Kernel Methods

CMSC 422

Slides adapted from Prof. CARPUAT

Slides credit: Piyush Rai

Beyond linear classification

- Problem: linear classifiers
  - Easy to implement and easy to optimize
  - But limited to linear decision boundaries

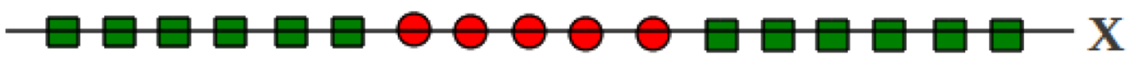
- What can we do about it?
  - Last week: Neural networks
    - Very expressive but harder to optimize (non-convex objective)
  - Today: Kernels

Kernel Methods

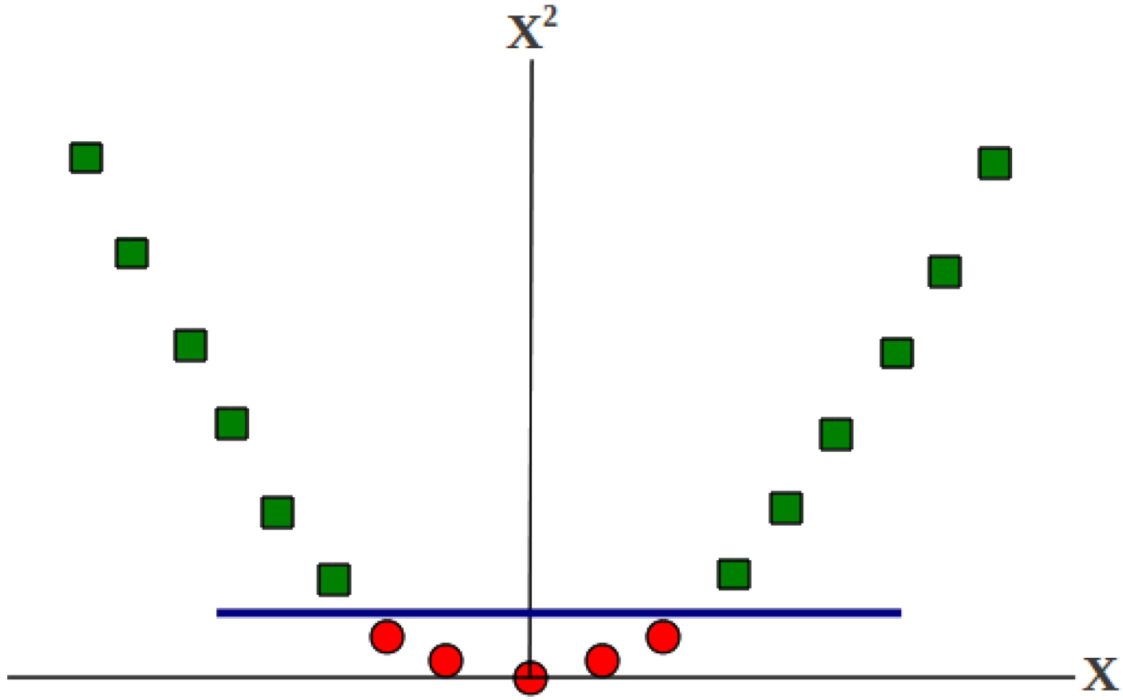
- Goal: keep advantages of linear models, but make them capture non-linear patterns in data!

- How?
  - By mapping data to higher dimensions where it exhibits linear patterns

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



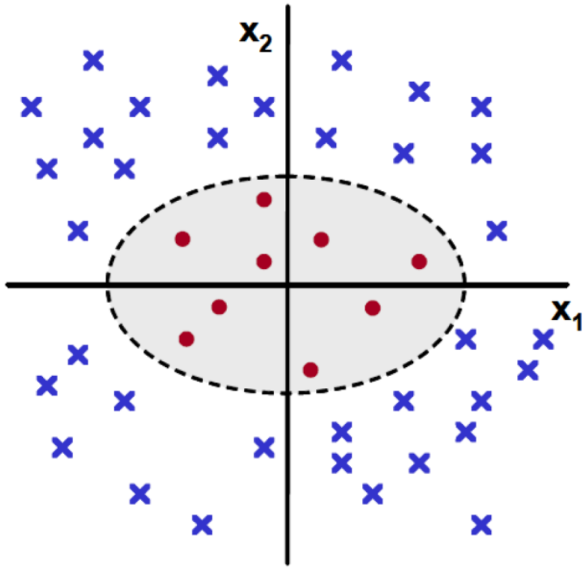
Non-linearly separable data in 1D



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

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

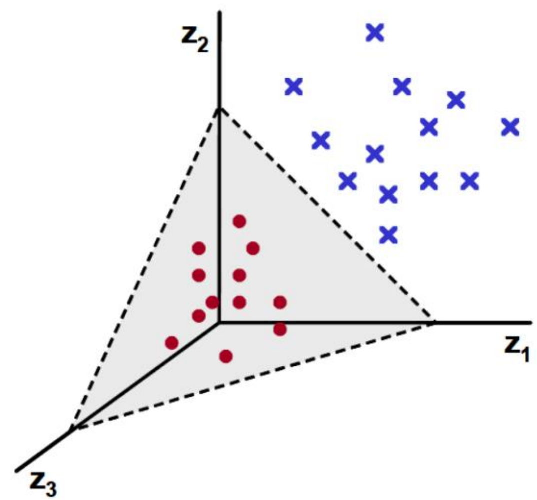
Classifying non-linearly separable data with a linear classifier: examples



Non-linearly
separable data in 2D

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

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



Defining feature mappings

- Map an original feature vector $\boldsymbol{x} = \langle x_1, x_2, x_3, \ldots, x_D \rangle$
  to an expanded version $\phi(\boldsymbol{x})$

- Example: quadratic feature mapping represents feature combinations

$$
\begin{aligned}
\phi(\boldsymbol{x}) = \langle 1, 2x_1, 2x_2, 2x_3, \ldots, 2x_D, \\
& x_1^2, x_1x_2, x_1x_3, \ldots, x_1x_D, \\
& x_2x_1, x_2^2, x_2x_3, \ldots, x_2x_D, \\
& x_3x_1, x_3x_2, x_3^2, \ldots, x_2x_D, \\
& \ldots, \\
& x_Dx_1, x_Dx_2, x_Dx_3, \ldots, x_D^2 \rangle
\end{aligned}
$$

Feature Mappings

- Pros: can help turn non-linear classification problem into linear problem

- Cons: “feature explosion” creates issues when training linear classifier in new feature space
  - More computationally expensive to train
  - More training examples needed to avoid overfitting

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**

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

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

Another example of Kernel Function (see CIML 11.1)

$$\begin{aligned}
\phi(\boldsymbol{x}) = \langle 1, 2x_1, 2x_2, 2x_3, \ldots, 2x_D, \\
x_1^2, x_1x_2, x_1x_3, \ldots, x_1x_D, \\
x_2x_1, x_2^2, x_2x_3, \ldots, x_2x_D, \\
x_3x_1, x_3x_2, x_3^2, \ldots, x_2x_D, \\
\ldots, \\
x_Dx_1, x_Dx_2, x_Dx_3, \ldots, x_D^2 \rangle
\end{aligned}$$

What is the function k(x,z) that can implicitly compute the dot product $\phi(\boldsymbol{x}) \cdot \phi(\boldsymbol{z})$?

$$\begin{aligned}
\phi(\boldsymbol{x}) \cdot \phi(\boldsymbol{z}) &= 1 + x_1z_1 + x_2z_2 + \cdots + x_Dz_D + x_1^2z_1^2 + \cdots + x_1x_Dz_1z_D + \\
&\quad \cdots + x_Dx_1z_Dz_1 + x_Dx_2z_Dz_2 + \cdots + x_D^2z_D^2 && (9.2) \\
&= 1 + 2\sum_d x_dz_d + \sum_d \sum_e x_dx_ez_dz_e && (9.3) \\
&= 1 + 2\boldsymbol{x} \cdot \boldsymbol{z} + (\boldsymbol{x} \cdot \boldsymbol{z})^2 && (9.4) \\
&= (1 + \boldsymbol{x} \cdot \boldsymbol{z})^2 && (9.5)
\end{aligned}$$

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

- 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**

"Kernelizing" the perceptron

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

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Algorithm 28 $\textsc{PerceptronTrain}(\mathbf{D}, \mathit{MaxIter})$

$\boldsymbol{w} \leftarrow \mathbf{0}$, $b \leftarrow 0$ // initialize weights and bias
for $\mathit{iter} = 1 \ldots \mathit{MaxIter}$ **do**
    for all $(x,y) \in \mathbf{D}$ **do**
        $a \leftarrow \boldsymbol{w} \cdot \phi(\boldsymbol{x}) + b$ // compute activation for this example
        if $ya \leq 0$ **then**
            $\boldsymbol{w} \leftarrow \boldsymbol{w} + y\, \phi(\boldsymbol{x})$ // update weights
            $b \leftarrow b + y$ // 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

  (on board + see CIML 11.2)

“Kernelizing” the perceptron

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

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

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

"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 $(x_n, y_n) \in \mathbf{D}$ **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
  - We'll talk about Support Vector Machines next

- 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