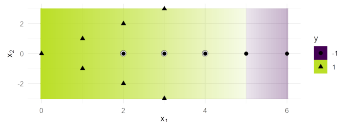
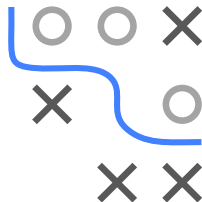


Introduction to Machine Learning

Nonlinear Support Vector Machines The Kernel Trick



Learning goals

- Know how to efficiently introduce non-linearity via the kernel trick
- Know common kernel functions (linear, polynomial, radial)
- Know how to compute predictions of the kernel SVM

DUAL SVM PROBLEM WITH FEATURE MAP

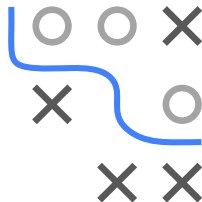
The dual (soft-margin) SVM is:

$$\begin{aligned} \max_{\alpha} \quad & \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y^{(i)} y^{(j)} \langle \phi(\mathbf{x}^{(i)}), \phi(\mathbf{x}^{(j)}) \rangle \\ \text{s.t.} \quad & 0 \leq \alpha_i \leq C, \\ & \sum_{i=1}^n \alpha_i y^{(i)} = 0, \end{aligned}$$

Here we replaced all features $\mathbf{x}^{(i)}$ with feature-generated, transformed versions $\phi(\mathbf{x}^{(i)})$.

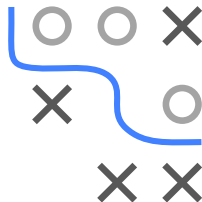
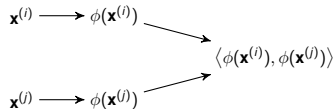
We see: The optimization problem only depends on **pair-wise inner products** of the inputs.

This now allows a trick to enable efficient solving.

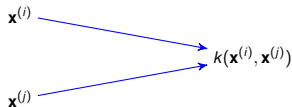


KERNEL = FEATURE MAP + INNER PRODUCT

Instead of first mapping the features to the higher-dimensional space and calculating the inner products afterwards,



it would be nice to have an efficient “shortcut” computation:



We will see: **Kernels** give us such a “shortcut”.

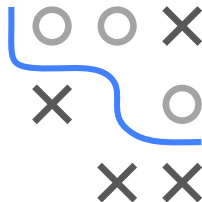
MERCER KERNEL

Definition: A (**Mercer**) **kernel** on a space \mathcal{X} is a continuous function

$$k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$$

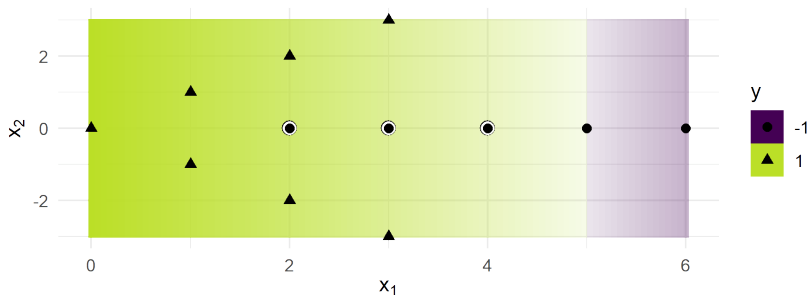
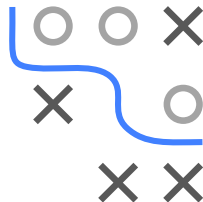
of two arguments with the properties

- Symmetry: $k(\mathbf{x}, \tilde{\mathbf{x}}) = k(\tilde{\mathbf{x}}, \mathbf{x})$ for all $\mathbf{x}, \tilde{\mathbf{x}} \in \mathcal{X}$.
- Positive definiteness: For each finite subset $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)}\}$ the **kernel Gram matrix** $\mathbf{K} \in \mathbb{R}^{n \times n}$ with entries $K_{ij} = k(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})$ is positive semi-definite.



CONSTANT AND LINEAR KERNEL

- Every constant function taking a non-negative value is a (very boring) kernel.
- An inner product is a kernel. We call the standard inner product $k(\mathbf{x}, \tilde{\mathbf{x}}) = \mathbf{x}^\top \tilde{\mathbf{x}}$ the **linear kernel**. This is simply our usual linear SVM as discussed.

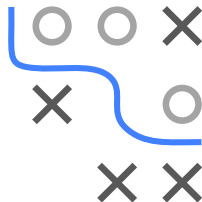


SUM AND PRODUCT KERNELS

A kernel can be constructed from other kernels k_1 and k_2 :

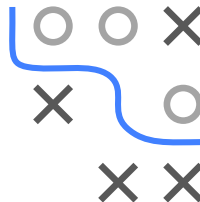
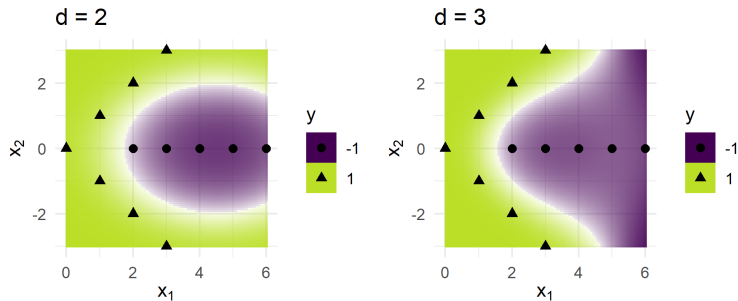
- For $\lambda \geq 0$, $\lambda \cdot k_1$ is a kernel.
- $k_1 + k_2$ is a kernel.
- $k_1 \cdot k_2$ is a kernel (thus also k_1^n).

The proofs remain as (simple) exercises.



POLYNOMIAL KERNEL

$$k(\mathbf{x}, \tilde{\mathbf{x}}) = (\mathbf{x}^\top \tilde{\mathbf{x}} + b)^d, \text{ for } b \geq 0, d \in \mathbb{N}$$



From the sum-product rules it directly follows that this is a kernel.

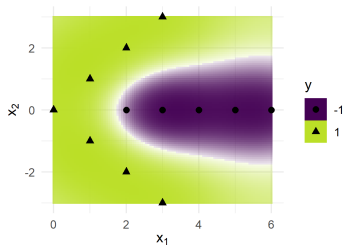
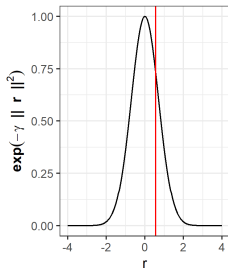
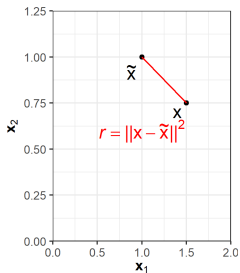
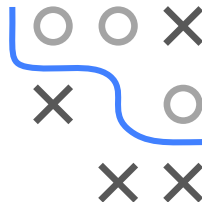
RBF KERNEL

The “radial” **Gaussian kernel** is defined as

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

or

$$k(\mathbf{x}, \tilde{\mathbf{x}}) = \exp(-\gamma\|\mathbf{x} - \tilde{\mathbf{x}}\|^2), \gamma > 0$$

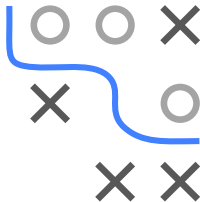


KERNEL SVM

We kernelize the dual (soft-margin) SVM problem by replacing all inner products $\langle \phi(\mathbf{x}^{(i)}), \phi(\mathbf{x}^{(j)}) \rangle$ by kernels $k(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})$

$$\begin{aligned} \max_{\alpha} \quad & \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y^{(i)} y^{(j)} \langle \phi(\mathbf{x}^{(i)}), \phi(\mathbf{x}^{(j)}) \rangle \\ \text{s.t.} \quad & 0 \leq \alpha_i \leq C, \\ & \sum_{i=1}^n \alpha_i y^{(i)} = 0. \end{aligned}$$

This problem is still convex because \mathbf{K} is psd!

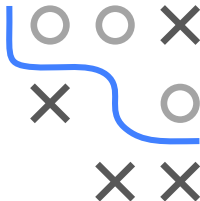


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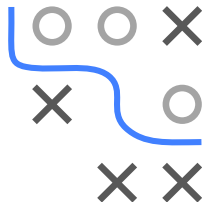
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In more compact matrix notation with \mathbf{K} denoting the kernel matrix:

$$\begin{aligned} \max_{\alpha \in \mathbb{R}^n} \quad & \mathbf{1}^\top \alpha - \frac{1}{2} \alpha^\top \text{diag}(\mathbf{y}) \mathbf{K} \text{diag}(\mathbf{y}) \alpha \\ \text{s.t.} \quad & \alpha^\top \mathbf{y} = 0, \\ & 0 \leq \alpha \leq C. \end{aligned}$$

This problem is still convex because \mathbf{K} is psd!



KERNEL SVM: PREDICTIONS

For the linear soft-margin SVM we had:

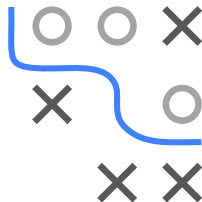
$$f(\mathbf{x}) = \hat{\theta}^T \mathbf{x} + \theta_0 \quad \text{and} \quad \hat{\theta} = \sum_{i=1}^n \alpha_i y^{(i)} \mathbf{x}^{(i)}$$

After the feature map this becomes:

$$f(\mathbf{x}) = \langle \hat{\theta}, \phi(\mathbf{x}) \rangle + \theta_0 \quad \text{and} \quad \hat{\theta} = \sum_{i=1}^n \alpha_i y^{(i)} \phi(\mathbf{x}^{(i)})$$

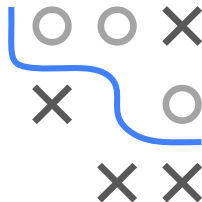
Assuming that the dot-product still follows its bi-linear rules in the mapped space and using the kernel trick again:

$$\begin{aligned} \langle \hat{\theta}, \phi(\mathbf{x}) \rangle &= \left\langle \sum_{i=1}^n \alpha_i y^{(i)} \phi(\mathbf{x}^{(i)}), \phi(\mathbf{x}) \right\rangle = \sum_{i=1}^n \alpha_i y^{(i)} \langle \phi(\mathbf{x}^{(i)}), \phi(\mathbf{x}) \rangle = \\ &= \sum_{i=1}^n \alpha_i y^{(i)} k(\mathbf{x}^{(i)}, \mathbf{x}), \quad \text{so:} \quad f(\mathbf{x}) = \sum_{i=1}^n \alpha_i y^{(i)} k(\mathbf{x}^{(i)}, \mathbf{x}) + \theta_0 \end{aligned}$$



MNIST EXAMPLE

- Through this kernelization we can now conveniently perform feature generation even for higher-dimensional data. Actually, this is how we computed all previous examples, too.
- We again consider MNIST with 28×28 bitmaps of gray values.
- A polynomial kernel extracts $\binom{d+p}{d} - 1$ features and for the RBF kernel the dimensionality would be infinite.
- We train SVMs again on 700 observations of the MNIST data set and use the rest of the data for testing; and use $C=1$.



0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3
 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4
 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5
 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6
 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7
 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8
 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9

	Error
linear	0.134
poly (d = 2)	0.119
RBF (gamma = 0.001)	0.12
RBF (gamma = 1)	0.184

