Kernel Learning And Its Application In Nonlinear Support Vector Machines

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Overview

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

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

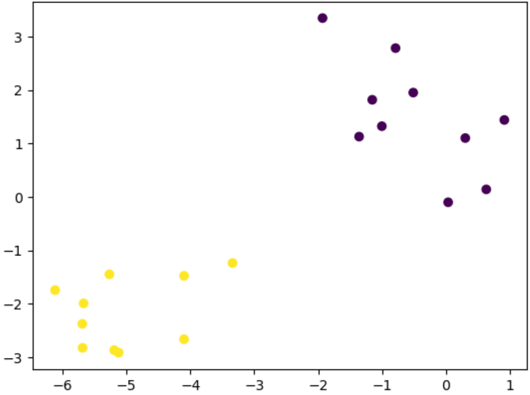

Figure: An example for linearly separable data.

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 powerfull tool for **classification** and **regression**.

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

$$\langle w, x \rangle + b = 0 \tag{1}$$

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

$$f(x) = sgn\left(\langle w, x \rangle + b\right) \tag{2}$$

can be used as similarity measures for unlabeld data.

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

$$\begin{aligned} \min_{w \in \mathcal{H}, b \in \mathbb{R}} \quad & \tau(w) = \frac{1}{2}\|w\|^2 \\ \text{subject to} \quad & y_i\left(\langle w, x \rangle + b\right) \geq 1 \; \forall i = 1, \ldots, m. \end{aligned} \tag{3}$$

The constraints in (3) 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 (3) can be re-written using the method of Lagrange multipliers. This leads to the Lagrangian

$$L(w, b, \alpha) = \frac{1}{2}\|w\|^2 - \sum_{i=1}^{m} \alpha_i \left(y_i \left(\langle w, x \rangle + b \right) - 1 \right) \tag{4}$$

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).

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

$$\frac{\partial}{\partial b} L(w, b, \alpha) = 0 \text{ and } \frac{\partial}{\partial w} L(w, b, \alpha) = 0 \tag{5}$$

leads to

$$\sum_{i=1}^{m} \alpha_i y_i = 0 \text{ and } w = \sum_{i=1}^{m} \alpha_i y_i x_i. \tag{6}$$

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 (6) into the Lagrangian (4) to eliminate the primal variables. This yields the dual optimization problem, which is usually solved in practice

$$
\begin{aligned}
\max_{\alpha \in \mathbb{R}^m} \quad & W(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle \\
\text{subject to} \quad & \alpha_i \geq 0 \ \forall i = 1, \ldots, m \text{ and } \sum_{i=1}^{m} \alpha_i y_i = 0.
\end{aligned}
\tag{7}
$$

Hyperplane classifiers - Dual optimization problem

Finally, the decision function can be re-written using (6) as

$$f(x) = sgn\left(\sum_{i=1}^{m} \alpha_i y_i \langle x, x_i \rangle + b\right), \tag{8}$$

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.

Maximum margin separator

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

Maximum margin separator

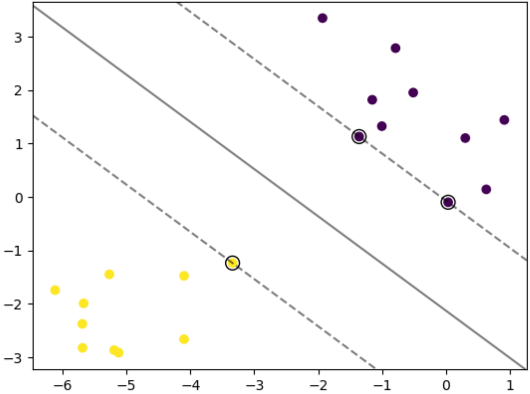

Figure: Implementation of a SVM with linearly separable data.

Limitations

Let's consider the following data set.

- Plot of nonlinear separable data -

Paragraphs of Text

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Bullet Points

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- Aliquam blandit faucibus nisi, sit amet dapibus enim tempus eu
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Multiple Columns

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)

$E = mc^2$

Verbatim

Example (Theorem Slide Code)

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

Figure

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

Citation

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

This statement requires citation [Smith, 2012].

References

John Smith (2012)
Title of the publication
Journal Name 12(3), 45 – 678.

The End