Slides adapted from Prof Carpuat and Duraiswami

CMSC 422 Introduction to Machine Learning

Lecture 22 Kernel Methods

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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

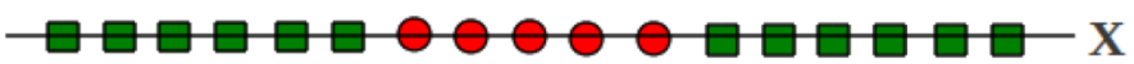
Kernel Methods

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

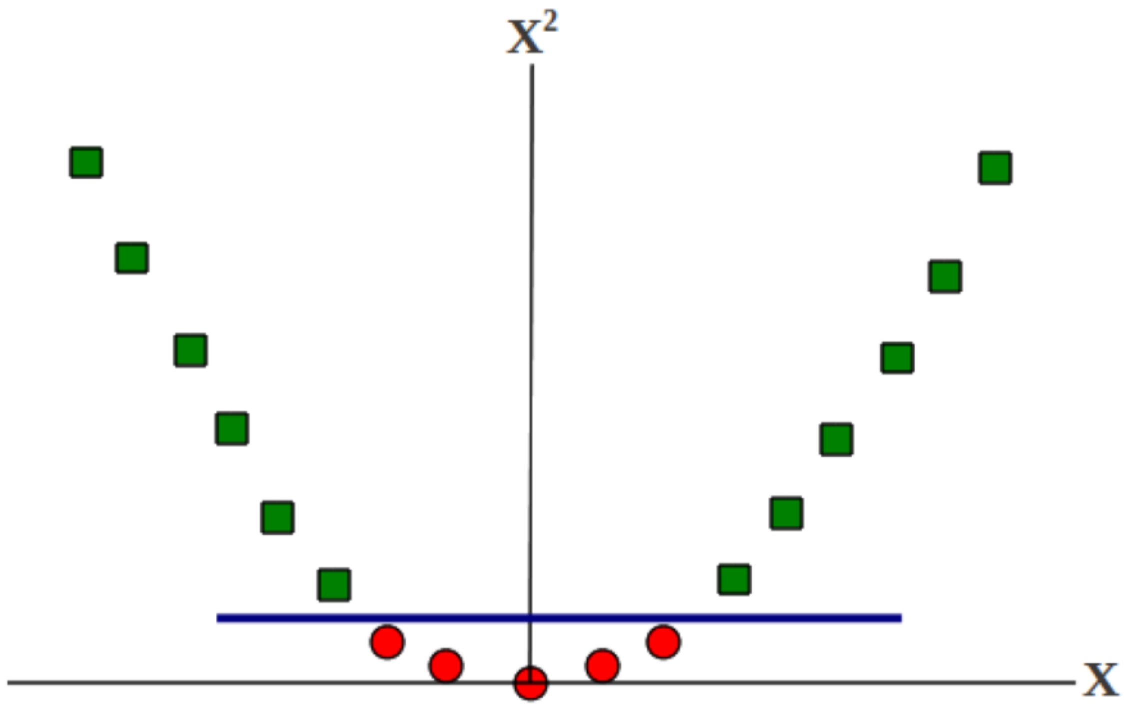
How?

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

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



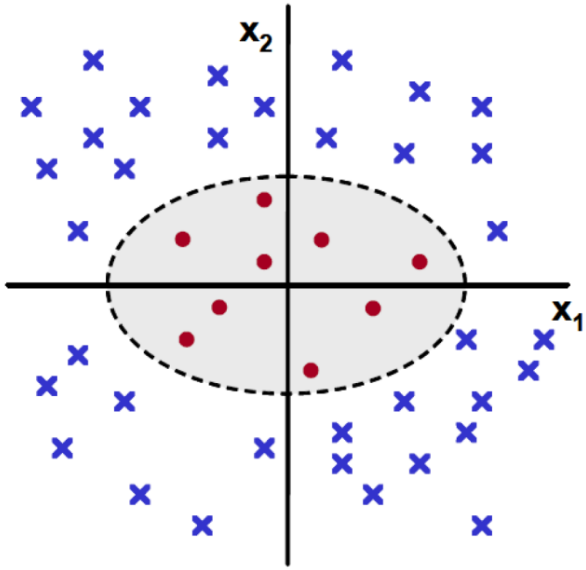
Non-linearly separable data in 1D



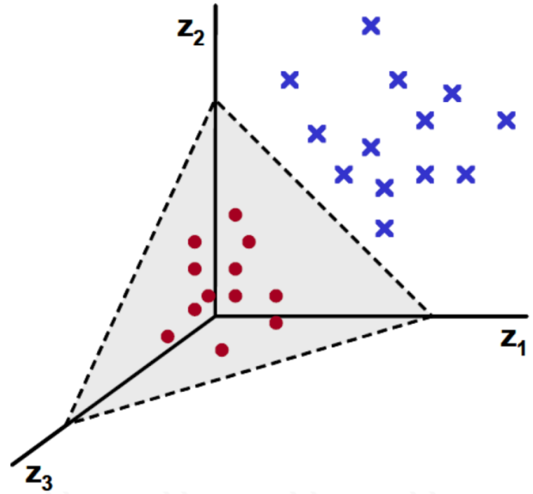
Becomes linearly separable in new 2D space
defined by the following mapping:

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

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 (from CIML)

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

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

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

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:

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

Fun Fact about RBF kernel

- The feature space of the kernel has an infinite number of dimensions; for $\sigma = 1$, its expansion is:

$$\exp\left(-\frac{1}{2}\|\mathbf{x}-\mathbf{x}'\|^2\right) = \sum_{j=0}^{\infty} \frac{(\mathbf{x}^\top \mathbf{x}')^j}{j!} \exp\left(-\frac{1}{2}\|\mathbf{x}\|^2\right) \exp\left(-\frac{1}{2}\|\mathbf{x}'\|^2\right)$$

$$= \sum_{j=0}^{\infty} \sum_{\sum n_i = j} \exp\left(-\frac{1}{2}\|\mathbf{x}\|^2\right) \frac{x_1^{n_1} \cdots x_k^{n_k}}{\sqrt{n_1! \cdots n_k!}} \exp\left(-\frac{1}{2}\|\mathbf{x}'\|^2\right) \frac{{x'}_1^{n_1} \cdots {x'}_k^{n_k}}{\sqrt{n_1! \cdots n_k!}}$$

- Since the value of the RBF kernel decreases with distance and ranges between zero (in the limit) and one (when $x = x'$), it has a ready interpretation as a similarity measure.

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

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

$\boldsymbol{w} \leftarrow \mathbf{0}$, $b \leftarrow 0$ // initialize weights and bias

for $\mathit{iter} = 1 \dots \mathit{MaxIter}$ **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 $\boldsymbol{w}, b$

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

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

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

"Kernelizing" the perceptron

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

```
α ← 0, b ← 0                                   // initialize coefficients and bias
for iter = 1 ... MaxIter do
    for all (x_n, y_n) ∈ D do
        a ← Σ_m α_m φ(x_m) · φ(x_n) + b        // compute activation for this example
        if y_n a ≤ 0 then
            α_n ← α_n + y_n                    // update coefficients
            b ← b + y                          // update bias
        end if
    end for
end for
return α, 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! Replace the inner product of $\phi(x_m) \cdot \phi(x_n)$ with some kernel function

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

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