Learning with Kernels

Advanced Signal Processing Seminar

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Outline

Intro – A Simple Learning Problem

Classification

- Sets $\mathcal{X}$ and $\mathcal{Y}$
- Each data point $\mathbf{x}_i$ is assigned a label y_i.
- Training data: $(\mathbf{x}^{(1)}, y^{(1)}), \ldots, (\mathbf{x}^{(m)}, y^{(m)})$
- Goal: classify an unseen data point $\mathbf{x}$, i.e. predict its label y
- Find $(\mathbf{x}, y)$ that is *similar* to the training examples.
- How to measure similarity?
  Use the standard inner product, for a vector space $\mathbb{R}^n$:

$$\langle \mathbf{a}, \mathbf{b} \rangle = \sum_{i=1}^{n} a_i b_i$$

Intro – Example

Prototype classifier

- Separate patterns from class A and B
- Classification criterion: distance to means of class samples (blackboard example)

Intro – Example

Prototype classifier

- Separate patterns from class A and B
- Classification criterion: distance to means of class samples
- Euclidean distance between two points: norm of difference vector $\mathbf{d}$

$$\begin{aligned} \|\mathbf{d}\| &= \|\mathbf{x}-\mathbf{y}\| \\ &= \sqrt{(x_1-y_1)^2+(x_2-y_2)^2+\cdots+(x_n-y_n)^2} \\ &= \sqrt{\langle \mathbf{x}-\mathbf{y}, \mathbf{x}-\mathbf{y}\rangle} \end{aligned}$$

Intro – Example

Prototype classifier - Summary

- If $\langle \bar{a} - \bar{b}, x \rangle > \theta$ then $\mathbf{x} \in A$ else $\in B$

  with $\theta = \frac{1}{2}(\langle \bar{a}, \bar{a} \rangle - \langle \bar{b}, \bar{b} \rangle)$

- Decision boundary along $\langle \bar{a} - \bar{b}, x \rangle = \theta$, orthogonal to distance vector of means

Intro – Inner Product Space

Definition

A vector space $\mathcal{X}$ over the reals $\mathbb{R}$ is an *inner product space* if there exists a real-valued symmetric bilinear map $\langle \mathbf{x}, \mathbf{x} \rangle \geq 0$.

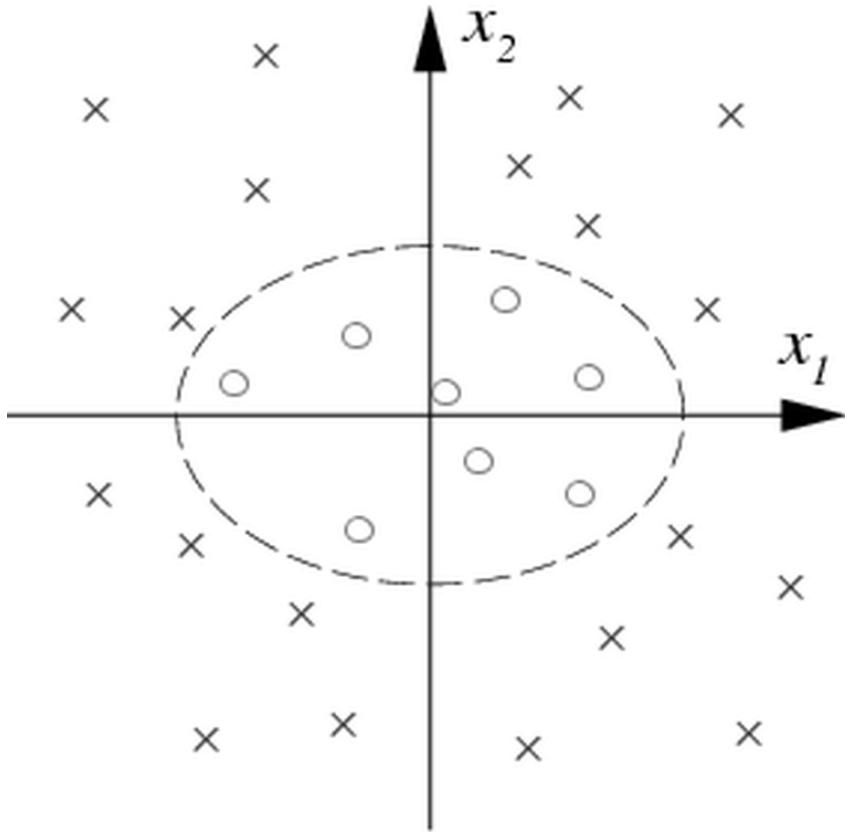
Angles and lengths

$$\cos\phi = \frac{\langle \mathbf{x}, \mathbf{y} \rangle}{\|\mathbf{x}\| \|\mathbf{y}\|}$$

$$\|\mathbf{x}\| = \sqrt{\langle \mathbf{x}, \mathbf{x} \rangle}$$

Mapping – Non-linear Problems

- How to separate these data sets?

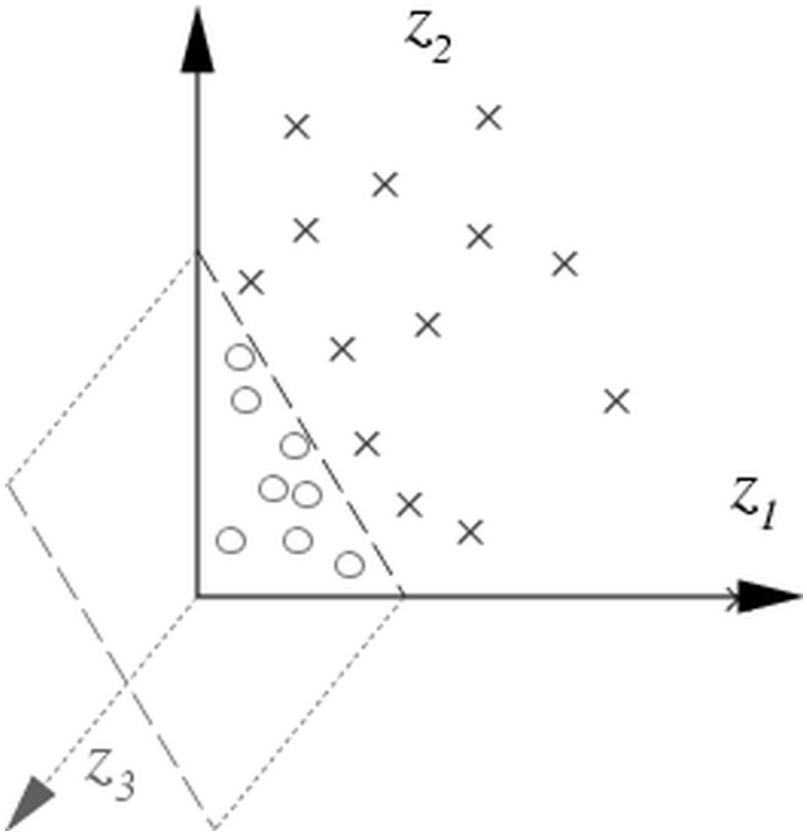


- Use a map to a space were the sets are separable!

Maps – Non-linear Problems

$$\Phi : \mathcal{X} \rightarrow \mathcal{Z}$$
$$\mathbf{x} \mapsto \mathbf{z}$$

Data can be separated by a *linear* hyperplane!



Maps – Non-linear Problems

- Example:

$$\begin{aligned} \Phi : \mathbb{R}^2 &\rightarrow \mathbb{R}^3 \\ (x_1, x_2) &\mapsto (z_1, z_2, z_3) := (x_1^2, \sqrt{2}x_1x_2, x_2^2) \end{aligned}$$

- For the similarity measure the feature space has to be an inner product space!

$$\langle \Phi(\mathbf{x}), \Phi(\mathbf{y}) \rangle = x_1^2 y_1^2 + 2x_1x_2y_1y_2 + y_1^2 y_2^2 = \langle \mathbf{x}, \mathbf{y} \rangle^2$$

$$\langle \mathbf{x}, \mathbf{y} \rangle^2 := k(\mathbf{x}, \mathbf{y}) \quad \text{is a kernel function}$$

Kernels – Definition

Definition

A kernel is a function k that for all $\mathbf{x}, \mathbf{y} \in \mathcal{X}$ satisfies

$$k(\mathbf{x}, \mathbf{y}) = \langle \Phi(\mathbf{x}), \Phi(\mathbf{y}) \rangle$$

where Φ is a mapping from $\mathcal{X}$ to an (inner product) feature space $\mathcal{Z}$

$$\Phi : \mathbf{x} \mapsto \Phi(\mathbf{x}) \in \mathcal{Z}$$

Kernels – The Kernel Trick

- Instead of $\langle \Phi(\mathbf{x}), \Phi(\mathbf{y}) \rangle$ compute $\langle \mathbf{x}, \mathbf{y} \rangle^2$.
- Compute inner product directly in the input space.
- No mapping to the feature space is necessary.
- Computationally more efficient!
- This is called the kernel trick.

Kernels – The Kernel Trick

Summary

- Any algorithm that only depends on inner products can benefit from the kernel trick.
- Kernels are a generalization of inner products.
- They can be seen as a nonlinear similarity measure.

Kernels – Examples for Kernel Functions

- Polynomial

$$k(\mathbf{x}, \mathbf{y}) = (\langle \mathbf{x}, \mathbf{y} \rangle + c)^d$$

- Sigmoid

$$k(\mathbf{x}, \mathbf{y}) = \tanh(\kappa \langle \mathbf{x}, \mathbf{y} \rangle + \Omega)$$

- Gaussian

$$k(\mathbf{x}, \mathbf{y}) = \exp(-(\mathbf{x} - \mathbf{y})^2 / (2\sigma^2))$$

Kernels – Positive Definite Kernels

- A Kernel can always be constructed by

$$k(\mathbf{x}, \mathbf{y}) = \langle \Phi(\mathbf{x}), \Phi(\mathbf{y}) \rangle$$

- How to find out if $k(.,.)$ defines an inner product in feature space without actually computing Φ?

- The kernel has to be *positive definite*.
  - Symmetric: $k(\mathbf{x}, \mathbf{y}) = k(\mathbf{y}, \mathbf{x})$.
  - Its *kernel matrix* or *Gram matrix* K is *positive semi-definite*.

$$K_{ij} := k(x_i, x_j) \quad \text{and} \quad v^T K v \geq 0 \quad \text{for all vectors v}$$

RKHS – Feature space

Construction of the feature space

- Define a feature map.
- Turn $\Phi(\mathcal{X})$ into a linear space.
- Endow it with a dot product satisfying

$$\langle k(.,x_i), k(.,x_j)\rangle = k(x_i,x_j)$$

- Complete the space to get a *reproducing kernel Hilbert space* (RKHS).

RKHS – The Reproducing Kernel Hilbert Space

Definition

A *Hilbert Space* $\mathcal{H}$ is an inner product space with the additional properties that it is *separable* and *complete*.

- Completeness refers to the property that every Cauchy sequence of elements of $\mathcal{H}$ converges to an element h of $\mathcal{H}$
- A space $\mathcal{H}$ is separable if for any $\epsilon > 0$ there is a finite set of elements $h_1, ..., h_N$ of $\mathcal{H}$ such that for all h of $\mathcal{H}$

$$\min_i \|h_i - h\| < \epsilon$$

RKHS – Turn It into a Linear Space

Form all linear combinations

$$
\begin{aligned}
f(.) &= \sum_{i=1}^{m} \alpha_i k(., x_i), \\
g(.) &= \sum_{j=1}^{m'} \beta_i k(., x'_j),
\end{aligned}
$$

$(m, m' \in \mathbb{N}, \alpha_i, \beta_i \in \mathbb{R}, x_i, x'_j \in \mathcal{X})$.

RKHS – Endow It with an Inner Product

$$\begin{aligned}\langle f, g\rangle &:= \sum_{i=1}^{m}\sum_{j=1}^{m'} \alpha_i \beta_j k(x_i, x'_j) \\ &= \sum_{i=1}^{m} \alpha_i g(x_i) = \sum_{j=1}^{m'} \beta_j f(x'_j)\end{aligned}$$

- This is well-defined, symmetric and bilinear.

RKHS – The Reproducing Kernel Property

Two special cases:

- Assume

$$f(.) = k(., x)$$

  In this case we have

$$\langle k(., x), g \rangle = g(x)$$

- If moreover

$$g(.) = k(., x')$$

  we have

$$\langle k(., x), k(., x') \rangle = k(x, x')$$

- k is called a *reproducing kernel*.

RKHS – The Reproducing Kernel Property

- Because of the reproducing property of the kernel, the feature space is called *reproducing kernel Hilbert space* (RKHS).

Discussion

Thank you for your attention!

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