TECHNISCHE UNIVERSITÄT KAISERSLAUTERN

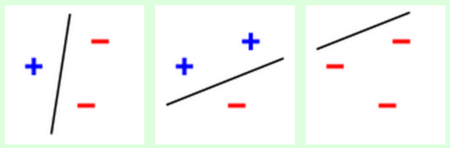
4.1 Kernel Methods

Machine Learning 1: Foundations

Marius Kloft *(TUK)*

Recap

In previous lectures: **Linear classification methods**



3 points shattered

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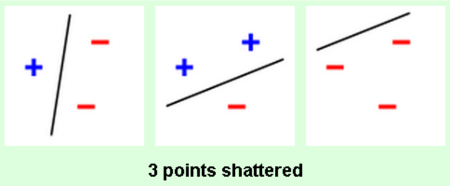
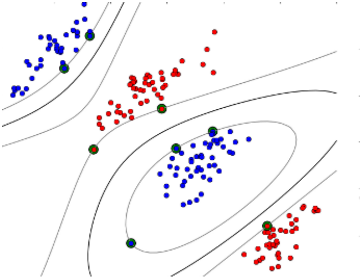
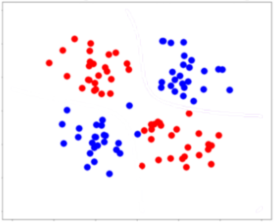


Will not work for non-linear data:



Limitations of Linear Classifiers

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



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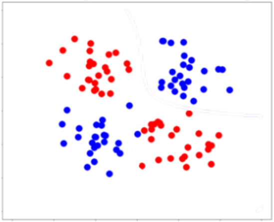

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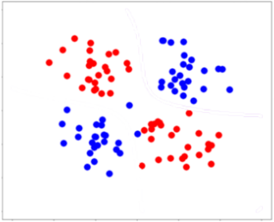

Non-linear algorithm we know so far: *k*-nearest neighbor algorithm

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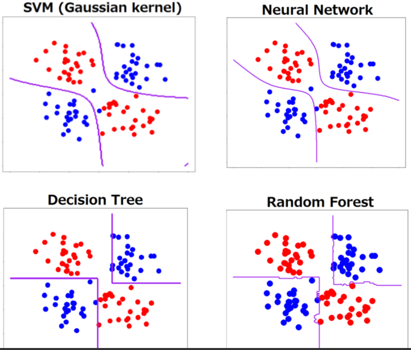
Other non-linear algorithms we will learn in this course:



Contents of this Class

Kernel Methods

Kernel methods is a paradigm to

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

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- convert linear learning machines (e.g., linear SVM)
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How does that work?

Core Idea

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

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

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

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

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

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Do all this very efficiently!

Example

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

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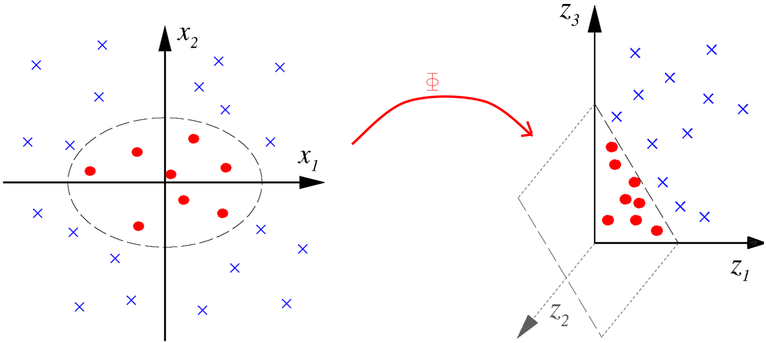

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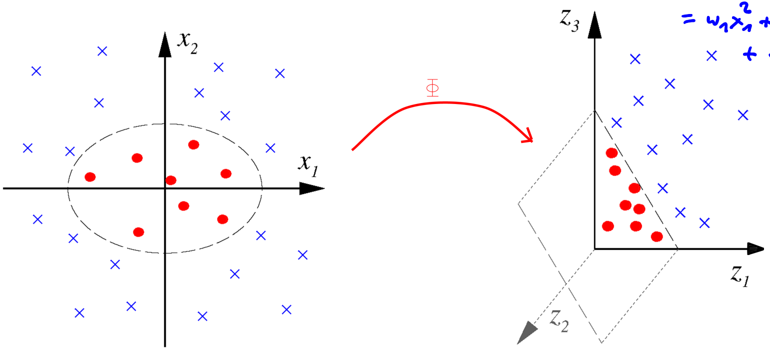
$f_w\begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix} = w_1 z_1 + w_2 z_2 + w_3 z_3$
$= w_1 x_1^2 + \sqrt{2} w_2 x_1 x_2 + w_3 x_2^2$



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

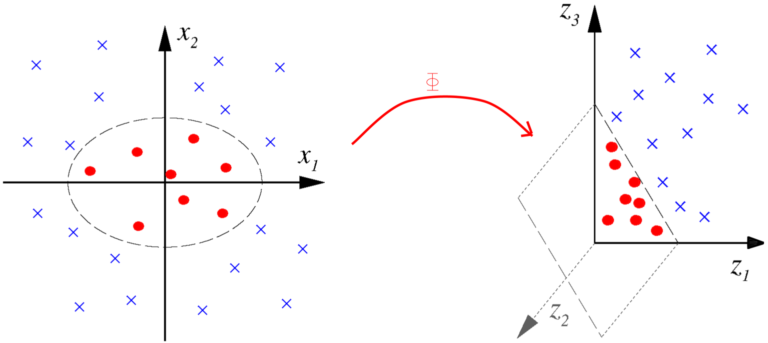
e.g. $w = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$, $b = -1$

$\Rightarrow f_w(x) = x_1^2 + x_2^2 - 1 \overset{!}{=} 0 \iff x_1^2 + x_2^2 = 1$

Example

Consider the map

$$\phi : \begin{array}{ccc} \overset{\mathbb{R}^d}{\mathbb{R}^2} & \rightarrow & \overset{\mathbb{R}^{\approx d^2}}{\mathbb{R}^3} \\ (x_1, x_2) & \mapsto & (x_1^2, \sqrt{2}x_1 x_2, x_2^2) \end{array}$$



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

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

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

$$
\begin{aligned}
\langle \phi(\mathbf{x}), \phi(\tilde{\mathbf{x}}) \rangle
&= \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) \rangle \\
&= x_1^2\tilde{x}_1^2 + 2x_1x_2\tilde{x}_1\tilde{x}_2 + x_2^2\tilde{x}_2^2 \\
&= (x_1\tilde{x}_1)^2 + 2(x_1\tilde{x}_1)(x_2\tilde{x}_2) + (x_2\tilde{x}_2)^2 \\
&= (x_1\tilde{x}_1 + x_2\tilde{x}_2)^2 \\
&= (\langle x, \tilde{x} \rangle)^2
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$k(\mathbf{x}, \tilde{\mathbf{x}}) := \langle \mathbf{x}, \tilde{\mathbf{x}} \rangle^2$ is an example of a **kernel**.

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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:

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

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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

To show: $k(x,\tilde{x}) := \langle x,\tilde{x}\rangle$ is a kernel,

① to show: k symmetric

to this end: $\forall x,\tilde{x}$: $k(x,\tilde{x}) = \langle x,\tilde{x}\rangle = \langle \tilde{x},x\rangle = k(\tilde{x},x)$ ✓

② to show: $\exists \phi : \mathbb{R}^d \to \mathbb{R}^D$: $\forall x,\tilde{x} \in \mathbb{R}^d$:

$$k(x,\tilde{x}) = \langle \phi(x),\phi(\tilde{x})\rangle$$

consider $\phi := id_{\mathbb{R}^d}$, $D := d$

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

$\square$

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.

e.g. $m = 2 \Rightarrow k(x, \tilde{x}) = (\langle x, \tilde{x} \rangle + c)^2$

quadratic 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:

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

Full proof: exercise sheet. $\square$

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Why the name 'polynomial kernel'?

Recall that in KM we use prediction functions

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

$$= \sum_{\substack{i \in \mathbb{N}^d: \\ \sum_j i_j \le m}} w_i \, x_1^{i_1} \cdots x_d^{i_d}$$

Example 3/3: Gaussian RBF Kernel

Definition

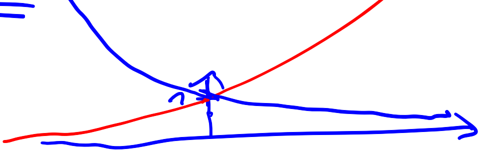
The **Gaussian RBF kernel** is defined as

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

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

Prop.: Gk is a kernel.

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

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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**.

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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:

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

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1. formulate learning machine such that it accesses the data only through inner products between data points
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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!!

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

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- but allow also for infinite-dimensional spaces $\mathbb{R}^{\text{“}\infty\text{”}}$.

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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 2/2

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"