\
&= \phi(\mathbf{x})^\top \phi(\mathbf{z})
\end{aligned}
$$

The above k implicitly defines a mapping ϕ to a higher dimensional space

$$\phi(\mathbf{x}) = \{x_1^2, \sqrt{2} x_1 x_2, x_2^2\}$$

Kernels: Formally defined

Recall: Each kernel k has an associated feature mapping ϕ

ϕ takes input $\mathbf{x} \in \mathcal{X}$ (input space) and maps it to $\mathcal{F}$ ("feature space")

Kernel $k(\mathbf{x}, \mathbf{z})$ takes two inputs and gives their similarity in $\mathcal{F}$ space

$$\begin{aligned} \phi &: \mathcal{X} \to \mathcal{F} \\ k &: \mathcal{X} \times \mathcal{X} \to \mathbb{R}, \quad k(\mathbf{x}, \mathbf{z}) = \phi(\mathbf{x})^\top \phi(\mathbf{z}) \end{aligned}$$

$\mathcal{F}$ needs to be a *vector space* with a *dot product* defined on it

Also called a *Hilbert Space*

Kernels: Mercer's condition

- Can *any* function be used as a kernel function?
  - No! it must satisfy Mercer's condition.

For k to be a kernel function

- There must exist a Hilbert Space $\mathcal{F}$ for which k defines a dot product
- The above is true if K is a positive definite function

$$\int d\mathbf{x} \int d\mathbf{z} f(\mathbf{x}) k(\mathbf{x}, \mathbf{z}) f(\mathbf{z}) > 0$$

For all square integrable functions f

Kernels: Constructing combinations of kernels

Let k_1, k_2 be two kernel functions then the following are as well

- $k(\mathbf{x}, \mathbf{z}) = k_1(\mathbf{x}, \mathbf{z}) + k_2(\mathbf{x}, \mathbf{z})$: direct sum
- $k(\mathbf{x}, \mathbf{z}) = \alpha k_1(\mathbf{x}, \mathbf{z})$: scalar product
- $k(\mathbf{x}, \mathbf{z}) = k_1(\mathbf{x}, \mathbf{z}) k_2(\mathbf{x}, \mathbf{z})$: direct product

Commonly Used Kernel Functions

Linear (trivial) Kernel:

$$k(\mathbf{x}, \mathbf{z}) = \mathbf{x}^\top \mathbf{z} \text{ (mapping function } \phi \text{ is identity - no mapping)}$$

Quadratic Kernel:

$$k(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^\top \mathbf{z})^2 \quad \text{or} \quad (1 + \mathbf{x}^\top \mathbf{z})^2$$

Polynomial Kernel (of degree d):

$$k(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^\top \mathbf{z})^d \quad \text{or} \quad (1 + \mathbf{x}^\top \mathbf{z})^d$$

Radial Basis Function (RBF) Kernel:

$$k(\mathbf{x}, \mathbf{z}) = \exp[-\gamma ||\mathbf{x} - \mathbf{z}||^2]$$

The Kernel Trick

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- Replace dot product $\phi(\mathbf{x})^\top \phi(\mathbf{z})$
  by **kernel function** $k(\mathbf{x}, \mathbf{z})$
  which computes the dot product **implicitly**

“Kernelizing” the perceptron

- Naïve approach: let’s explicitly train a perceptron in the new feature space

Algorithm 28 PERCEPTRONTRAIN($\mathbf{D}$, $MaxIter$)

```
w ← 0, b ← 0                                  // initialize weights and bias
for iter = 1 ... MaxIter do
    for all (x,y) ∈ D do
        a ← w · φ(x) + b                      // compute activation for this example
        if ya ≤ 0 then
            w ← w + y φ(x)                    // update weights
            b ← b + y                         // update bias
        end if
    end for
end for
return w, b
```

Can we apply the Kernel trick?
Not yet, we need to rewrite the algorithm using dot products between examples

“Kernelizing” the perceptron

- Perceptron Representer Theorem

“During a run of the perceptron algorithm, the weight vector w can always be represented as a linear combination of the expanded training data”

Proof by induction

(in CIML)

“Kernelizing” the perceptron

- We can use the perceptron representer theorem to compute activations as a **dot product** between examples

$$\boldsymbol{w} \cdot \phi(\boldsymbol{x}) + b = \left(\sum_n \alpha_n \phi(\boldsymbol{x}_n) \right) \cdot \phi(\boldsymbol{x}) + b \quad \text{definition of } \boldsymbol{w} \tag{9.6}$$

$$= \sum_n \alpha_n \left[\phi(\boldsymbol{x}_n) \cdot \phi(\boldsymbol{x}) \right] + b \quad \text{dot products are linear} \tag{9.7}$$

“Kernelizing” the perceptron

Algorithm 29 KernelizedPerceptronTrain($\mathbf{D}$, *MaxIter*)

$\boldsymbol{\alpha} \leftarrow \mathbf{0}$, $b \leftarrow 0$ // initialize coefficients and bias
for $iter = 1 \ldots MaxIter$ **do**
  for all $(\boldsymbol{x}_n, y_n) \in \mathbf{D}$ **do**
    $a \leftarrow \sum_m \alpha_m \phi(\boldsymbol{x}_m) \cdot \phi(\boldsymbol{x}_n) + b$ // compute activation for this example
    if $y_n a \leq 0$ **then**
      $\alpha_n \leftarrow \alpha_n + y_n$ // update coefficients
      $b \leftarrow b + y$ // update bias
    end if
  end for
end for
return $\boldsymbol{\alpha}$, b

- Same training algorithm, but doesn’t explicitly refers to weights w anymore only depends on dot products between examples
- We can apply the kernel trick!

Kernel Methods

- Goal: keep advantages of linear models, but make them capture non-linear patterns in data!
- How?
  - By **mapping data to higher dimensions** where it exhibits linear patterns
  - By **rewriting linear models** so that the **mapping never needs to be explicitly computed**

Discussion

- Other algorithms can be kernelized:
  - See CIML for K-means

- Do Kernels address all the downsides of "feature explosion"?
  - Helps reduce computation cost during training
  - But overfitting remains an issue

What you should know

- Kernel functions
  - What they are, why they are useful, how they relate to feature combination
- Kernelized perceptron
  - You should be able to derive it and implement it

Support Vector Machines

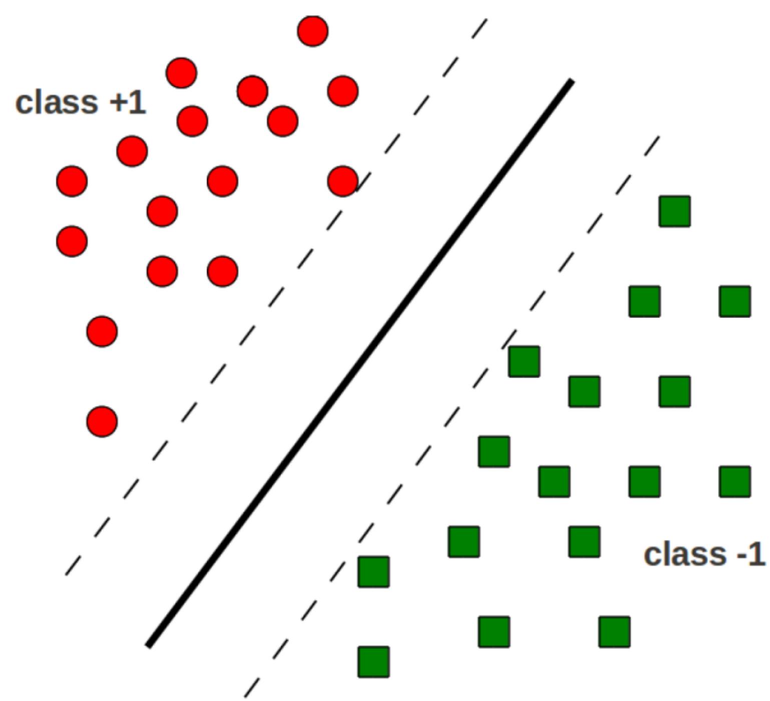
Back to linear classification

- So far: we've seen that kernels can help capture non-linear patterns in data while keeping the advantages of a linear classifier

- Support Vector Machines
  - A hyperplane-based classification algorithm
  - Highly influential
  - Backed by solid theoretical grounding (Vapnik & Cortes, 1995)
  - Easy to kernelize

The Maximum Margin Principle

- Find the hyperplane with maximum separation margin on the training data



Margin of a data set D

$$margin(\mathbf{D}, \boldsymbol{w}, b) = \begin{cases} \min_{(x,y)\in\mathbf{D}} y(\boldsymbol{w}\cdot\boldsymbol{x} + b) & \text{if } \boldsymbol{w} \text{ separates } \mathbf{D} \\ -\infty & \text{otherwise} \end{cases} \tag{3.8}$$

Distance between the hyperplane (w,b) and the nearest point in D

$$margin(\mathbf{D}) = \sup_{\boldsymbol{w},b} margin(\mathbf{D}, \boldsymbol{w}, b) \tag{3.9}$$

Largest attainable margin on D

Support Vector Machine (SVM)

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

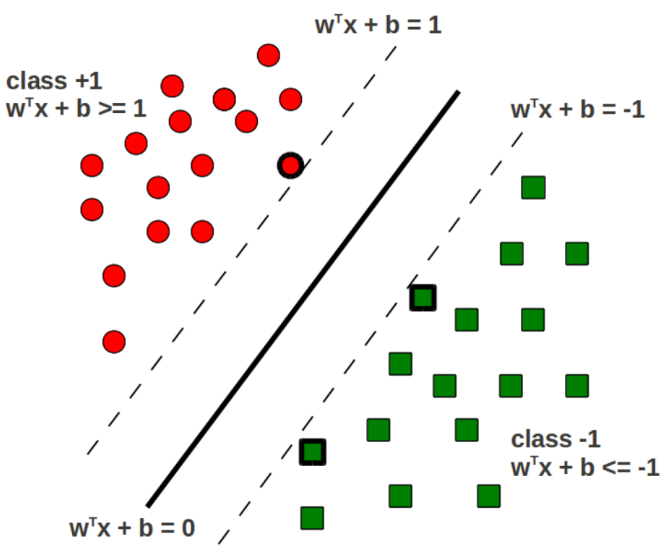
Prediction rule: $y = sign(\mathbf{w}^T\mathbf{x} + b)$

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 (**w**,b) that achieve the maximum margin

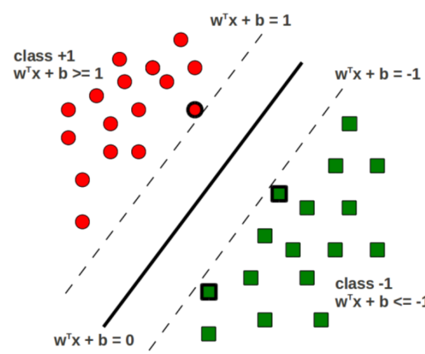


- Assume the hyperplane is such that
  - $\mathbf{w}^T\mathbf{x}_n + b \geq 1$ for $y_n = +1$
  - $\mathbf{w}^T\mathbf{x}_n + b \leq -1$ for $y_n = -1$
  - Equivalently, $y_n(\mathbf{w}^T\mathbf{x}_n + b) \geq 1$
    $\Rightarrow \min_{1\leq n\leq N} |\mathbf{w}^T\mathbf{x}_n + b| = 1$
  - The hyperplane's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

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

The Optimization Problem

We want to maximize the margin $\gamma = \frac{1}{||\mathbf{w}||}$



Maximizing the margin γ = minimizing $||\mathbf{w}||$ (the norm)

Our optimization problem would be:

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

Large Margin = Good Generalization

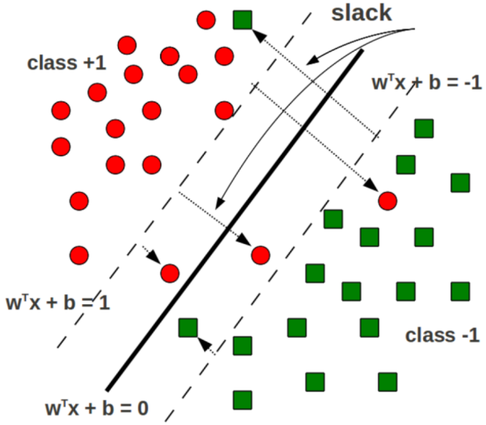
- Intuitively, large margins mean good generalization
  - Large margin => small $||\mathbf{w}||$
  - small $||\mathbf{w}||$ => regularized/simple solutions
- (Learning theory gives a more formal justification)

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

Soft SVM

- Same optimization as :

$$\min_{\mathbf{w},b} \frac{\|\mathbf{w}\|^2}{2} + C\underbrace{\sum_{n=1}^{N} \max\left\{1 - y_n(\mathbf{w}^t\mathbf{x}_n), 0\right\}}_{\text{Hinge loss!}}$$

- Why?

- Have you seen this loss function before?