# 4.1 Kernel Methods

*Machine Learning 1: Foundations*

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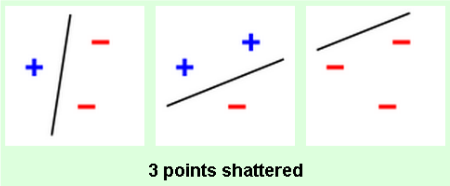
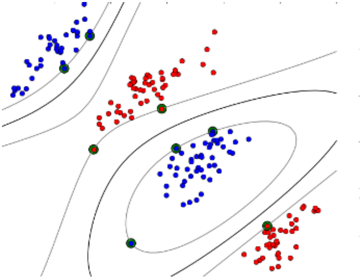
# Recap

In previous lectures: **Linear classification methods**

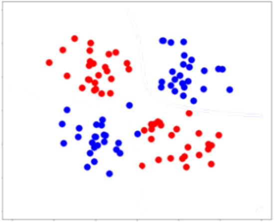



Will not work for non-linear data:



# Limitations of Linear Classifiers

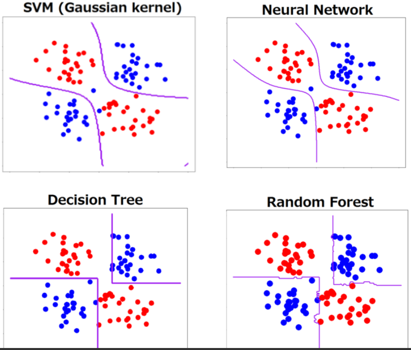
For instance, we cannot solve the XOR problem with a linear classifier:



Non-linear algorithm we know so far: *k*-nearest neighbor algorithm

- too simplistic and inaccurate

Other non-linear algorithms we will learn in this course:



# Contents of this Class

1. Kernel Methods
2. Kernel SVM

# Kernel Methods

**Kernel methods** is a paradigm to

- convert linear learning machines (e.g., linear SVM)
- into non-linear ones (e.g., kernel SVM)

How does that work?

# Core Idea

1. Define, in a clever way, a non-linear map

$$\phi : \mathbb{R}^d \rightarrow \mathbb{R}^D ,$$

   where $\mathbb{R}^D$ is a very high-dimensional space ($D >> d$)

2. Map the inputs into that space,

$$\mathbf{x}_i \mapsto \phi(\mathbf{x}_i), \quad i = 1, \ldots, n$$

3. Separate the data linearly in that space

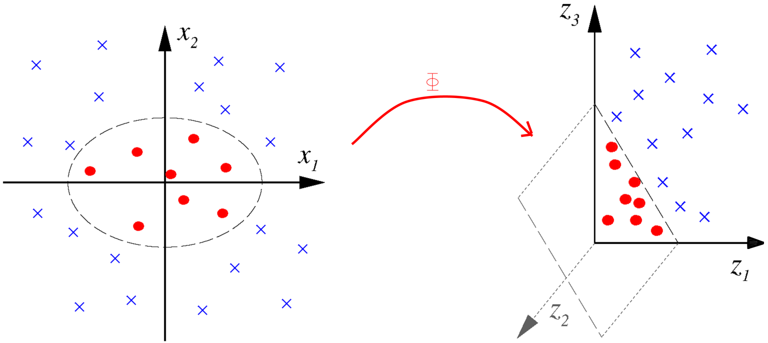
$$f(\mathbf{x}) = \mathrm{sign}(\langle \mathbf{w}, \phi(\mathbf{x}) \rangle + b)$$

4. Corresponds to non-linear separation in the input space

**Do all this very efficiently!**

# Example

Consider the map $\phi : \begin{array}{ccc} \mathbb{R}^2 & \to & \mathbb{R}^3 \\ (x_1, x_2) & \mapsto & (x_1^2, \sqrt{2}x_1 x_2, x_2^2) \end{array}$




Key idea: linear separation in the image space $\mathbb{R}^3$ corresponds to non-linear separation in the input space $\mathbb{R}^2$.

Problem: the image space is usually too high-dimensional to perform any operations in it $\Rightarrow$ **kernel trick**.

# Kernel Trick: Example

Say $\mathbf{x} = (x_1, x_2)$ and $\tilde{\mathbf{x}} = (\tilde{x}_1, \tilde{x}_2)$ are two data points in $\mathbb{R}^2$.

- We first map the two points into the higher-dimensional space, using the map $\phi(\mathbf{x}) = (x_1^2, \sqrt{2}x_1x_2, x_2^2)$.

Now let's try computing their inner product in that space:

$$
\begin{aligned}
&\langle \phi(\mathbf{x}), \phi(\tilde{\mathbf{x}}) \rangle \\
&\overset{\text{def.}}{=} \left\langle (x_1^2, \sqrt{2}x_1x_2, x_2^2), (\tilde{x}_1^2, \sqrt{2}\tilde{x}_1\tilde{x}_2, \tilde{x}_2^2) \right\rangle \\
&= (x_1\tilde{x}_1)^2 + 2(x_1\tilde{x}_1x_2\tilde{x}_2) + (x_2\tilde{x}_2)^2 \\
&= \langle \mathbf{x}, \tilde{\mathbf{x}} \rangle^2
\end{aligned}
$$

Result: we computed a higher-dimensional inner product via a lower-dimensional one!

$k(\mathbf{x}, \tilde{\mathbf{x}}) := \langle \mathbf{x}, \tilde{\mathbf{x}} \rangle^2$ is an example of a **kernel**.

# Kernel Trick: Formal Definition

## Kernel Trick

1. Formulate the (linear) learning machine (training and prediction) solely in terms of inner products
2. Replace the inner products $\langle \mathbf{x}_i, \mathbf{x}_j \rangle$ by the kernel $k(\mathbf{x}_i, \mathbf{x}_j)$

Remarks:

- The kernel trick can be applied only to **linear** learning machines, and not to all of them:
  - only to those that can be formulated in a way that they access the training data only through inner products between pairs of data points.

# Kernel

## Definition

A function $k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is called **kernel function** (or simply "**kernel**") if all of the following holds

1. it is a symmetric
2. there exists a map $\phi : \mathbb{R}^d \to \mathcal{H}$ (called **kernel feature map** into some high-dimensional **kernel feature space** $\mathcal{H}$ (e.g., $\mathcal{H} = \mathbb{R}^l$ or $\mathcal{H} = \mathbb{R}^{\text{“}\infty\text{”}}$) such that:

$$\forall \mathbf{x}, \tilde{\mathbf{x}} \in \mathbb{R}^d : \quad k(\mathbf{x}, \tilde{\mathbf{x}}) = \langle \phi(\mathbf{x}), \phi(\tilde{\mathbf{x}}) \rangle \ .$$

In a nutshell: "k computes inner products in some high-dimensional space"

Additional practical requirement:

- $k$ should be very efficiently computable!

# Example 1: Linear Kernel

## Definition

The **linear kernel** is defined as

$$k(\mathbf{x}, \tilde{\mathbf{x}}) := \langle \mathbf{x}, \tilde{\mathbf{x}} \rangle \, .$$

## Proposition

The **linear kernel** is a kernel.

# Proof

1. By the symmetry of the inner product, we have, for all $\mathbf{x}, \tilde{\mathbf{x}} \in \mathbb{R}^d$:

$$k(\mathbf{x}, \tilde{\mathbf{x}}) \overset{(\star)}{=} \langle \mathbf{x}, \tilde{\mathbf{x}} \rangle = \langle \tilde{\mathbf{x}}, \mathbf{x} \rangle \overset{(\star)}{=} k(\tilde{\mathbf{x}}, \mathbf{x}),$$

   where $(\star)$ is by the definition of the linear kernel. Thus the linear kernel is symmetric.

2. We choose the identify map $\phi := \mathrm{id}$ and the kernel feature space $\mathcal{H} := \mathbb{R}^d$. Then, for all $\mathbf{x}, \tilde{\mathbf{x}} \in \mathbb{R}^d$, we have:

$$\begin{aligned} & k(\mathbf{x}, \tilde{\mathbf{x}}) \\ & \overset{(\star)}{=} \langle \mathbf{x}, \tilde{\mathbf{x}} \rangle \\ & \overset{(\star)}{=} \langle \mathrm{id}(\mathbf{x}), \mathrm{id}(\tilde{\mathbf{x}}) \rangle \\ & = \langle \phi(\mathbf{x}), \phi(\tilde{\mathbf{x}}) \rangle , \end{aligned}$$

   where again $(\star)$ is by the definition of the linear kernel. $\square$

# Example 2/3: Polynomial Kernel

**Definition**

The **polynomial kernel of degree** $m \in \mathbb{N}$ is defined as

$$k(\mathbf{x}, \tilde{\mathbf{x}}) := (\langle \mathbf{x}, \tilde{\mathbf{x}} \rangle + c)^m$$

where $c \geq 0$ is a parameter.

**Proposition**

The **polynomial kernel** is a kernel.

# Proof Idea

One can verify that, for the right choice of the coefficients $c_i \in \mathbb{R}$, the following map is a kernel feature map for the polynomial kernel:

$$\phi : \mathbf{x} \mapsto c_i (x_1^{i_1} \cdots x_d^{i_d})_{i=(i_1,\ldots,i_d)\in\mathbb{N}_0^d : \sum_{j=1}^n i_j \leq m} \,. \tag{1}$$

Full proof: exercise sheet. $\square$

**Why the name 'polynomial kernel'?**

Recall from Slide 6 that, in kernel methods, we use the classifier

$$f(\mathbf{x}) = \langle \mathbf{w}, \phi(\mathbf{x}) \rangle \,. \tag{2}$$

Plugging (1) into (2), we obtain

$$f(\mathbf{x}) = \sum_{i=(i_1,\ldots,i_d)\in\mathbb{N}_0^d : \sum_{j=1}^n i_j = m} w_i x_1^{i_1} \cdots x_d^{i_d} \,.$$

Thus $f$ is a polynomial.

# Example 3/3: Gaussian RBF Kernel

## Definition

The **Gaussian RBF kernel** is defined as

$$k(\mathbf{x}, \tilde{\mathbf{x}}) := \exp\left(-\frac{1}{2\sigma^2}\|\mathbf{x}-\tilde{\mathbf{x}}\|^2\right).$$

The parameter $\sigma^2 > 0$ is called **kernel width** (or bandwith).

Note: This is the most widely used kernel function in practice!
Proof: exercise sheet

Oftentimes the Gaussian RBF kernel is simply called ‘Gaussian kernel’ or ‘RBF’ kernel.

# Properties of Kernels

**Theorem**

1. If $k$ is a kernel and $c \in \mathbb{R}_+$, then $ck$ is a kernel.
2. If $k_1$ and $k_2$ are kernels, then $k_1 + k_2$ is a kernel.
3. If $k_1$ and $k_2$ are kernels, then $k_1 * k_2$ is a kernel.

Proof: is an exercise on the current exercise sheet.

# Kernel matrix

## Definition

Let $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d$ be the input data, and let $k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ be a kernel function. Then the matrix

$$K := \begin{pmatrix} k(\mathbf{x}_1, \mathbf{x}_1) & \ldots & k(\mathbf{x}_1, \mathbf{x}_n) \\ \vdots & & \vdots \\ k(\mathbf{x}_n, \mathbf{x}_1) & \ldots & k(\mathbf{x}_n, \mathbf{x}_n) \end{pmatrix} \in \mathbb{R}^{n \times n}$$

is called **kernel matrix**.

Equivalent characterization of kernels:

## Theorem

A function $k : \mathbb{R}^d \times \mathbb{R}^d \to \mathcal{H}$ is a kernel if and only if for any $n \in \mathbb{N}$ and any input points $\mathbf{x}_1, \ldots, \mathbf{x}_n$ the matrix $K$ is positive semi-definite (meaning $\forall \mathbf{v} \in \mathbb{R}^n : \mathbf{v}^\top K \mathbf{v} \geq 0$).

# Conclusion: Kernel Methods

Idea:

- Map the data into a high-dimensional space and use a simple linear separation there, corresponding to a non-linear classifier in the input space:

$$f(\mathbf{x}) = \text{sign}(\langle \mathbf{w}, \phi(\mathbf{x}) \rangle + b).$$

Kernel trick

- for the sake of efficiency, perform that mapping only implicitly via a kernel function

Kernelization of a learning machine

1. formulate learning machine such that it accesses the data only through inner products between data points
2. replace all occurrences of these inner products by kernel

Next week:

How to represent learning machines in terms of scalar products $\langle \mathbf{x}_i, \mathbf{x}_j \rangle$ & Example of kernelization of SVM.

# Appendix

Further Information
(non-mandatory class content)

# Full Story: More Precise Definition of Kernels. Sorry!!

Problem:

- In the definition of kernels, we used the notion of a kernel feature space $\mathcal{H}$, without defining it!

We said it should:

- cover the case $\mathcal{H} = \mathbb{R}^d$
- but allow also for infinite-dimensional spaces $\mathbb{R}^{\text{``}\infty\text{''}}$.

**Definition**

A **Hilbert space** $\mathcal{H}$ is a real vector space together with an inner product such that any Cauchy sequence converges in $\mathcal{H}$.

Remark:

- For ML purposes it suffices to think of a Hilbert space as a generalization of $\mathbb{R}^d$ to infinitely many dimensions

Examples of Hilbert spaces:

- $\mathcal{H} := \mathbb{R}^d$, for any $d \in \mathbb{N}$
- $\mathcal{H} := \left\{ \mathbf{x} = (x_1, x_2, x_3, \ldots) \in \mathbb{R}^{\text{``}\infty\text{''}} : \sum_{i=1}^{\infty} x_i < \infty \right\}$

# More Precise Definition of Kernels

**Definition**

A symmetric function $k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is called **kernel function** (or simply "**kernel**") if and only if there exists a map $\phi : \mathbb{R}^d \to \mathcal{H}$ into a Hilbert space $\mathcal{H}$ (called **kernel feature space**) such that

$$\forall \mathbf{x}, \tilde{\mathbf{x}} \in \mathbb{R}^d : \quad k(\mathbf{x}, \tilde{\mathbf{x}}) = \langle \phi(\mathbf{x}), \phi(\tilde{\mathbf{x}}) \rangle \ .$$

"k computes inner products in some Hilbert space"