Lecture VI: Support Vector Machines

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Linear SVM’s
The margin and the expected classification error
Maximum Margin Linear classifiers
Linear classifiers for non-linearly separable data

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The “kernel trick”
Kernels
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Extensions
$L_1$ SVM
Multi-class and One class SVM
SV Regression

Reading HTF Ch.: Ch. 12.1–3, Murphy Ch.: Ch 14 (14.1,14.2–14.2.4 kernels, 14.4 and equations (14.28,14.29) kernel trick, 14.5.1.–3 Support Vector Machines), Bach Ch.: 7.1–7.4, 7.7
Additional Reading: C. Burges - “A tutorial on SVM for pattern recognition”
These notes: Appendices (convex optimization) are optional.
A VC bound

\[ L_{01}(\theta) \leq \hat{L}_{01}(\theta) + \sqrt{\frac{h[1 + \log(2n/h)] + \log(4/\delta)}{n}} R(h) \]  \quad \text{w.p.} > 1 - \delta  \tag{1}

with \( h = \text{VCdim} \mathcal{F} \) and \( \delta < 1 \) the confidence.

A linear classifier is denoted as \( f(x; w, b) = w^T x + b \), where \( x \) takes label equal to \( \text{sgn}(f(x; w, b)) \). The margin of \( f \) on data point \( x^i \) is as usual equal to \( y^i f(x^i; w, b) \).
The margin and the expected classification error

The following two theorems suggest that large margin is a predictor of good generalization error.

**Theorem** Let $\mathcal{F}_\rho$ be the class of hyperplanes $f(x) = w^T x$, $x, w \in \mathbb{R}^n$, that are $\rho$ away from any data point\(^1\) in the training set $\mathcal{D}$. Then,

$$\text{VCdim } \mathcal{F}_\rho \leq 1 + \min \left( d, \frac{R_D^2}{\rho^2} \right) \quad (2)$$

where $R_D$ is the radius of the smallest ball that encloses the dataset.

**Theorem** Let $\mathcal{F} = \{\text{sgn} (w^T x), ||w|| \leq \Lambda, ||x|| \leq R\}$ and let $\rho > 0$ be any “margin”. Then for any $f \in \mathcal{F}$, w.p $1 - \delta$ over training sets

$$L_{01}(f) \leq \hat{L}_\rho + \sqrt{\frac{c}{n} \left( \frac{R^2\Lambda^2}{\rho^2} \ln n^2 + \ln \frac{1}{\delta} \right)} \quad (3)$$

where $c$ is a universal constant and $\hat{L}_\rho$ is the fraction of the training examples for which

$$y^i w^T x_i < \rho \quad (4)$$

A data point $i$ that satisfies (4) for some $\rho$ is called a margin error. For $\rho = 0$ the margin error rate $\hat{L}_\rho$ is equal to $\hat{L}_{01}$. Note that $\rho$ has a different meaning in the two Theorems above.

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\(^1\)In other words, a set $\mathcal{D}$ is shattered only if all the linear classifiers pass at least $\rho$ away from its points.
Maximum Margin Linear classifiers

Support Vector Machines appeared from the convergence of Three Good Ideas

**Assume** (for the moment) that the data are linearly separable.

- Then, there are an infinity of linear classifiers that have $\hat{L}_{01} = 0$. Which one to choose?

**First idea** Select the classifier that has maximum margin $\rho$ on the training set.

By SRM, we should choose the $(w, b)$ parameters that minimize $\hat{L}(w, b) + R(h_{w,b})$, where $h_{w,b}$ is given by (2):

- For any parameters $(w, b)$ that perfectly classify the data $\hat{L}(w, b) = 0$.
- Among these, the best $(w, b)$ is the one that minimizes $R(h_{w,b})$
- $R(h)$ increases with $h$, and $h_{w,b}$ decreases when $\rho$ increases
- Hence, by SRM we should choose

$$\argmax_{\rho, w, b:\hat{L}(w, b) = 0} \rho, \quad \text{s.t. } d(x, H_{w,b}) \geq \rho \text{ for } i = 1 : n,$$

where $d()$ denotes the Euclidean distance and $H_{w,b} = \{ x | w^T x + b = 0 \}$ is the decision boundary of the linear classifier.

- Because $d(x, H_{w,b}) = \frac{|w^T x + b|}{||w||}$ (proof in a few slides) (5) becomes

$$\argmax_{\rho, w, b:\hat{L}(w, b) = 0} \rho, \quad \text{s.t. } \frac{|w^T x^i + b|}{||w||} \geq \rho \text{ for } i = 1 : n,$$

(6)
Maximum Margin Linear classifiers

We continue to transform (6)

- If all data correctly classified, then \( y^i(w^T x^i + b) = |w^T x^i + b| \). Therefore (6) has the same solution as

\[
\arg\max_{\rho, w, b} \rho, \quad \text{s.t.} \quad \frac{y^i(w^T x^i + b)}{||w||} \geq \rho \text{ for } i = 1 : n, \tag{7}
\]

- Note now that the problem (7) is underdetermined. Setting \( w \leftarrow Cw, b \leftarrow Cb \) with \( C > 0 \) does not change anything.
- We add a cleverly chosen constraint to remove the indeterminacy; this is \( ||w|| = 1/\rho \), which allows us to eliminate the variable \( \rho \). We get

\[
\arg\max_{w, b} \frac{1}{||w||}, \quad \text{s.t.} \quad y^i(w^T x^i + b) \geq 1 \text{ for } i = 1 : n, \tag{8}
\]

Note: the successive problems (5),(6),(7),… are equivalent in the sense that their optimal solution is the same.
Alternative derivation of (8)

First idea
Select the classifier that has maximum margin on the training set, by the alternative definition of margin.

Formally, define $\min_{i=1:n} y^i f(x^i)$ be the margin of classifier $f$ on $\mathcal{D}$. Let $f(x) = w^T x + b$, and choose $w, b$ that

$$\max_{w \in \mathbb{R}^n, b \in \mathbb{R}} \min_{i=1:n} y^i (w^T x^i + b)$$

Remarks

- (if data is linearly separable), there exist classifiers with margins $> 0$
- one can arbitrarily increase the margin of such a classifier by multiplying $w$ and $b$ by a positive constant.
- Hence, we need to “normalize” the set of candidate classifiers by requiring instead

$$\max_{w, b} \min_{i=1:n} d(x, H_{w,b}), \text{ s.t. } y^i (w^T x^i + b) \geq 1 \text{ for } i = 1 : n,$$

(9)

where $d()$ denotes the Euclidean distance and $H_{w,b} = \{ x \mid w^T x + b = 0 \}$ is the decision boundary of the linear classifier.
- Under the conditions of (9), because there are points for which $|w^T x + b| = 1$, maximizing $d(x, H_{w,b})$ over $w, b$ for such a point is the same as

$$\max_{w, b} \frac{1}{||w||}, \text{ s.t. } \min_{i} y_i (w^T x + b) = 1$$

(10)
The **Second idea** is to formulate (8) as a **quadratic** optimization problem.

\[
\min_{w,b} \frac{1}{2} ||w||^2 \quad \text{s.t.} \quad y^i(w^T x^i + b) \geq 1 \quad \text{for all } i = 1 : n
\]  

(11)

This is the **Linear SVM (primal) optimization problem**

- This problem has a strongly convex **objective** \( ||w||^2 \), and **constraints** \( y^i(w^T x^i + b) \) linear in \((w, b)\).
- Hence this is a convex problem, and can be studied with the tools of convex optimization.
The distance of a point $x$ to a hyperplane $H_{w,b}$

$$d(x, H_{w,b}) = \frac{|w^T x + b|}{||w||}$$

(12)

Intuition: denote

$$\tilde{w} = \frac{w}{||w||}, \tilde{b} = \frac{b}{||w||}, x' = \tilde{w}^T x.$$ 

(13)

Obviously $H_{w,b} = H_{\tilde{w},\tilde{b}}$, and $x'$ is the length of the projection of point $x$ on the direction of $w$. The distance is measured along the normal through $x$ to $H$; note that if $x' = -\tilde{b}$ then $x \in H_{w,b}$ and $d(x, H_{w,b}) = 0$; in general, the distance along this line will be $|x' - (-\tilde{b})|$. 
Optimization with Lagrange multipliers

2 The **Lagrangean** of (11) is

\[ L(w, b, \alpha) = \frac{1}{2}||w||^2 - \sum \alpha_i[y_i(w^T x_i + b) - 1]. \]  

(14)

**[KKT conditions]**

At the optimum of (11)

\[ w = \sum \alpha_i y_i x_i \quad \text{with} \quad \alpha_i \geq 0 \]  

(15)

and \( b = y_i - w^T x_i \) for any \( i \) with \( \alpha_i > 0 \).

- **Support vector** is a data point \( x^i \) such that \( \alpha_i > 0 \).
- According to (15), the final decision boundary is determined by the support vectors (i.e. does not depend explicitly on any data point that is not a support vector).

\[ ^2 \text{The derivations of these results are in the Appendix} \]
Dual SVM optimization problem

- Any convex optimization problem has a **dual** problem. In SVM, it is both illuminating and practical to solve the dual problem.
- The dual to problem (11) is

\[
\max_{\alpha_{1:n}} \sum_i \alpha_i - \frac{1}{2} \sum_i \alpha_i \alpha_j y^i y^j x^i \mathbf{T} x_j \quad \text{s.t} \quad \alpha_i \geq 0 \text{ for all } i \text{ and } \sum_i \alpha_i y^i = 0. \tag{16}
\]

- This is a **quadratic** problem with \( n \) variables on a convex domain.
- Dual problem in matrix form
  - Denote \( \alpha = [\alpha_i]_{i=1:n}, y = [y^i]_{i=1:n}, G_{ij} = x^i \mathbf{T} x_j, \bar{G}_{ij} = y^i y^j x^i \mathbf{T} x_j, \)
  - \( G = [G_{ij}] \in \mathbb{R}^{n \times n}, \bar{G} = [\bar{G}_{ij}] \in \mathbb{R}^{n \times n} \).

\[
\max_{\alpha \in \mathbb{R}^n} 1^T \alpha - \frac{1}{2} \alpha^T \bar{G} \alpha \quad \text{s.t} \quad \alpha \succeq 0 \text{ and } y^T \alpha = 0. \tag{17}
\]

- \( g(\alpha) = 1^T \alpha - \frac{1}{2} \alpha^T \bar{G} \alpha \) is the **dual objective function**
- \( G \) is called the **Gram matrix** of the data. Note that \( \bar{G} = \text{diag} y^{1:n^T} G \text{diag} y^{1:n} \).

- At the dual optimum
  - \( \alpha_i > 0 \) for constraints that are satisfied with equality, i.e. **tight**
  - \( \alpha_i = 0 \) for the **slack** constraints
Non-linearly separable problems and their duals

The **C-SVM**

\[
\begin{align*}
\text{minimize}_{w,b,\xi} & \quad \frac{1}{2}||w||^2 + C \sum_i \xi_i \\
\text{s.t.} & \quad y_i(w^T x_i + b) \geq 1 - \xi_i \\
& \quad \xi_i \geq 0
\end{align*}
\] (18)

In the above, \(\xi_i\) are the **slack variables**. Dual\(^3\):

\[
\begin{align*}
\text{maximize}_\alpha & \quad \sum_i \alpha_i - \frac{1}{2} \sum_i \sum_j \alpha_i \alpha_j y_i y_j x_i^T x_j \\
\text{s.t.} & \quad C \geq \alpha_i \geq 0 \text{ for all } i \\
& \quad \sum_i \alpha_i y_i = 0
\end{align*}
\] (19)

\(\Rightarrow\) two types of SV

- \(\alpha_i < C\) data point \(x^i\) is “on the margin” \(\Leftrightarrow\) \(y_i(w^T x_i + b) = 1\) (original SV)
- \(\alpha_i = C\) data point \(x^i\) cannot be classified with margin 1 (**margin error**) \(\Leftrightarrow\) \(y_i(w^T x_i + b) < 1\)

---

\(^3\)Lagrangian \(L(w, b, \xi, \alpha, \mu) = \frac{1}{2}||w||^2 + C \sum_i \xi_i - \sum_i \alpha_i[y_i(w^T x_i + b) - 1 + \xi_i] - \sum_i \mu_i \xi_i\) with \(\alpha_i \geq 0, \xi_i \geq 0, \mu_i \geq 0\)
The $\nu$-SVM

$$\text{minimize}_{w, b, \xi, \rho} \quad \frac{1}{2}||w||^2 - \nu \rho + \frac{1}{n} \sum_i \xi_i \quad (20)$$

s.t. \quad y^i(w^T x^i + b) \geq \rho - \xi_i \quad (21)

\quad \xi_i \geq 0 \quad (22)

\quad \rho \geq 0 \quad (23)

where $\nu \in [0, 1]$ is a parameter.

Dual$^4$:

$$\text{maximize}_\alpha \quad -\frac{1}{2} \sum_i \alpha_i \alpha_j y^i y^j x^i T x^j \quad (24)$$

s.t. \quad \frac{1}{n} \geq \alpha_i \geq 0 \text{ for all } i \quad (25)

\quad \sum_i \alpha_i y^i = 0 \quad (26)

\quad \sum_i \alpha_i \geq \nu \quad (27)

Properties If $\rho > 0$ then:

- $\nu$ is an upper bound on $\#\text{margin errors}/n$ (if $\sum_i \alpha_i = \nu$)
- $\nu$ is a lower bound on $\#\text{(original support vectors + margin errors)}/n$
- $\nu$-SVM leads to the same $w, b$ as C-SVM with $C = 1/\nu$

$^4$Lagrangian $L(w, b, \xi, \rho, \alpha, \mu, \delta) = \frac{1}{2}||w||^2 - \nu \rho + \frac{1}{n} \sum_i \xi_i - \sum_i \alpha_i [y^i(w^T x^i + b) - \rho + \xi_i] - \sum_i \mu_i \xi_i - \delta \rho$ with $\alpha_i \geq 0, \delta \geq 0, \mu_i \geq 0$
A simple error bound

\[ L_{01}(f_n) \leq E \left[ \frac{\text{#support vectors of } f_{n+1}}{n + 1} \right] \]  \hspace{1cm} (28)

where \( f_n \) denotes the SVM trained on a sample of size \( n \).

Exercise Use the Homework 6 to prove this result.
Non-linear SVM

How to use linear classifier on data that is not linearly separable?

An old trick

1. Map the data \( x^{1:n} \) to a higher dimensional space

\[
    x \rightarrow z = \phi(x) \in \mathcal{H}, \text{ with } \dim \mathcal{H} \gg n.
\]

2. Construct a linear classifier \( w^T z + b \) for the data in \( \mathcal{H} \)

In other words, we are implementing the non-linear classifier

\[
    f(x) = w^T \phi(x) + b = w_1 \phi_1(x) + w_2 \phi_2(x) + \ldots + w_m \phi_m(x) + b
\]
Example

- Data \( \{(x, y)\} \) below are not linearly separable

\[ \begin{array}{ccc|ccc} x & y & z \\ \hline -1 & -1 & 1 & -1 & -1 & 1 \\ -1 & 1 & -1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ \end{array} \]

- We map them to 3 dimensions by

\[ z = \phi(x) = [x_1 \ x_2 \ x_1x_2]. \]

- Now the classes can be separated by the hypeplane \( z_3 = 0 \) (which happens to be the maximum margin hyperplane). Hence,
  - \( w = [0 \ 0 \ 1] \) (a vector in \( \mathcal{H} \))
  - \( b = 0 \)
  - and the classification rule is \( f(\phi(x)) = w^T \phi(x) + b \).
- If we write \( f \) as a function of the original \( x \) we get

\[ f(x) = x_1x_2 \]

a quadratic classifier.
Non-linear SV problem

- **Primal problem** minimize $\frac{1}{2}||w||^2$ s.t. $y^i(w^T\phi(x^i) + b) - 1 \geq 0$ for all $i$.
- **Dual problem**

$$
\max_{\alpha_1:n} \sum_i \alpha_i - \frac{1}{2} \sum_i \alpha_i \alpha_j y^i y_j \phi(x^i)^T \phi(x_j) \quad \text{s.t. } \alpha_i \geq 0 \text{ for all } i \text{ and } \sum_i y^i \alpha_i = 0
$$

(30)

$$
G_{ij} = \phi(x^i)^T \phi(x^j) \quad \text{and} \quad \tilde{G} = y^T G y
$$

(31)

- $\tilde{G}_{ij}$ has been redefined in terms of $\phi$

- **Dual problem**

$$
\max_{\alpha} 1^T \alpha - \frac{1}{2} \alpha^T \tilde{G} \alpha \quad \text{s.t. } \alpha_i \geq 0, \ y^T \alpha = 0
$$

(32)

- Same as (17)!
The “Kernel Trick”

Third idea The result (32) is the celebrated kernel trick of the SVM literature. We can make the following remarks.

1. The $\phi$ vectors enter the SVM optimization problem only through the Gram matrix, thus only as the scalar products $\phi(x^i)^T \phi(x_j)$. We denote by $K(x, x')$ the function

$$K(x, x') = K(x', x) = \phi(x)^T \phi(x')$$ (33)

$K$ is called the kernel function. If $K$ can be computed efficiently, then the Gram matrix $G$ can also be computed efficiently. This is exactly what one does in practice: we choose $\phi$ implicitly by choosing a kernel $K$. Hereby we also ensure that $K$ can be computed efficiently.

2. Once $G$ is obtained, the SVM optimization is independent of the dimension of $x$ and of the dimension of $z = \phi(x)$. The complexity of the SVM optimization depends only on $n$ the number of examples. This means that we can choose a very high dimensional $\phi$ without any penalty on the optimization cost.

3. Classifying a new point $x$. As we know, the SVM classification rule is

$$f(x) = w^T \phi(x) + b = \sum_{i=1}^{n} \alpha_i y^i \phi(x^i)^T \phi(x) = \sum_{i=1}^{n} \alpha_i y^i K(x^i, x)$$ (34)

Hence, the classification rule is expressed in terms of the support vectors and the kernel only. No operations other than scalar product are performed in the high dimensional space $H$. 
Kernels

The previous section shows why SVMs are often called kernel machines. If we choose a kernel, we have all the benefits of a mapping in high dimensions, without ever carrying on any operations in that high dimensional space. The most usual kernel functions are

\[ K(x, x') = (1 + x^T x')^p \]  the polynomial kernel of degree \( p \)

\[ K(x, x') = \tanh(\sigma x^T x' - \beta) \]  the “neural network” kernel

\[ K(x, x') = e^{-\frac{||x-x'||^2}{\sigma^2}} \]  the Gaussian or radial basis function (RBF) kernel

it’s \( \phi \) is \( \infty \)-dimensional
The Mercer condition

- How do we verify that a chosen $K$ is is a valid kernel, i.e. that there exists a $\phi$ so that $K(x, x') = \phi(x)^T \phi(x')$?
- This property is ensured by a positivity condition known as the Mercer condition.

Mercer condition

Let $(\mathcal{X}, \mu)$ be a finite measure space. A symmetric function $K : \mathcal{X} \times \mathcal{X}$, can be written in the form $K(x, x') = \phi(x)^T \phi(x')$ for some $\phi : \mathcal{X} \to \mathcal{H} \subset \mathbb{R}^m$ iff

$$\int_{\mathcal{X}^2} K(x, x') g(x) g(x') d\mu(x) d\mu(x') \geq 0 \quad \text{for all } g \text{ such that } \|g(x)\|_{L^2} < \infty$$

(35)

- In other words, $K$ must be a positive semidefinite operator on $L_2$.
- If $K$ satisfies the Mercer condition, there is no guarantee that the corresponding $\phi$ is unique, or that it is finite-dimensional.
Quadratic kernel

- C-SVM, polynomial degree 2 kernel, $n = 200, C = 10000$
- The two ellipses show that a constant shift to the data ($x^i \leftarrow x^i + v, v \in \mathbb{R}^n$) can affect non-linear kernel classifiers.
RBF kernel and Support Vectors
Prediction with SVM

- Estimating $b$
  - For any $i$ support vector, $w^T x^i + b = y^i$ because the classification is tight
  - Alternatively, if there are slack variables, $w^T x^i + b = y^i(1 - \xi_i)$
  - Hence, $b = y^i(1 - \xi_i) - w^T x^i$

- For non-linear SVM, where $w$ is not known explicitly, $w = \sum_j \alpha_j y^j \phi(x^j)$. Hence, $b = y^i(1 - \xi_i) - \sum_{j=1}^n \alpha_j y^j K(x^i, x^j)$ for any $i$ support vector

- Given new $x$

\[
\hat{y}(x) = \text{sgn}(w^T x + b) = \text{sgn} \left( \sum_{i=1}^n \alpha_i y^i K(x^i, x) + b \right). \tag{36}
\]
L1-SVM

- If the regularization $\|w\|^2$, based on $l_2$ norm, is replaced with the $l_1$ norm $\|w\|_1$, we obtain what is known as the **Linear L1-SVM**

\[
\min_{w,b} \|w\|_1 + C \sum_i \xi_i \quad \text{s.t} \quad y^i(w^T x^i + b) \geq 1 - \xi_i, \ \xi_i \geq 0 \text{ for all } i = 1 : n \quad (37)
\]

- The use of the $l_1$ norm promotes sparsity in the entries of $w$

- The **Non-linear L1-SVM** is

\[
f(x) = \sum_i (\alpha_i^+ + \alpha_i^-) y^i K(x_i, x) + b \quad \text{classifier} \quad (38)
\]

\[
\min_{\alpha_+, b} \sum_i (\alpha_i^+ + \alpha_i^-) + C \sum_i \xi_i \quad \text{s.t} \quad y^i f(x^i) \geq 1 - \xi_i, \ \xi_i, \alpha_i^\pm \geq 0 \text{ for all } i = 1 \quad (39)
\]

- This formulation enforces $\alpha_i^+ = 0$ or $\alpha_i^- = 0$ for all $i$. If we set $w_i = \alpha_i^+ - \alpha_i^-$, we can write $f(x) = \sum_i w_i y^i K(x^i, x) + b$, a linear classifier in the non-linear features $K(x^i, x)$.

- The L1-SVM problems are **Linear Programs**

- The dual L1-SVM problems are also **linear programs**

- The L1-SVM is no longer a Maximum Margin classifier
Multi-class and One class SVM

Multiclass SVM
For a problem with $K$ possible classes, we construct $K$ separating hyperplanes $w_r^T x + b_r = 0$.

\[
\begin{align*}
\text{minimize} & & \frac{1}{2} \sum_{r=1}^{K} ||w_r||^2 + \frac{C}{n} \sum_{i,r} \xi_{i,r} \\
\text{s.t.} & & w_{y_i}^T x_i^i + b_{y_i} \geq w_r^T x_i + b_r + 1 - \xi_{i,r} \quad \text{for all } i = 1 : n, \ r \neq y_i \\
& & \xi_{i,r} \geq 0
\end{align*}
\] (40)

One-class SVM This SVM finds the “support regions” of the data, by separating the data from the origin by a hyperplane. It’s mostly used with the Gaussian kernel, that projects the data on the unit sphere. The formulation below is identical to the $\nu$-SVM where all points have label 1.

\[
\begin{align*}
\text{minimize} & & \frac{1}{2} ||w||^2 - \nu \rho + \frac{1}{n} \sum_i \xi_i \\
\text{s.t.} & & w^T x_i + b \geq \rho - \xi_i \\
& & \xi_i \geq 0 \\
& & \rho \geq 0
\end{align*}
\] (43)
SV Regression

The idea is to construct a “tolerance interval” of $\pm \epsilon$ around the regressor $f$ and to penalize data points for being outside this tolerance margin. In words, we try to construct the smoothest function that goes within $\epsilon$ of the data points.

$$\text{minimize} \quad \frac{1}{2}||w||^2 + C \sum_i (\xi_i^+ + \xi_i^-)$$

s.t. \quad $\epsilon + \xi_i^+ \geq w^T x_i + b - y_i \geq -\epsilon - \xi_i^-$

$$\xi_i^\pm \geq 0$$

$$\rho \geq 0$$

The above problem is a linear regression, but with the kernel trick we obtain a kernel regressor of the form $f(x) = \sum_i (\alpha_i^- - \alpha_i^+) K(x_i, x) + b$
Convex optimization in a nutshell

A set $D \subseteq \mathbb{R}^n$ is **convex** iff for every two points $x^1, x^2 \in D$ the line segment defined by $x = tx^1 + (1 - t)x^2$, $t \in [0, 1]$ is also in $D$. A function $f : D \rightarrow R$ is **convex** iff, for any $x^1, x^2 \in D$ and for any $t \in [0, 1]$ for which $tx^1 + (1 - t)x^2 \in D$ the following inequality holds

$$f(tx^1 + (1 - t)x^2) \leq tf(x^1) + (1 - t)f(x^2)$$

(51)

If $f$ is convex, then the set $\{x \mid f(x) \leq c\}$ is convex for any value of $c$. Convex functions defined on convex sets have very interesting properties which have engendered the field called **convex optimization**.

The optimization problem

$$\min_x f_0(x)$$

s.t. $f_i(x) \leq 0$ for $i = 1, \ldots m$

is a **convex optimization problem** if all the functions $f, f_i$ are convex. Note that in this case the feasible domain $A = \bigcap_i \{x \mid f_i(x) \leq 0\}$ is a convex set.
It is known that if $A$ has a non empty interior then the convex optimization problem has at most one optimum $x^*$. If $A$ is also bounded, $x^*$ always exists. Assuming that $x^*$ exists, there are two possible cases: (1) The \textbf{unconstrained minimum} of $f_0$ lies in $A$. In this case, the optimum can be found by solving the equations $\frac{\partial f_0}{\partial x} = 0$. (2) The unconstrained minimum of $f_0$ lies outside $A$. Figure 1 depicts what happens at the optimum $x^*$ in this case.
Figure: (a) One constraint optimization. (b) Four constraint optimization. At the optimum only constraints $g_1, g_4$ are active. $f$ denotes the objective ($f_0$ in text) and $g$ denote the constraints ($f_i$ in text).

Assume there is only one constraint $f_1$. The domain $A$ is the inside of the curve $f_1(x) = 0$. The optimum $x^*$ is the point where a level curve $f_0(x) = c$ is tangent to $f_1 = 0$ from the outside. In this point, the gradients of two curves lie along the same line, pointing in opposite directions. Therefore, we can write $\frac{\partial f_0}{\partial x} = -\alpha \frac{\partial f_1}{\partial x}$. Equivalently, we have that at $x^*$, $\frac{\partial f_0}{\partial x} + \alpha \frac{\partial f_1}{\partial x} = 0$. Note that this is a necessary but not a sufficient condition. The above set of equations represents the Karush-Kuhn-Tucker optimality conditions (KKT).
With more than one constraint, the KKT conditions are equivalent to requiring that the gradient of $f_0$ lies in the subspace spanned by the gradients of the constraints.

$$\frac{\partial f_0}{\partial x} = - \sum_i \alpha_i \frac{\partial f_i}{\partial x} \text{ with } \alpha_i \geq 0 \text{ for all } i \quad (53)$$

Note that if a certain constraint $f_i$ does not participate in the boundary of $D$ at $x^*$, i.e if the constraint is not active, the coefficient $\alpha_i$ should be 0. Equation (53) can be rewritten as

$$\frac{\partial}{\partial x} \left[ f_0(x) + \sum_i \alpha_i f_i(x) \right] = 0 \text{ for some } \alpha_i \geq 0 \text{ for } i = 1, \ldots m \quad (54)$$

The optimum $x^*$ has to satisfy the equation above. The new function $L(x, \alpha)$ is the Lagrangean of the problem and the variables $\alpha_i$ are called Lagrange multipliers. The Lagrangean is convex in $x$ and affine (i.e linear + constant) in $\alpha$. 
The dual problem Define the function

\[ g(\alpha) = \inf_x L(x, \alpha) \quad \alpha = (\alpha_i), \alpha_i \geq 0 \]  \quad (55)

In the above, the infimum is over all the values of \( x \) for which \( f_0, f_i \) are defined, not just \( A \) (but everything still holds if the infimum is only taken over \( A \)). Two facts are important about \( g \):

- \( g(\alpha) \leq L(x, \alpha) \leq f(x) \) for any \( x \in A, \alpha \geq 0 \), i.e. \( g \) is a lower bound for \( f_0 \), and implicitly for the optimal value \( f_0(x^*) \), for any value of \( \alpha \geq 0 \).
- \( g(\alpha) \) is concave (i.e. \( -g(\alpha) \) is convex).

We also can derive from (54) that if \( x^* \) exists then for an appropriate value \( \alpha^* \) we have

\[ g(\alpha^*) = L(x^*, \alpha^*) = f_0(x^*) + 0 \]  \quad (56)

and therefore \( g(\alpha^*) \) must be the unique maximum of \( g(\alpha) \). The second term in \( L \) above is zero because \( x^* \) is on the boundary of \( A \); hence for the active constraints \( f_i(x^*) = 0 \) and for the inactive constraints \( \alpha^*_i = 0 \).
This surprising relationship shows that by solving the dual problem

\[
\begin{align*}
\max & \quad g(\alpha) \\
\text{s.t.} & \quad \alpha \geq 0
\end{align*}
\]

we can obtain the values \( \alpha^* \) that plugged into (53 will allow us to find the solution \( x^* \) to our original (primal) problem. The constraints of the dual are simpler than the constraints of the primal. In practice, it is surprisingly often possible to compute the function \( g(\alpha) \) explicitly. Below we give a simple example thereof. This is also the case of the SVM optimization problem, which will be discussed in section 5.
A simple optimization example
Take as an example the convex optimization problem

$$\min \frac{1}{2}x^2 \quad \text{s.t.} \quad x + 1 \leq 0$$  \hspace{1cm} (58)$$

By inspection the solution is $x^* = -1$.

Let us now apply to it the convex optimization machinery. We have

$$L(x, \alpha) = \frac{1}{2}x^2 + \alpha(x + 1)$$  \hspace{1cm} (59)$$
defined for $x \in \mathbb{R}$ and $\alpha \geq 0$.

$$g(\alpha) = \inf_x \left[ \frac{1}{2}x^2 + \alpha(x + 1) \right]$$  \hspace{1cm} (60)$$

$$= \inf_x \left[ \frac{1}{2}(x + \alpha)^2 - \frac{1}{2}\alpha^2 + \alpha \right]$$  \hspace{1cm} (61)$$

$$= -\frac{1}{2}\alpha^2 + \alpha$$  \hspace{1cm} (62)$$

$$= \frac{1}{2}\alpha(2 - \alpha) \quad \text{attained for} \quad x = -\alpha$$  \hspace{1cm} (63)$$

The dual problem is

$$\max \frac{1}{2}\alpha(2 - \alpha) \quad \text{s.t.} \quad \alpha \geq 0$$  \hspace{1cm} (64)$$

and its solution is $\alpha = 1$ which, using equation (63) leads to $x = -1$.

From the KKT condition

$$\frac{\partial L}{\partial x} = x + \alpha = 0$$  \hspace{1cm} (65)$$

we also obtain $x^* = -\alpha^* = -1$. 
Figure 2 depicts the function $L$. Note that $L$ is convex in $x$ (a parabola) and that along the $\alpha$ axis the graph of $L$ consists of lines. The areas of $L$ that fall outside the admissible domain $x \leq -1, \alpha \geq 0$ are in flat (green) color. The crossection $L(x, \alpha = 0)$ represents the plot of $f$. The constrained minimum of $f$ is at $x = -1$, the unconstrained one is at $x = 0$ outside the admissible domain. Note that $g(\alpha) = L(-\alpha, \alpha)$ is concave, and that in the admissible domain it is always below the graph of $f$. The (red) dot is the optimum $(x^*, \alpha^*)$, which represents a saddle point for $h$. The line $L(x = -1, \alpha)$ is horizontal (because $f_1 = x + 1 = 0$) and thus $L(x^*, \alpha^*) = L(x^*, \alpha) = f(x^*)$.

**Figure:** The surface $L(x, \alpha)$ for the problem $\min \ \frac{1}{2} x^2 \ \text{s.t.} \ x + 1 \leq 0$. 
The SVM solution by convex optimization

The SVM optimization problem

$$\min_w \frac{1}{2} ||w||^2 \ \text{s.t.} \ y^i(w^T x^i + b) \geq 1 \ \text{for all} \ i$$  \hspace{1cm} (66)

is a convex (quadratic) optimization problem where

$$f_0(w, b) = \frac{1}{2} ||w||^2$$  \hspace{1cm} (67)

$$f_i(w, b) = -y^i w^T x^i + 1 - y^i b$$  \hspace{1cm} (68)

Hence,

$$L(w, b, \alpha) = \frac{1}{2} ||w||^2 + \sum_i \alpha_i [1 - y^i b - y^i x^i T w]$$  \hspace{1cm} (69)

Equating the partial derivatives of $h$ w.r.t $w, b$ with 0 we get

$$\frac{\partial L}{\partial w} = w - \sum_i \alpha_i y^i x^i$$  \hspace{1cm} (70)

$$\frac{\partial L}{\partial b} = \sum_i \alpha_i y^i$$  \hspace{1cm} (71)

or, equivalently

$$w = \sum_i \alpha_i y^i x^i \quad 0 = \sum_i \alpha_i y^i$$  \hspace{1cm} (72)

Hence, the normal $w$ to the optimal separating hyperplane is a linear combination of data points.
Sparsity of solution Moreover, we know that only those $\alpha_i$ corresponding to active constraints will be non-zero. In the case of SVM, these represent points that are classified with $y_i(w^T x_i + b) = 1$. We call these points support points or support vectors. The solution of the SVM problem does not depend on all the data points, it depends only on the support vectors and therefore is sparse.

Computing the solution. SVM solvers use the dual problem to compute the solution. Below we derive the dual for the SVM problem. $g(\alpha)$ is computed explicitly by replacing equation (72) in (69). After a simple calculation we obtain

$$g(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} y_i y_j x_i^T x_j \alpha_i \alpha_j$$

or, in vector/matrix notation

$$g(\alpha) = 1^T \alpha - \frac{1}{2} \alpha^T G \alpha$$

where $G = [G_{ij}]_{ij} = [y^i y_j x_i^T x_j]_{ij}$. 
A simple SVM problem

Data: 4 vectors in the plane and their labels

\[
\begin{align*}
x_1 &= (-2,-2) & y_1 &= +1 \\
x_2 &= (-1,1) & y_2 &= +1 \\
x_3 &= (1,1) & y_3 &= -1 \\
x_4 &= (2,-2) & y_4 &= -1
\end{align*}
\]

The Gramm matrix \( G = [x^i \, ^T \, x_j]_{i,j=1:l} \)

\[
G = \begin{bmatrix}
8 & 0 & -4 & 0 \\
0 & 2 & 0 & -4 \\
-4 & 0 & 2 & 0 \\
0 & -4 & 0 & 8
\end{bmatrix}
\]

The dual function to be maximized (subject to \( \alpha_i \geq 0 \)) is

\[
g(\alpha) = \sum_i \alpha_i - \frac{1}{2} \sum_i \alpha_i \alpha_j y_i y_j x_i \, ^T \, x_j
\]

\[
= \alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 - 4\alpha_1^2 - \alpha_2^2 - \alpha_3^2 - 4\alpha_4^2 - 4\alpha_1\alpha_3 - 4\alpha_2\alpha_4
\]

\[
= (2\alpha_1 + \alpha_3) - (2\alpha_1 + \alpha_3)^2 - \alpha_1 + (\alpha_2 + 2\alpha_4) - (\alpha_2 + 2\alpha_4)^2 - \alpha_4
\]

The parts depending on \( \alpha_1, \alpha_3 \) and \( \alpha_2, \alpha_4 \) can be maximized separately.
After some short calculations we obtain:

\[
\begin{align*}
\alpha_1 &= 0 & \alpha_4 &= 0 \\
\alpha_2 &= \frac{1}{2} & \alpha_3 &= \frac{1}{2}
\end{align*}
\]

Hence, the support vectors are \(x_2\) and \(x_3\). From these, we obtain

\[
\begin{align*}
w &= \sum_i \alpha_i y^i x^i = \frac{1}{2} (x_2 - x_3) = (-1, 0) \\
b &= y_2 - w^T x_2 = 0
\end{align*}
\]

The results are depicted in the figure below: