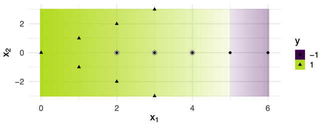
Introduction to Machine Learning

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:

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

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,

$$
\begin{tikzcd}
\mathbf{x}^{(i)} \arrow[r] & \phi(\mathbf{x}^{(i)}) \arrow[dr] & \\
 & & \left\langle \phi(\mathbf{x}^{(i)}), \phi(\mathbf{x}^{(j)}) \right\rangle \\
\mathbf{x}^{(j)} \arrow[r] & \phi(\mathbf{x}^{(j)}) \arrow[ur] &
\end{tikzcd}
$$

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

$$
\begin{tikzcd}
\mathbf{x}^{(i)} \arrow[dr] & \\
 & k(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) \\
\mathbf{x}^{(j)} \arrow[ur] &
\end{tikzcd}
$$

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

MERCER KERNEL

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

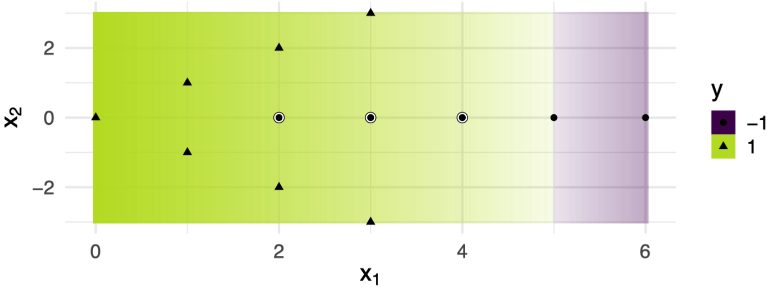
$$k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$$

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 $\left\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)}\right\}$ the **kernel Gram matrix $\boldsymbol{K} \in \mathbb{R}^{n \times n}$** 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

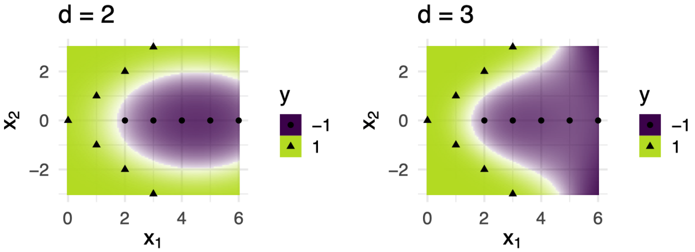
A kernel can be constructed from other kernels k_1 and k_2:

- 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.

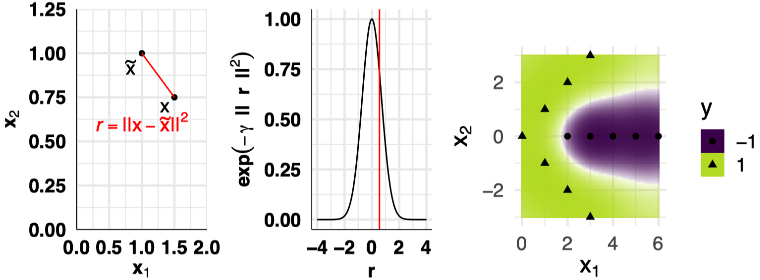
RBF KERNEL

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 $\left\langle \phi\left(\mathbf{x}^{(i)}\right), \phi\left(\mathbf{x}^{(j)}\right)\right\rangle$ 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)} \left\langle \phi\left(\mathbf{x}^{(i)}\right), \phi\left(\mathbf{x}^{(j)}\right)\right\rangle \\
\text{s.t.} \quad & 0 \leq \alpha_i \leq C, \\
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This problem is still convex because $\boldsymbol{K}$ is psd!

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\end{aligned}
$$

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

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

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

KERNEL SVM: PREDICTIONS

For the linear soft-margin SVM we had:

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

After the feature map this becomes:

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

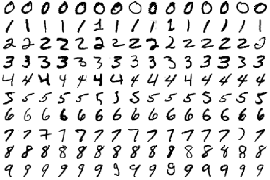
Assuming that the dot-product still follows its bi-linear rules in the mapped space and using the kernel trick again:

$$\left\langle \hat{\boldsymbol{\theta}}, \phi(\mathbf{x}) \right\rangle = \left\langle \sum_{i=1}^{n} \alpha_i y^{(i)} \phi(\mathbf{x}^{(i)}), \phi(\mathbf{x}) \right\rangle = \sum_{i=1}^{n} \alpha_i y^{(i)} \left\langle \phi(\mathbf{x}^{(i)}), \phi(\mathbf{x}) \right\rangle =$$

$$= \sum_{i=1}^{n} \alpha_i y^{(i)} k(\mathbf{x}^{(i)}, \mathbf{x}), \qquad \text{so:} \qquad f(\mathbf{x}) = \sum_{i=1}^{n} \alpha_i y^{(i)} k(\mathbf{x}^{(i)}, \mathbf{x}) + \theta_0$$

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.



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

FINAL COMMENTS

- The kernel trick allows us to make linear machines non-linear in a very efficient manner.
- Linear separation in high-dimensional spaces is **very flexible**.
- Learning takes place in the feature space, while predictions are computed in the input space.
- Both the polynomial and Gaussian kernels can be computed in linear time. Computing inner products of features is **much faster** than computing the features themselves.
- What if a good feature map ϕ is already available? Then this feature map canonically induces a kernel by defining $k(\mathbf{x}, \tilde{\mathbf{x}}) = \langle \phi(\mathbf{x}), \phi(\tilde{\mathbf{x}}) \rangle$. There is no problem with an explicit feature representation as long as it is efficiently computable.