Support Vector Machines (SVM)

Jérémie Gince

Département de physique Université de Sherbrooke

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Context

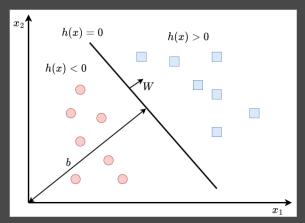


Figure: Two classes being separate by a line with the parameters W and b and the estimator $h(\cdot)$.



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Hinge Loss

The hinge loss used to maximize the margins of a binary classifier is the following:

$$E_{\mathsf{hinge}}(\theta|\mathcal{D}) = \sum_{\{x^t, y^t\} \in \mathcal{D}} \mathsf{max} \big(0, \ 1 - y^t h(x^t|\theta) \big) + E_{\mathsf{regularization}}(\theta). \tag{1}$$

- lacksquare if $y^t=1$ and $h^t>0 o \mathsf{good}$ classification with $E\in [0,1)$
- \blacksquare if $y^t=1$ and $h^t<0$ \to bad classification with E>0
- lacksquare if $y^t=-1$ and $h^t<0 o$ good classification with $E\in[0,1)$
- \blacksquare if $y^t = -1$ and $h^t > 0 \rightarrow$ bad classification with E > 0

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Estimator

The linear separator is defined by the decision function

$$h^{t}(x^{t}|W,b) = \sum_{j=1}^{M} W_{j}x_{j}^{t} + b$$
 (2)

$$\hat{y}^t = \phi(h^t(x^t|W, b)) \tag{3}$$

with a training dataset $\mathcal{D} = \left\{ x^t, y^t \right\}$ where

- lacksquare x_j^t is j-th entry of the input t of size M;
- W_j is the j-th weight from the vector W of size M;
- b is the bias as a scalar;
- $\phi(\cdot)$ is the activation function which is often sign (\cdot) in a binary classifier;
- ullet y^t is the target class t;
- \hat{y}^t is the predicted class t.



Changing the decision space

It's possible that the data $\mathcal D$ are not linearly separable in the initial space $\mathcal S_0$ but they are in another space $\mathcal S_1$. Then we can use a transformation $\psi:\mathbb R^M\mapsto\mathbb R^N.$

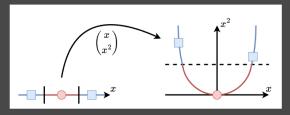


Figure: Two classes not separable in initial space but are separable after the transformation $\psi(x) = \begin{pmatrix} x & x^2 \end{pmatrix}^T$.

■ The linear separator will be

$$h(x) = W^T \psi(x) + b.$$

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SVM

In a SVM, the parameters \boldsymbol{W} of the separator are

$$W = \sum_{t} \alpha^{t} y^{t} \psi(x^{t}) \tag{5}$$

with $\alpha^t \geq 0$, a parameter associated with x^t . This lead to

$$h(x) = \sum_{t} \alpha^t y^t (\psi(x^t))^T \psi(x) + b.$$
 (6)



The Kernel

The kernel function is defined as

$$K(x,y) = (\psi(x))^T \psi(y). \tag{7}$$

Using the kernel definition, the SVM decision function is

$$h(x) = \sum_{t} \alpha^t y^t K(x^t, x) + b. \tag{8}$$

The computing of $\psi(\cdot)$ is now hidden in the new kernel function, so this $\psi(\cdot)$ can be "unknown" from the SVM decision function.



Considering that some α^t are null, we can write the prediction function as

$$h(x) = \sum_{s} \alpha^{s} y^{s} K(x^{s}, x) + b, \tag{9}$$

$$\hat{y} = \phi(h(x)) \tag{10}$$

where

■ the index s are associated with the non-zero α^t . The x^s are what we called, the support vectors.



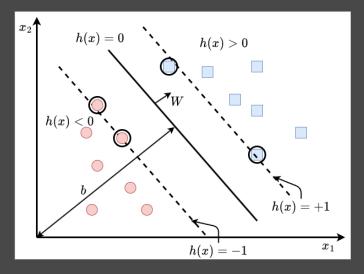


Figure: Binary classification. The dots lines represent the margins of the classifier and the circled data are the support vectors.



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Finding the parameters

To Learn the parameters α^t and b of the SVM classifier, we can do a gradient descent in L iterations. The updates are

$$\ \ \ \Delta\alpha^t = -\eta \frac{\partial E(\alpha,b|\mathcal{D})}{\partial\alpha^t}$$
 ,

with the user-defined error function $E(\cdot)$ and the learning rate η . The update of the parameters will be

$$\alpha_{\kappa} = \begin{cases} 0 & \text{if } \alpha_{\kappa-1} + \Delta \alpha^t < 0\\ \alpha_{\kappa-1} + \Delta \alpha^t & \text{else,} \end{cases}$$
 (11)

$$b_{\kappa} = b_{\kappa-1} + \Delta b, \quad \forall \kappa \in \{1, \dots, L\}.$$
 (12)



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Hinge Loss

The following hinge loss is generally used for SVM:

$$E_{\mathsf{hinge}}(\alpha, b | \mathcal{D}) = \sum_{\{x^t, y^t\} \in \mathcal{D}} \mathsf{max} \left(0, \ 1 - y^t h(x^t | \alpha, b) \right) + \lambda \frac{1}{2} \sum_{\alpha^s \in \alpha} (\alpha^s)^2, \tag{13}$$

where λ is the regularization coefficient and generally $\lambda \in [0, 1]$.



Advantages/Disadvantages

Advantages:

- Effective in high dimensional spaces.
- Still effective in cases where number of dimensions is greater than the number of samples.
- Uses a subset of training points in the decision function (called support vectors), so it is also memory efficient.
- Versatile: user-defined Kernel for the decision function.

Disadvantages:

- If the number of features is much greater than the number of samples, avoid over-fitting in choosing Kernel functions and regularization term is crucial.
- SVMs do not directly provide probability estimates.

Advantages and disadvantages taken from scikit-learn.

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Code

- Repository: https://github.com/JeremieGince/Learning_SVM
- Google Colab: Learning_SVM.google.colab



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Support vector machines (SVM)

SVM is a special type of linear separator with following goals:

Maximize the distance between the separating hyperplane and the training data:

$$d_{h^t,x^t} = \frac{\left| W^T x^t + b \right|}{\|W\|} = \frac{y^t (W^T x^t + b)}{\|W\|} \tag{14}$$

 \blacksquare Find the weights W and b in order to have

$$d_{h^t, x^t} \ge \rho, \ \forall t \tag{15}$$

where ρ is the margin.

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Lagrange multipliers

In order to achieve those goals, we have to use the Lagrange multipliers.

- It's a method used to optimize a function f(x) under a constraint g(x) written in a way that g(x) = 0,
- with the Lagrangian

$$\mathcal{L}(x,\alpha) = f(x) + \alpha g(x). \tag{16}$$

■ The stationary points of the Lagrangian and the optimal solution of f(x) is then found with

$$\nabla \mathcal{L}(x,\alpha) = 0. \tag{17}$$



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Lagrangian multipliers - Example

Suppose we want to maximize the function $f(q_i) = q_1 + q_2$ with the constraint $q_1^2 + q_2^2 = 1$. The constraint will then be noted as

$$g(q_i) = q_1^2 + q_2^2 - 1 = 0, (18)$$

and the Lagrangian as

$$\mathcal{L}(q_i, \alpha) = f(q_i) + \alpha g(q_i) \tag{19}$$

$$\implies \mathcal{L}(q_i, \alpha) = q_1 + q_2 + \alpha (q_1^2 + q_2^2 - 1).$$
 (20)



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The gradient of the Lagrangian will be

$$\nabla \mathcal{L}(q_i, \alpha) = \left[\frac{\partial \mathcal{L}(q_i)}{\partial q_1}, \quad \frac{\partial \mathcal{L}(q_i)}{\partial q_1}, \quad \frac{\partial \mathcal{L}(q_i)}{\partial \alpha} \right], \tag{21}$$

$$= [1 + 2\alpha q_1, \quad 1 + 2\alpha q_2, \quad q_1^2 + q_2^2 - 1], \tag{22}$$

$$= \begin{bmatrix} 1 + 2\alpha q_1 = 0, \\ 1 + 2\alpha q_2 = 0, \\ q_1^2 + q_2^2 - 1 = 0 \end{bmatrix}, \tag{23}$$

$$q_1 = q_2 = -\frac{1}{2\alpha},\tag{24}$$

$$\implies \alpha^{(1)} = +\frac{1}{\sqrt{2}}, \ \alpha^{(2)} = -\frac{1}{\sqrt{2}}.$$
 (25)

Since $f(-\frac{1}{2\alpha^{(1)}},-\frac{1}{2\alpha^{(1)}})=-\sqrt{2}$ and $f(-\frac{1}{2\alpha^{(2)}},-\frac{1}{2\alpha^{(2)}})=\sqrt{2}$, the Lagrange multiplier that maximize our function $f(q_i)$ is $\alpha^{(2)}$.

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Lagrange multipliers with inequality

If the constraint is $g(x) \ge 0$, the conditions for optimality will be

- $g(x) \ge 0$;
- $\alpha \geq 0$;
- $\alpha q(x) = 0.$

Then to minimize f(x) with $g(x) \ge 0$, we have to optimize the Lagrangian

$$\mathcal{L}(x,\alpha) = f(x) - \alpha g(x) \tag{26}$$

with $\alpha > 0$.



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SVM

The problem:

- Minimize $\frac{1}{2}||W||^2$
- with the constraint $y^t(W^Tx^t + b) \ge 1 \ \forall t$

Re-writing using the Lagrangian multiplier:

$$\mathcal{L}_{p} = \frac{1}{2} \|W\|^{2} - \sum_{t} \alpha^{t} \left[y^{t} (W^{T} x^{t} + b) - 1 \right]$$

$$\frac{1}{2} \|W\|^{2} - \sum_{t} t t (W^{T} t + b) + \sum_{t} t$$

$$\frac{1}{2} \|W\|^{2} - \sum_{t} t t (W^{T} t + b) + \sum_{t} t$$

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$$\frac{1}{2} \|W\|^{2} - \sum_{t} t t (W^{T} t + b) + \sum_{t} t ($$

$$= \frac{1}{2} \|W\|^2 - \sum_{t} \alpha^t y^t (W^T x^t + b) + \sum_{t} \alpha^t$$
 (28)

with \mathcal{L}_p , the primal form of the Lagrangian.



Simplification - dual form

Since we want to find an stationary point of \mathcal{L}_p :

$$\frac{\partial \mathcal{L}_p}{\partial W} = 0 = W - \sum_t \alpha^t y^t x^t, \tag{29}$$

$$\implies W = \sum_{t} \alpha^{t} y^{t} x^{t}, \tag{30}$$

and

$$\frac{\partial \mathcal{L}_p}{\partial b} = 0 = \sum_{t} \alpha^t y^t. \tag{31}$$



The dual form can be written as

$$\mathcal{L}_{d} = \frac{1}{2} (W^{T} W) - W^{T} \underbrace{\sum_{t} \alpha^{t} y^{t} x^{t}}_{\text{VI}} - b \underbrace{\sum_{t} \alpha^{t} y^{t}}_{\text{O}} + \sum_{t} \alpha^{t}$$
(32)

$$= -\frac{1}{2} (W^T W) + \sum_{t} \alpha^t \tag{33}$$

$$\implies \mathcal{L}_d = -\frac{1}{2} \sum_{t} \sum_{s} \alpha^t \alpha^s y^t y^s (x^t)^T x^s + \sum_{t} \alpha^t$$
 (34)

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Dual form

Re-writing the problem using the dual form.

- Maximize $-\frac{1}{2}\sum_t\sum_s\alpha^t\alpha^sy^ty^s(x^t)^Tx^s + \sum_t\alpha^t$
- With the constraints $\sum_t \alpha^t y^t = 0$ and $\alpha^t \ge 0 \ \forall t$
- \rightarrow In practice, a majority of α^t will be zero;
- \rightarrow The data x^t with $\alpha^t > 0$ are called the support vectors.



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Changing the decision space

It's possible that the data \mathcal{D} are not linearly separable in the initial space S_0 but are in another space S_1 . Then we can use a transformation $\psi: \mathbb{R}^M \mapsto \mathbb{R}^N$ that $x \mapsto \psi(x)$.

The linear separator will be

$$h(x) = W^T \psi(x) + b \tag{35}$$

In the dual form:

$$W = \sum_{t} \alpha^t y^t \psi(x^t) \tag{36}$$

$$h(x) = \sum_{t} W^{T} \psi(x) + b = \sum_{t} \alpha^{t} y^{t} (\psi(x^{t}))^{T} \psi(x) + b$$
 (37)



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The Kernel

The kernel function is defined as

$$K(x,y) = (\psi(x))^T \psi(y). \tag{38}$$

Using the kernel definition, the SVM decision function is

$$h(x) = \sum_{t} \alpha^t y^t K(x^t, x) + b. \tag{39}$$

The computing of $\psi(\cdot)$ is now hidden in the new kernel function, so this $\psi(\cdot)$ can be "unknown" from the SVM decision function.



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The resulting prediction function of the SVM:

$$h(x) = \sum_{x^s} \alpha^s y^s K(x^s, x) + b, \tag{40}$$

$$\hat{y} = \phi(h(x)). \tag{41}$$

Reminder: x^s is the support vector s associated with the non-zero Lagrangian multiplier α^s .



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The End



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