

Kernel Learning And Its Application In Nonlinear Support Vector Machines

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1 Introduction

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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. $(x_1, y_1), \dots, (x_m, y_m) \in \mathcal{X} \times \{-1, 1\}$.

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

Linearly separable data classes

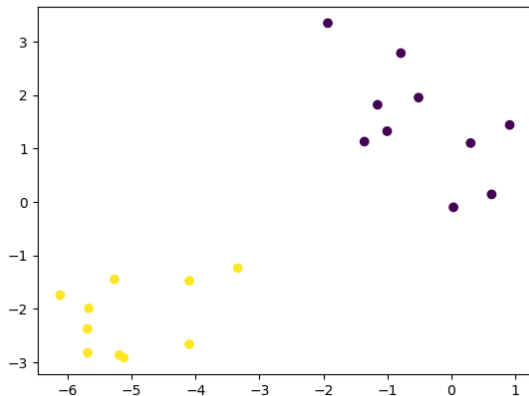


Figure: An example for linearly separable data.

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 relevant topic and an even more powerful tool for **classification** and **regression**.

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

$$\begin{aligned} k : \mathcal{X} \times \mathcal{X} &\rightarrow \mathbb{R} \\ (x, x') &\mapsto k(x, x') \end{aligned} \tag{1}$$

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

$$\langle x, x' \rangle = \sum_{i=1}^n x_i x'_i. \quad (2)$$

Futhermore this allows a calculation of the **norm** (length) of a single vector x as

$$\|x\| = \sqrt{\langle x, x \rangle}. \quad (3)$$

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

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

where $w \in \mathcal{H}$, $b \in \mathbb{R}$ shall be considered [p.11 Kernel Learning Book].
Furthermore decision functions

$$f(x) = \text{sgn}(\langle w, x \rangle + b) \quad (5)$$

can be assigned.

Hyperplane classifiers - A constrained optimization problem

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

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

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 [Chap 7, Kernel Learning Book].

Hyperplane classifiers - Lagrangian

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

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

subject to $\alpha_i \geq 0 \ \forall i = 1, \dots, m$. 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).

Hyperplane classifiers - KKT conditions

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

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

leads to

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

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).

Hyperplane classifiers - Dual optimization problem

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

$$\begin{aligned} \max_{\alpha \in \mathbb{R}^m} \quad & W(\alpha) = \sum_{i=1}^m \alpha_i - \frac{1}{2} \sum_{i,j=1}^m \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle \\ \text{subject to} \quad & \alpha_i \geq 0 \quad \forall i = 1, \dots, m \text{ and } \sum_{i=1}^m \alpha_i y_i = 0. \end{aligned} \tag{10}$$

Hyperplane classifiers - Dual optimization problem

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

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

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

Maximum margin separator

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

Maximum margin separator

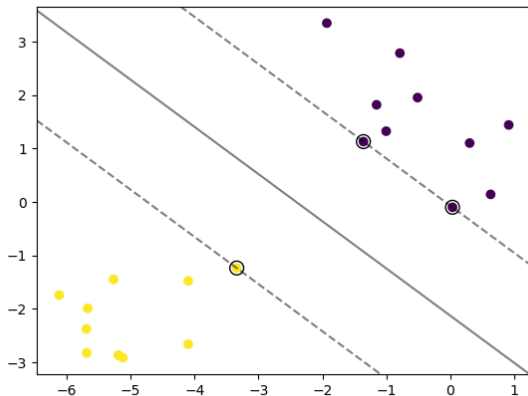


Figure: Implementation of a SVM with linearly separable data.

Limitations

Let's consider the following data set.

- Plot of nonlinear separable data -

Paragraphs of Text

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Heading

- 1 Statement
- 2 Explanation
- 3 Example

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Table

Treatments	Response 1	Response 2
Treatment 1	0.0003262	0.562
Treatment 2	0.0015681	0.910
Treatment 3	0.0009271	0.296

Table: Table caption

Theorem

Theorem (Mass–energy equivalence)

$$E = mc^2$$

Example (Theorem Slide Code)

```
\begin{frame}  
\frametitle{Theorem}  
\begin{theorem}[Mass--energy equivalence]  
$E = mc^2$  
\end{theorem}  
\end{frame}
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Figure

Uncomment the code on this slide to include your own image from the same directory as the template .TeX file.

An example of the `\cite` command to cite within the presentation:

This statement requires citation [Smith, 2012].



John Smith (2012)

Title of the publication

Journal Name 12(3), 45 – 678.

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