Kernel Learning And Its Application In Nonlinear Support Vector Machines

Anastasia S., Sven N., Joshua S.

Otto-Friedrich-University Bamberg

anastasia.sinitsyna@stud.uni-bamberg.de
sven-jason-waldemar.nekula@stud.uni-bamberg.de
joshua-guenter.simon@stud.uni-bamberg.de

June 9, 2021

Overview

Linearly separable data classes

First, let's consider a given data set $\mathcal{X}$ of labeled points (inputs) with individual labels $y_i \in \{-1, 1\}$, e.g. $(x_1, y_1), ..., (x_m, y_m) \in \mathcal{X} \times \{-1, 1\}$.

Our goal is to implement a classification method, which is able to classify new and unlabeld data points with the right or "best" label.
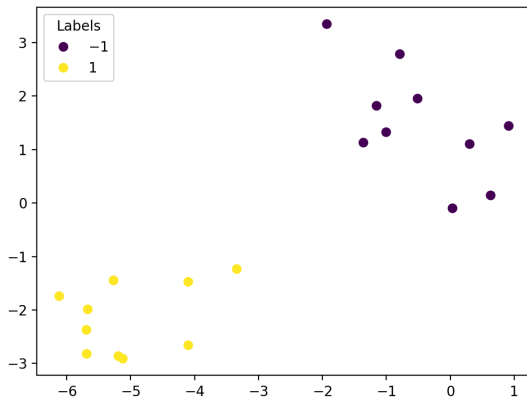
Linearly separable data classes

Figure: An example for linearly separable data.

Linearly separable data classes

In machine learning, a well established classification method are the so called **Support Vector Machines** (SVM). Developed by Vladimir Vapnik and his coworkers in the 1990s, SVMs are still a relevent topic and an even more powerful tool for **classification** and **regression**.

Similarity

To perform a classification, a similarity measure is needed. Finding a suitable measure is a core problem of machine learning. For now let's consider

$$k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$$
$$(x, x') \mapsto k(x, x') \tag{1}$$

where k is a function that, given two patterns x and x', returns a real number characterizing their similarity. This function k is called a **kernel**. Unless stated otherwise, $k(x, x') = k(x', x)$.

Dot product and vector norm

A simple type of similarity measure is a **dot product**. Given two vectors $x, x' \in \mathbb{R}^n$ the canonical dot product is defined as

$$\langle x, x' \rangle = (x')^T x = \sum_{i=1}^{n} [x_i][x']_i, \tag{2}$$

where $[x]_i$ denotes the ith entry of x. Futhermore this allows a calculation of the **norm** (length) of a single vector x as

$$\|x\| = \sqrt{\langle x, x \rangle}. \tag{3}$$

Dot product and vector norm

Given a vector space $\mathcal{V}$ (mostly over $\mathbb{R}$ or $\mathbb{C}$) and a dot product, one can define a so called **dot product space** or **Pre-Hilbert space** $\mathcal{H}$, where every pair of elements $x, x' \in \mathcal{V}$ is assigned to a scalar value, the dot product of x and x' [Bronstein, 2020].

More properties of vector spaces, dot products and norms can be found in [Liesen, 2015].

Hyperplane classifiers

The underlying learning algorithm of SVMs yields to find a hyperplane in some dot product space $\mathcal{H}$, which separates the data. A hyperplane of the form

$$\langle w, x \rangle + b = 0 \qquad (4)$$

where $w \in \mathcal{H}, b \in \mathbb{R}$ shall be considered [Schölkopf, 2002](p. 11). Futhermore decision functions

$$f(x) = sgn\left(\langle w, x \rangle + b\right) \qquad (5)$$

can be assigned.

The **optimal hyperplane** can be calculated by finding the normal vector that leads to the largest margin. Thus we need to solve the optimization problem

$$\min_{w \in \mathcal{H}, b \in \mathbb{R}} \quad \tau(w) = \frac{1}{2}\|w\|^2$$
$$\text{subject to} \quad y_i \left(\langle w, x \rangle + b\right) \geq 1 \ \forall i = 1, \ldots, m. \tag{6}$$

The constraints in (6) ensure that $f(x_i)$ will be $+1$ for $y_i = +1$ and -1 for $y_i = -1$. The ≥ 1 on the right hand side of the constraints effectively fixes the scaling of w. This leads to the maximum margin hyperplane. A detailed explanation can be found in [Schölkopf, 2002](Chap 7).

The constrained optimization problem in (6) can be re-written using the method of Lagrange multipliers. This leads to the Lagrangian

$$L(w, b, \alpha) = \frac{1}{2}\|w\|^2 - \sum_{i=1}^{m} \alpha_i \left(y_i \left(\langle w, x \rangle + b \right) - 1 \right) \tag{7}$$

subject to $\alpha_i \geq 0 \ \forall i = 1, \ldots, m$. Here, α_i are the Lagrange multipliers. The Lagrangian L has to be minimized with respect to the primal variables w and b and maximized with respect to the dual variables α_i (in other words, a saddle point has to be found).

The Karush-Kuhn-Tucker (KKT) complementarity conditions of optimization theory state, that at the saddle point, the derivatives of L with respect to the primal variables must vanish, since

$$\frac{\partial}{\partial b} L(w, b, \alpha) = 0 \text{ and } \frac{\partial}{\partial w} L(w, b, \alpha) = 0 \tag{8}$$

leads to

$$\sum_{i=1}^{m} \alpha_i y_i = 0 \text{ and } w = \sum_{i=1}^{m} \alpha_i y_i x_i. \tag{9}$$

The solution vector w thus has an expansion in terms of a subset of the training patterns, namely those patterns with non-zero α_i, called Support Vectors (SVs).

We can again re-write our optimization problem by substituting (9) into the Lagrangian (7) to eliminate the primal variables. This yields the dual optimization problem, which is usually solved in practice

$$\max_{\alpha \in \mathbb{R}^m} \quad W(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle \tag{10}$$

$$\text{subject to} \quad \alpha_i \geq 0 \ \forall i = 1, \ldots, m \text{ and } \sum_{i=1}^{m} \alpha_i y_i = 0.$$

Finally, the decision function can be re-written using (9) as

$$f(x) = sgn\left(\sum_{i=1}^{m} \alpha_i y_i \langle x, x_i \rangle + b\right), \tag{11}$$

where b can be computed by exploiting $\alpha_i \left[y_i \left(\langle x_i, w \rangle + b \right) - 1 \right] = 0$, which follows from the KKT conditions.

Details on mathematical optimization and convex constrained problems can be found in [Jarre, 2019]. Explanations on dealing with nonlinear problems are given in [Reinhardt, 2012].

Maximum margin separator

We now have all the theoretical background to go back to our inital classification problem. We can implement a SVM as a maximum margin separator for the given data set $\mathcal{X}$.

Maximum margin separator

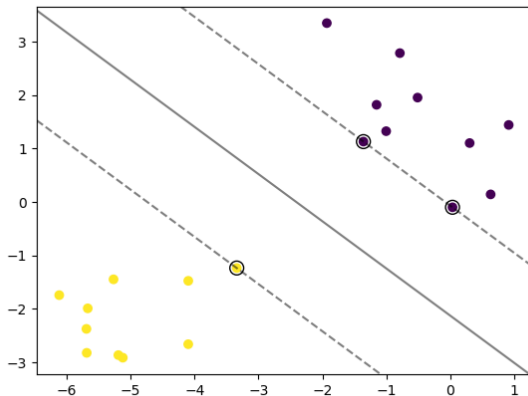Figure: Implementation of a SVM using the 'linear' Kernel.

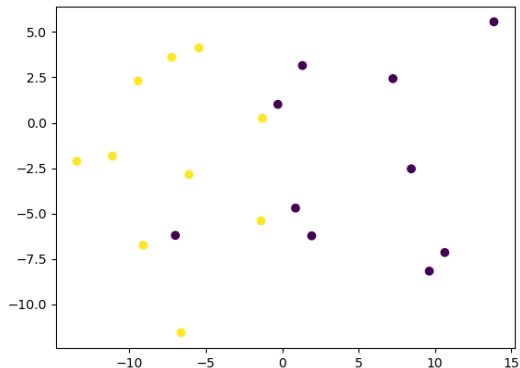# Limitations

Let's consider the following data set.

Figure: Linearly separable or not?

Soft Margin Hyperplanes

We introduce a slack variable

$$\xi_i \geq 0 \ \forall i = 1, \ldots, m \quad (12)$$

in the simplest case, this leads to

$$\min_{w \in \mathcal{H}, \xi \in \mathbb{R}^n} \quad \tau(w, \xi) = \frac{1}{2}\|w\|^2 + \frac{C}{m} \sum_{i=1}^{m} \xi_i$$

$$\text{subject to} \quad y_i \left(\langle w, x \rangle + b \right) \geq 1 - \xi_i \ \forall i = 1, \ldots, m. \quad (13)$$

By making ξ_i large enough, the constraint can always be met, which is why we penalize them in the objective function with $\frac{C}{m}$, where $C \in \mathbb{R}$ is a regularization parameter.

Soft Margin Hyperplanes

Our dual optimization problem also gets re-written as

$$\max_{\alpha \in \mathbb{R}^m} \quad W(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle$$

$$\text{subject to} \quad 0 \leq \alpha_i \leq \frac{C}{m} \ \forall i = 1, \ldots, m \text{ and } \sum_{i=1}^{m} \alpha_i y_i = 0. \tag{14}$$

This classifier is referred to as C-SV classifier and can be used to prevent overfitting by allowing the classifier to make false classifications.
More classifiers using soft margins can be found in
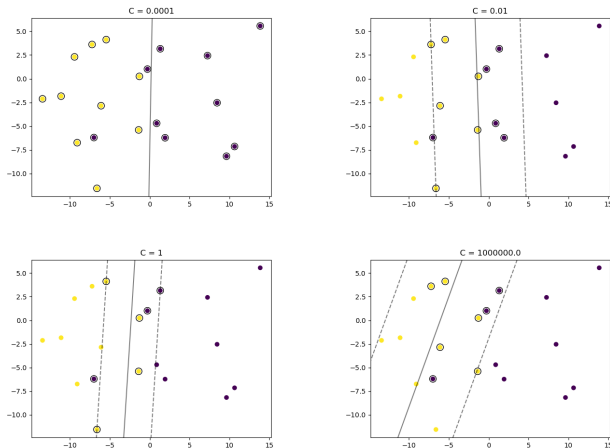[Schölkopf, 2002](Chap. 7.5).

Soft Margin Hyperplanes

Figure: Implementation of a SVM using the 'linear' kernel with different soft margins.

Limitations
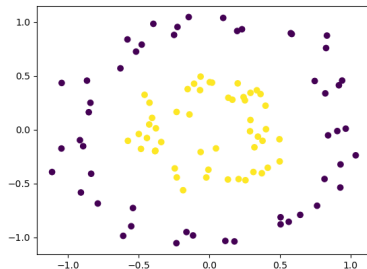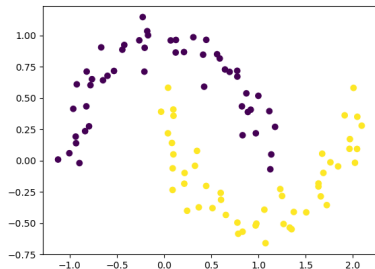
Let's consider the following data sets.

Figure: Two examples of data that can't be linearly separated.

Limitations

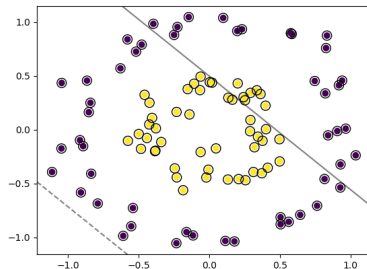What happens if you try to seperate them linearly?
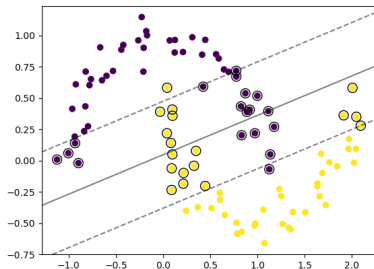

Figure: SVMs using the 'linear' Kernel.

The kernel trick

To extend the introduced SVM algorithm, we can substitute (11) by applying a kernel of the form

$$k(x, x') = \langle \Phi(x), \Phi(x') \rangle \tag{15}$$

where

$$
\begin{aligned}
\Phi : \mathcal{X} &\to \mathcal{H} \\
(x) &\mapsto \Phi(x)
\end{aligned} \tag{16}
$$

is a function that maps an input from $\mathcal{X}$ into a dot product space $\mathcal{H}$. This is referred to as the **kernel trick**.

The kernel trick

We then obtain decision functions of the form

$$f(x) = sgn\left(\sum_{i=1}^{m} \alpha_i y_i \langle \Phi(x), \Phi(x_i) \rangle + b\right) \quad (17)$$

$$= sgn\left(\sum_{i=1}^{m} \alpha_i y_i k(x, x_i) + b\right) \quad (18)$$

and the optimization problem

$$\max_{\alpha \in \mathbb{R}^m} \quad W(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j k(x, x_i)$$

$$\text{subject to} \quad \alpha_i \geq 0 \; \forall i = 1, \ldots, m \text{ and } \sum_{i=1}^{m} \alpha_i y_i = 0. \quad (19)$$

The kernel trick

The $m \times m$ Matrix K with elements $K_{ij} = k(x_i, x_j)$ is called the **Gram matrix** (or kernel matrix) of k.

A kernel k is called **positive definite kernel**, when the Gram matrix K is positive definite.

As stated in [Schölkopf, 2002](Chap. 2): *Given an algorithm which is formulated in terms of a positive definite kernel k, one can construct an alternative algorithm by replacing k by another positive definite kernel $\tilde{k}$.*

The kernel trick

The kernel trick can be applied since all feature vectors only occurred in dot products. A more precise explanation can be found in [Schölkopf, 2002](Chap. 2).

A suitable kernel

Going back to our problem of non linearly separable data, we can use a kernel function of the form

$$k(x, x') = \exp\left(-\frac{\|x - x'\|^2}{2\sigma^2}\right), \tag{20}$$

a so called **Gaussian radial basis function** (GRBF or RBF kernels) with $\sigma > 0$.

Solving the nonlinear problem

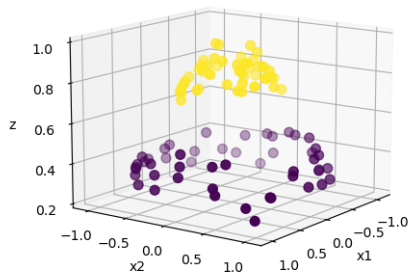Figure: Data points mapped into a 3-dimensional space using the 'rbf' kernel.
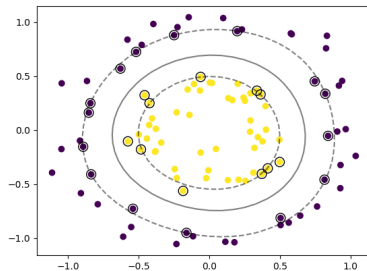
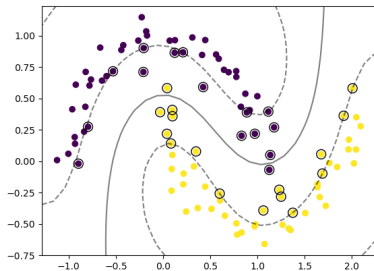# Solving the nonlinear problem

Figure: SVMs using the 'rbf' Kernel.

Examples of kernels

An overview of common kernels:

- **Linear**: $k(x, x') = \langle x, x' \rangle$
- **Polynomial**: $k(x, x') = \langle x, x' \rangle^d, d \in \mathbb{N}$
- **Inhomogeneous Polynomial**: $k(x, x') = (\langle x, x' \rangle + c)^d, d \in \mathbb{N}, c \geq 0$
- **Gaussian**: $k(x, x') = \exp\left(-\frac{\|x - x'\|^2}{2\sigma^2}\right), \sigma > 0$
- **Sigmoid**: $k(x, x') = \tanh(\kappa \langle x, x' \rangle + \vartheta), \kappa > 0, \vartheta < 0$

These kernels are implemented in the Python modul scikit-learn
sklearn.svm based on the libsvm implementation in C++ by Chih-Chung
Chang and Chih-Jen Lin [Chang, 2011].

More kernel applications

Some interessting kernel applications:

- Image recognition/classification (with SVMs) for example in
  - Handwriting recognition
  - Tumor detection
- Computer vision and computer graphics, 3D reconstruction
- Kernel principal component analysis

References

📄 Schölkopf, Bernhard, Alexander J. Smola
Learning with Kernels: Support Vector Machines, Regularization, Optimization, and Beyond. MIT press, 2002.

📄 Liesen, Jörg, Volker Mehrmann
Lineare Algebra. Wiesbaden, Germany: Springer, 2015.

📄 Jarre, Florian, Josef Stoer
Optimierung: Einführung in mathematische Theorie und Methoden. Springer-Verlag, 2019.

📄 Reinhardt, Rüdiger, Armin Hoffmann, Tobias Gerlach
Nichtlineare Optimierung: Theorie, Numerik und Experimente. Springer-Verlag, 2012.

📄 Bronstein, Ilja N., et al.
Taschenbuch der Mathematik. 11. Auflage, Springer-Verlag, 2020.

📄 Chang, Chih-Chung, Chih-Jen Lin
LIBSVM : A library for support vector machines. ACM Transactions on Intelligent Systems and Technology, 2:27:1–27:27, 2011. Software available at https://www.csie.ntu.edu.tw/~cjlin/libsvm.

Time for your questions!

Follow our development on GitHub
https://github.com/JoshuaSimon/Kernel-Learning