Support Vector Machine
(SVM)

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Context

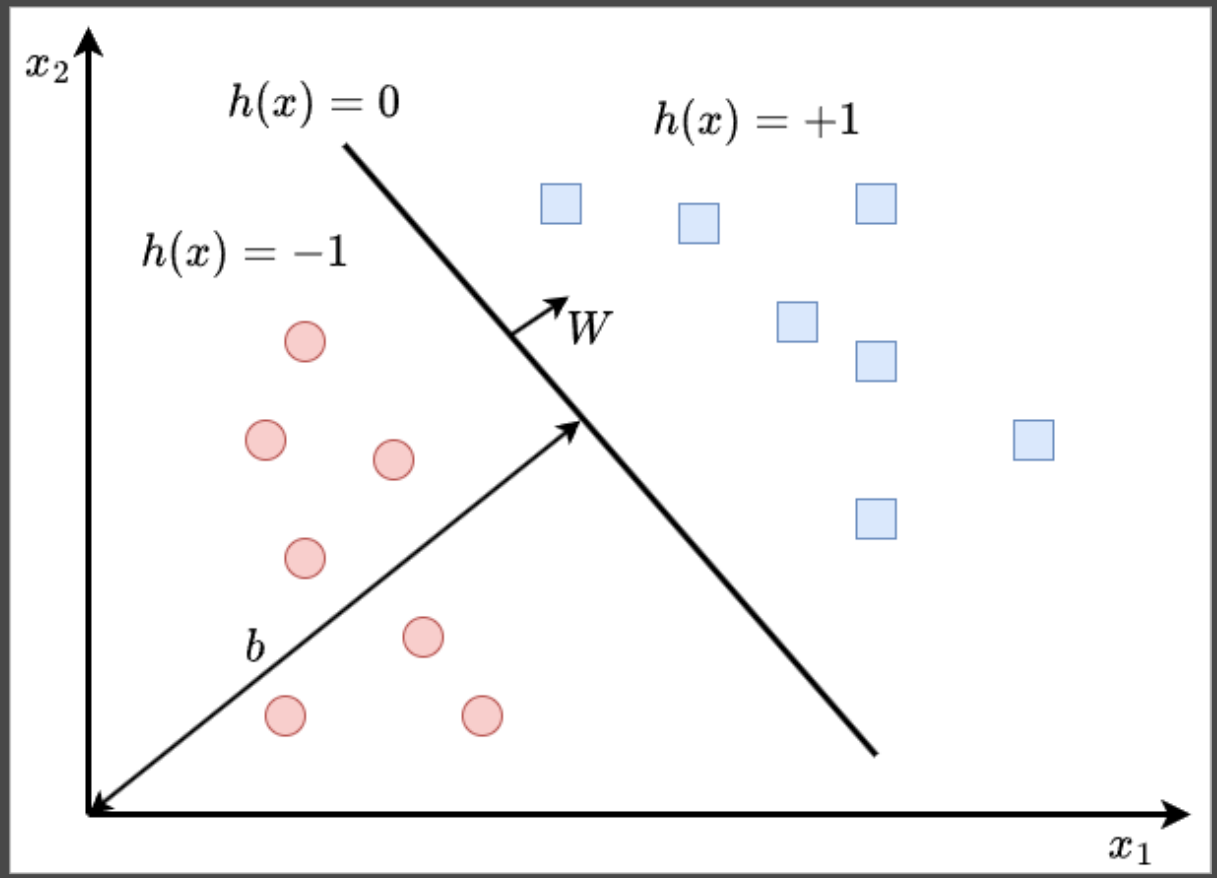

Figure: Two classes being separate by a line with the parameters W and b and the estimator $h(\cdot)$.

Hinge Loss

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

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

- if $y^t = 1$ and $h^t > 0 \rightarrow$ good classification with $E \in [0, 1)$
- if $y^t = 1$ and $h^t < 0 \rightarrow$ bad classification with $E > 0$
- if $y^t = -1$ and $h^t < 0 \rightarrow$ good classification with $E \in [0, 1)$
- if $y^t = -1$ and $h^t > 0 \rightarrow$ bad classification with $E > 0$

Estimator

The linear separator is defined by the decision function

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

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

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

- 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;
- 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 $\psi : \mathbb{R}^M \mapsto \mathbb{R}^N$.

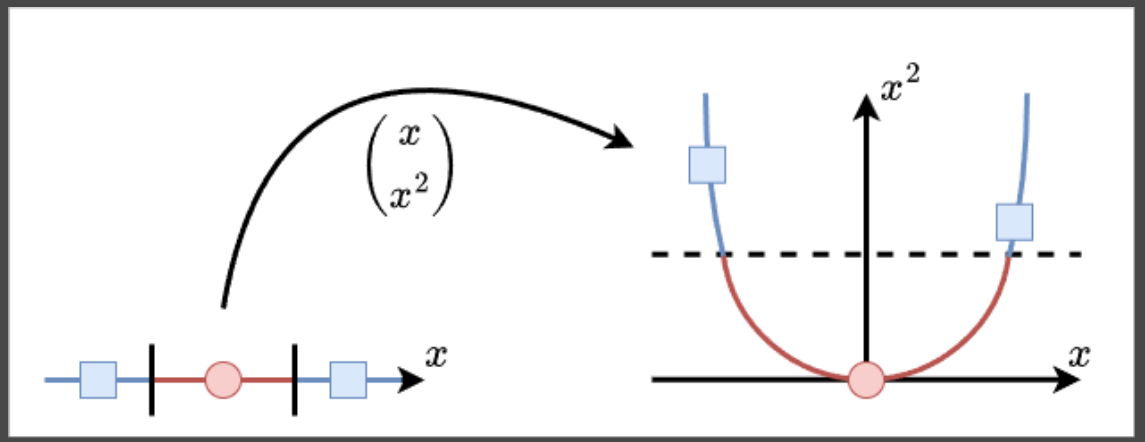

Figure: Two classes not separable in initial space but are separable after the transformation $\psi(x) = \begin{pmatrix} x & x^2 \end{pmatrix}^T$.

- The linear separator will be

$$h(x) = W^T \psi(x) + b. \tag{4}$$

SVM

In a SVM, the parameters W of the separator are

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

with α^t, a parameter associated with x^t. This lead to

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

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.

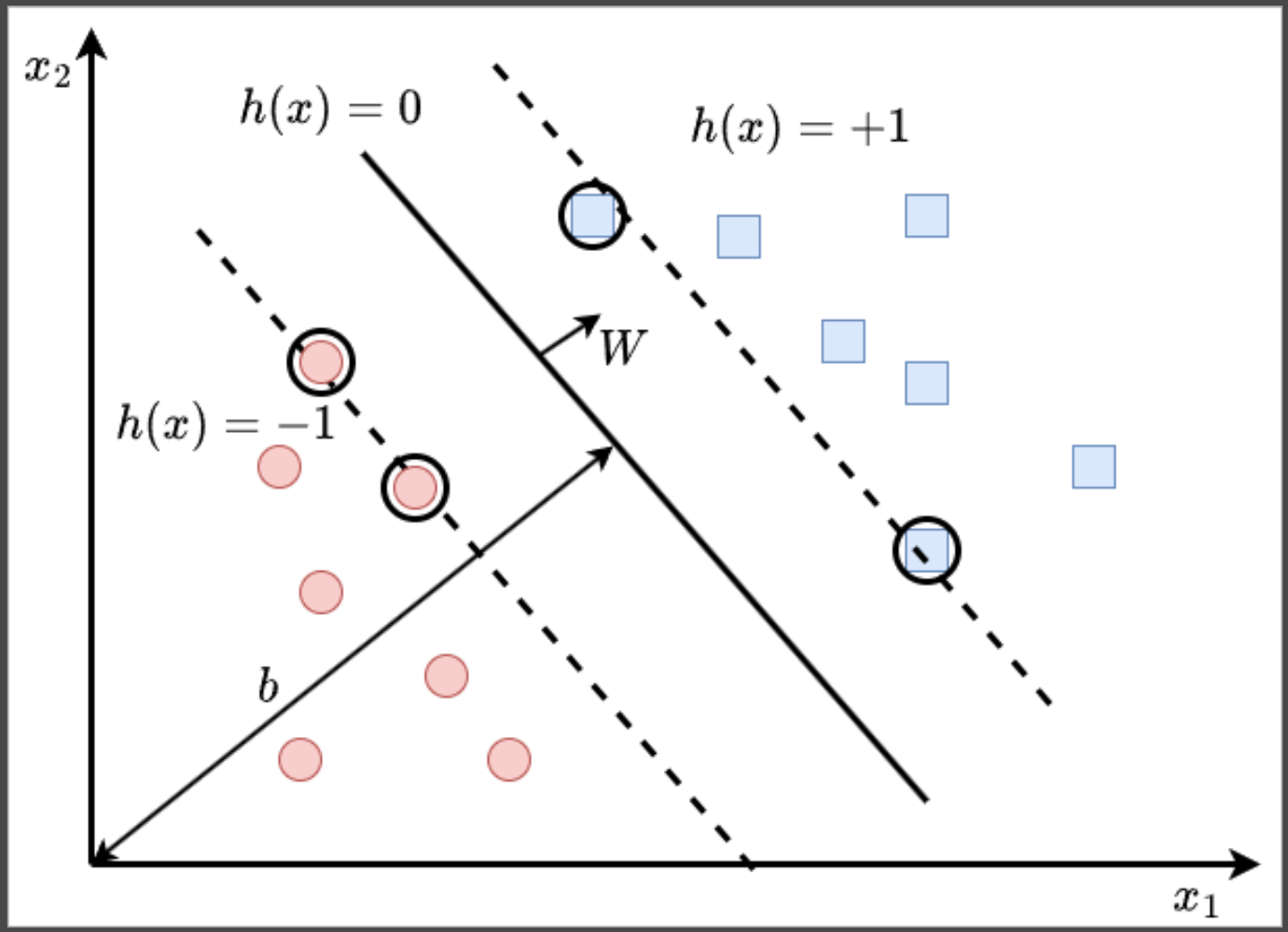

Figure: Binary classification. The dots lines represent the margins of the classifier and the circled data are the support vectors.

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

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

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

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

$$b_\kappa = b_{\kappa-1} + \Delta b, \quad \forall \kappa \in \{1, \ldots, L\}. \tag{12}$$

Hinge Loss

The hinge loss is generally used for SVM.

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

Code

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

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:

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

- Find the weights W and b in order to have

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

where ρ is the margin.

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

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

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

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

and the Lagrangian as

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

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

The gradient of the Lagrangian will be

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

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

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

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

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

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 $\alpha^{(2)}$.

Lagrange multipliers with inequality

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

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

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

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

with $\alpha \geq 0$.

SVM

The problem:

- Minimize $\frac{1}{2}\|W\|^2$
- with the constraint $y^t\left(W^T x^t + b\right) \geq 1 \; \forall t$

Re-writing using the Lagrangian multiplier:

$$\mathcal{L}_p = \frac{1}{2}\|W\|^2 - \sum_t \alpha^t \left[y^t\left(W^T x^t + b\right) - 1\right] \tag{27}$$

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

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

$$\mathcal{L}_d = \frac{1}{2}(W^T W) - W^T \underbrace{\sum_t \alpha^t y^t x^t}_{W} - b \underbrace{\sum_t \alpha^t y^t}_{0} + \sum_t \alpha^t \tag{32}$$

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

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

Dual form

Re-writing the problem using the dual form.

- Maximize $-\frac{1}{2}\sum_t \sum_s \alpha^t \alpha^s y^t y^s \left(x^t\right)^T x^s + \sum_t \alpha^t$
- With the constraints $\sum_t \alpha^t y^t = 0$ and $\alpha^t \geq 0 \; \forall t$

$\rightarrow$ In practice, a majority of α^t will be zero;

$\rightarrow$ The data x^t with $\alpha^t > 0$ are called the support vectors.

Changing the decision space

It's possible that the data $\mathcal{D}$ are not linearly separable in the initial space $\mathcal{S}_0$ but are in another space $\mathcal{S}_1$. 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:

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

$$h(x) = \sum_t W^T \psi(x) + b = \sum_t \alpha^t y^t \left(\psi(x^t)\right)^T \psi(x) + b \tag{37}$$

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.

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.

The End

Questions

1. Why do we want to use SVM and not deep neural networks?
2. Why don't we show the quantum advantage with auto-encoders?
3. What are the specific objectives of the project?
4. Do we have a specific dataset in mind?