Support vector machines

Course of Machine Learning
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Idea

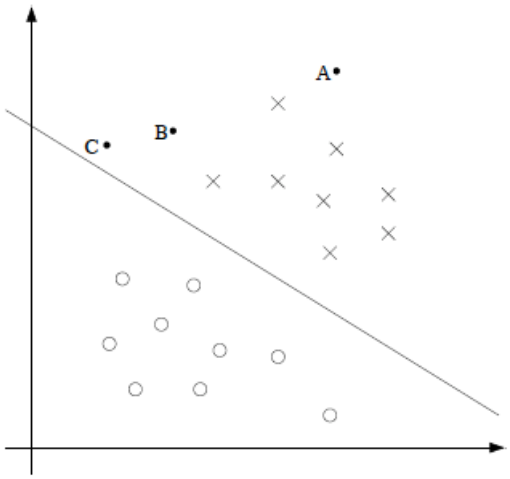
The binary classification problem is approached in a direct way, that is:

We try and find a plane that separates the classes in feature space (indeed, a "best" plane, according to a reasonable characteristic)

If this is not possible, we get creative in two ways:

- We soften what we mean by "separates", and
- We enrich and enlarge the feature space so that separation is (more) possible

Margins



A can be assigned to $\mathcal{C}_1$ with greater confidence than B and even greater confidence than C.

Binary classifiers

Consider a binary classifier which, for any element $\mathbf{x}$, returns a value $y \in \{-1, 1\}$, where we assume that $\mathbf{x}$ is assigned to $\mathcal{C}_0$ if $y = -1$ and to $\mathcal{C}_1$ if $y = 1$.

Moreover, we consider linear classifier such as

$$h(\mathbf{x}) = g(\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_i) + w_0)$$

where $g(z) = 1$ if $z \geq 0$ and $g(z) = -1$ if $z < 0$. The prediction on the class of $\mathbf{x}$ is then provided by deriving a value in $\{-1, 1\}$ just as in the case of a perceptron, that is with no estimation of the probabilities $p(\mathcal{C}_i|\mathbf{x})$ that $\mathbf{x}$ belongs to each class.

Margins

For any training set item $(\mathbf{x}_i, t_i)$, the *functional margin* of $(\mathbf{w}, w_0)$ wrt such item is defined as

$$\overline{\gamma}_i = t_i(\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_i) + w_0)$$

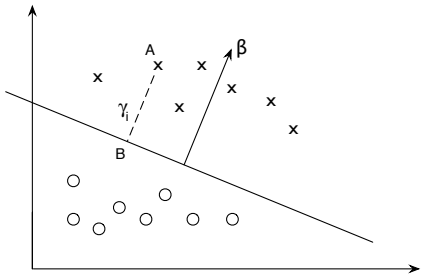
Observe that the resulting prediction is correct iff $\overline{\gamma}_i > 0$. Moreover, larger values of $\overline{\gamma}_i$ denote greater confidence on the prediction.

Given a training set $\mathcal{T} = \{(\mathbf{x}_1, t_1), \ldots, (\mathbf{x}_n, t_n)\}$ the functional margin of $(\mathbf{w}, w_0)$ wrt $\mathcal{T}$ is the minimum functional margin for all items in $\mathcal{T}$

$$\overline{\gamma} = \min_i \overline{\gamma}_i$$

Margins

The *geometric margin* γ_i of a training set item $\mathbf{x}_i, t_i$ is defined as the product of t_i and the distance from $\mathbf{x}_i$ to the boundary hyperplane, that is as the length of the line segment from $\mathbf{x}_i$ to its projection on the boundary hyperplane



Margins

Since, in general, the distance of a point $\overline{\mathbf{x}}$ from a hyperplane $\mathbf{w}^T\mathbf{x} = 0$ is $\frac{\mathbf{w}^T\overline{\mathbf{x}}}{||\mathbf{w}||}$, it results

$$\gamma_i = t_i \left(\frac{\mathbf{w}^T}{||\mathbf{w}||}\boldsymbol{\phi}(\mathbf{x}_i) + \frac{w_0}{||\mathbf{w}||} \right) = \frac{\overline{\gamma}_i}{||\mathbf{w}||}$$

So, differently from $\overline{\gamma}_i$, the geometric margin γ_i is invariant wrt parameter scaling. In fact, by substituting $c\mathbf{w}$ to $\mathbf{w}$ and cw_0 to w_0, we get

$$\overline{\gamma}_i = t_i(c\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_i) + cw_0) = ct_i(\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_i) + w_0)$$

$$\gamma_i = t_i \left(\frac{c\mathbf{w}^T}{||c\mathbf{w}||}\boldsymbol{\phi}(\mathbf{x}_i) + \frac{cw_0}{||c\mathbf{w}||} \right) = t_i \left(\frac{\mathbf{w}^T}{||\mathbf{w}||}\boldsymbol{\phi}(\mathbf{x}_i) + \frac{w_0}{||\mathbf{w}||} \right)$$

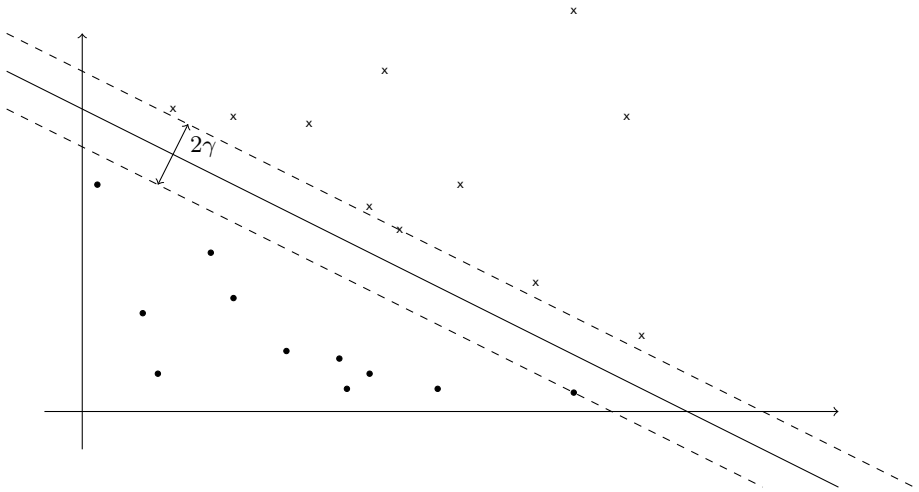
Margins

- The geometric margin wrt the training set $\mathcal{T} = \{(\mathbf{x}_1, t_1), \ldots, (\mathbf{x}_n, t_n)\}$ is then defined as the smallest geometric margin for all items $(\mathbf{x}_i, t_i)$

  $$\gamma = \min_i \gamma_i$$

- a useful interpretation of γ is as half the width of the largest strip, centered on the hyperplane $\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}) + w_0 = 0$, containing none of the points $\mathbf{x}_1, \ldots, \mathbf{x}_n$
- the hyperplanes on the boundary of such strip, each at distance γ from the hyperplane and passing (at least one of them) through some point $\mathbf{x}_i$ are said *maximum margin hyperplanes*.

Margins



Optimal margin classifiers

Given a training set $\mathcal{T}$, we wish to find the hyperplanes which separates the two classes (if one does exist) and has maximum γ: by making the distance between the hyperplanes and the set of points corresponding to elements as large as possible, the confidence on the provided classification increases.

Assume classes are linearly separable in the training set: hence, there exists a hyperplane (an infinity of them, indeed) separating elements in C_1 from elements in C_2. In order to find the one among those hyperplanes which maximizes γ, we have to solve the following optimization problem

$$\max_{\mathbf{w},w_0} \gamma$$
$$\text{where } \gamma_i = \frac{t_i}{||\mathbf{w}||}(\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_i) + w_0) \geq \gamma \qquad i = 1, \ldots, n$$

That is,

$$\max_{\mathbf{w},w_0} \gamma$$
$$\text{where } t_i(\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_i) + w_0) \geq \gamma\,||\mathbf{w}|| \qquad i = 1, \ldots, n$$

Optimal margin classifiers

As observed, if all parameters are scaled by any constant c, all geometric margins γ_i between elements and hyperplane are unchanged: we may then exploit this freedom to introduce the constraint

$$\gamma = \min_i t_i(\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_i) + w_0) = 1$$

This can be obtained by assuming $||w|| = \frac{1}{\gamma}$, which corresponds to considering a scale where the maximum margin has width 2. This results, for each element $\mathbf{x}_i, t_i$, into a constraint

$$\gamma_i = t_i(\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_i) + w_0) \geq 1$$

An element (point) is said *active* if the equality holds, that is if

$$t_i(\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_i) + w_0) = 1$$

and *inactive* if this does not hold. Observe that, by definition, there must exists at least one active point.

Optimal margin classifiers

For any element $\mathbf{x}, t$,

1. $t(\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}) + w_0) > 1$ if $\boldsymbol{\phi}(\mathbf{x})$ is in the region corresponding to its class, outside the margin strip
2. $t(\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}) + w_0) = 1$ if $\boldsymbol{\phi}(\mathbf{x})$ is in the region corresponding to its class, on the maximum margin hyperplane

3. $0 < t(\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}) + w_0) < 1$ if $\boldsymbol{\phi}(\mathbf{x})$ is in the region corresponding to its class, inside the margin strip
4. $t(\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}) + w_0) = 0$ if $\boldsymbol{\phi}(\mathbf{x})$ is on the separating hyperplane
5. $-1 < t(\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}) + w_0) < 0$ if $\boldsymbol{\phi}(\mathbf{x})$ is in the region corresponding to the other class, inside the margin strip
6. $t(\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}) + w_0) = -1$ if $\boldsymbol{\phi}(\mathbf{x})$ is in the region corresponding to the other class, on the maximum margin hyperplane
7. $t(\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}) + w_0) < -1$ if $\boldsymbol{\phi}(\mathbf{x})$ is in the region corresponding to the other class, outside the margin strip

Optimal margin classifiers

The optimization problem, is then transformed into

$$\begin{aligned} &\max_{\mathbf{w}, w_0} \gamma = ||\mathbf{w}||^{-1} \\ &\text{where } t_i(\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_i) + w_0) \geq 1 \qquad i = 1, \ldots, n \end{aligned}$$

Maximizing $||\mathbf{w}||^{-1}$ is equivalent to minimizing $||\mathbf{w}||^2$ (we prefer minimizing $||\mathbf{w}||^2$ instead of $||\mathbf{w}||$ since it is smooth everywhere): hence we may formulate the problem as

$$\begin{aligned} &\min_{\mathbf{w}, w_0} \frac{1}{2} ||\mathbf{w}||^2 \\ &\text{where } t_i(\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_i) + w_0) \geq 1 \qquad i = 1, \ldots, n \end{aligned}$$

This is a *convex quadratic* optimization problem. The function to be minimized is in fact convex and the set of points satisfying the constraint is a convex polyhedron (intersection of half-spaces).

Duality

From optimization theory it derives that, given the problem structure (linear constraints + convexity):

- there exists a *dual formulation* of the problem
- the optimum of the dual problem is the same the the original (*primal*) problem

Karush-Kuhn-Tucker theorem

Consider the optimization problem

$$\begin{aligned} &\min_{\mathbf{x} \in \Omega} f(\mathbf{x}) \\ &g_i(\mathbf{x}) \geq 0 \qquad i = 1, \ldots, k \\ &h_j(\mathbf{x}) = 0 \qquad i = 1, \ldots, k' \end{aligned}$$

where $f(\mathbf{x})$, $g_i(\mathbf{x})$, $h_j(\mathbf{x})$ are convex functions and Ω is a convex set.

Define the *Lagrangian*

$$L(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\mu}) = h(\mathbf{x}) + \sum_{i=1}^{k} \lambda_i g_i(\mathbf{x}) + \sum_{j=1}^{k'} \mu_j h_j(\mathbf{x})$$

and the minimum

$$\theta(\boldsymbol{\lambda}, \boldsymbol{\mu}) = \min_{\mathbf{x}} L(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\mu})$$

Then, the solution of the original problem is the same as the solution of

$$\begin{aligned} &\max_{\boldsymbol{\lambda}, \boldsymbol{\mu}} \theta(\boldsymbol{\lambda}, \boldsymbol{\mu}) \\ &\lambda_i \geq 0 \qquad i = 1, \ldots, k \end{aligned}$$

Karush-Kuhn-Tucker theorem

The following necessary and sufficient conditions apply for the existence of an optimum $(\mathbf{x}^*, \boldsymbol{\lambda}^*, \boldsymbol{\mu}^*)$.

$$\begin{aligned}
\frac{\partial L(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\mu})}{\partial \mathbf{x}}\Big|_{\mathbf{x}^*, \boldsymbol{\lambda}^*, \boldsymbol{\mu}^*} &= \mathbf{0} \\
\frac{\partial L(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\mu})}{\partial \lambda_i}\Big|_{\mathbf{x}^*, \boldsymbol{\lambda}^*, \boldsymbol{\mu}^*} &= g_i(\mathbf{x}^*) \geq 0 \qquad i = 1, \ldots, k \\
\frac{\partial L(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\mu})}{\partial \mu_j}\Big|_{\mathbf{x}^*, \boldsymbol{\lambda}^*, \boldsymbol{\mu}^*} &= h_j(\mathbf{x}^*) = 0 \qquad i = j, \ldots, k' \\
\lambda_i^* &\geq 0 \qquad i = 1, \ldots, k \\
\lambda_i^* g_i(\mathbf{x}^*) &= 0 \qquad i = 1, \ldots, k
\end{aligned}$$

Note: the last condition states that a Lagrangian multiplier λ_i^* can be non-zero only if $g_i(\mathbf{x}^*) = 0$, that is of $\mathbf{x}^*$ is"at the limit" for the constraint $g_i(\mathbf{x})$. In this case, the constraint is said *active*.

Applying Kuhn-Tucker theorem

In our case,

- $f(\mathbf{x})$ corresponds to $\frac{1}{2}\,||\mathbf{w}||^2$
- $g_i(x)$ corresponds to $t_i(\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_i) + w_0) - 1 \geq 0$
- there is no $h_j(\mathbf{x})$
- Ω is the intersection of a set of hyperplanes, that is a polyhedron, hence convex.

By the KKT theorem, the solution is then the same as the solution of

$$\begin{aligned}
\max_{\boldsymbol{\lambda}} \min_{\mathbf{w}, w_0} L(\mathbf{w}, w_0, \boldsymbol{\lambda}) &= \max_{\boldsymbol{\lambda}} \min_{\mathbf{w}, b} \left(\frac{1}{2}\mathbf{w}^T\mathbf{w} - \sum_{i=1}^{n} \lambda_i \left(t_i(\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_i) + w_0) - 1 \right) \right) \\
&= \max_{\boldsymbol{\lambda}} \min_{\mathbf{w}, w_0} \left(\frac{1}{2}\mathbf{w}^T\mathbf{w} - \sum_{i=1}^{n} \lambda_i t_i(\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_i) + w_0) + \sum_{i=1}^{n} \lambda_i \right)
\end{aligned}$$

under the constraints

$$\lambda_i \geq 0 \qquad i = 1, \ldots, k$$

Applying the KKT conditions

Since the KKT conditions hold for the maximum point, it must be, at that point:

$$\begin{aligned}
\frac{\partial L(\mathbf{w}, w_0, \boldsymbol{\lambda})}{\partial \mathbf{w}} &= \mathbf{w} - \sum_{i=1}^{n} \lambda_i t_i \boldsymbol{\phi}(\mathbf{x}_i) = \mathbf{0} \\
\frac{\partial L(\mathbf{w}, w_0, \boldsymbol{\lambda})}{\partial w_0} &= \sum_{i=1}^{n} \lambda_i t_i = 0 \\
t_i(\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_i) + w_0) - 1 &\geq 0 \qquad i = 1, \ldots, n \\
\lambda_i &\geq 0 \qquad i = 1, \ldots, n \\
\lambda_i \left(t_i(\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_i) + w_0) - 1 \right) &= 0 \qquad i = 1, \ldots, n
\end{aligned}$$

Lagrange method: dual problem

We may apply the above relations to drop $\mathbf{w}$ and w_0 from $L(\mathbf{w}, w_0, \lambda)$ and from all constraints. As a result, we get a new *dual* formulation of the problem

$$\max_{\boldsymbol{\lambda}} \overline{L}(\boldsymbol{\lambda}) = \max_{\boldsymbol{\lambda}} \left(\sum_{i=1}^{n} \lambda_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \lambda_i \lambda_j t_i t_j \boldsymbol{\phi}(\mathbf{x}_i)\boldsymbol{\phi}(\mathbf{x}_j) \right)$$

where

$$\lambda_i \geq 0 \qquad i = \ldots, n$$
$$\sum_{i=1}^{n} \lambda_i t_i = 0$$

Dual problem and kernel function

By defining the *kernel function*

$$\kappa(\mathbf{x}_i, \mathbf{x}_j) = \boldsymbol{\phi}(\mathbf{x}_i)^T \boldsymbol{\phi}(\mathbf{x}_j)$$

the dual problem's formulation can be given as

$$\max_{\boldsymbol{\lambda}} \tilde{L}(\boldsymbol{\lambda}) = \max_{\boldsymbol{\lambda}} \left(\sum_{i=1}^{n} \lambda_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \lambda_i \lambda_j t_i t_j \kappa(\mathbf{x}_i, \mathbf{x}_j) \right)$$
$$\lambda_i \geq 0 \qquad i = 1, \ldots, n$$
$$\sum_{i=1}^{n} \lambda_i t_i = 0$$

Passing from primal to dual

Disadvantage The number variables increases from m to n (in particualar, if $\boldsymbol{\phi}(\mathbf{x}) = \mathbf{x}$, from d to n).

Advantage The number of variables to be considered, which are relevant for classification, turns out to be quite smaller than n.

Deriving coefficients

By solving the dual problem, the optimal values of Langrangian multipliers $\boldsymbol{\lambda}^*$ are obtained.

The optimal values of parameters $\mathbf{w}^*$ are then derived through the relations

$$w_i^* = \sum_{j=1}^{n} \lambda_j^* t_j \phi_i(\mathbf{x}_j) \qquad\qquad i = 1, \ldots, m$$

The value of w_0^* can be obtained by observing that, for any support vector $\mathbf{x}_k$ (characterized by the condition $\lambda_k \geq 0$), it must be

$$\begin{aligned} 1 &= t_k \left(\boldsymbol{\phi}(\mathbf{x}_i)^T \mathbf{w}^* + w_0^* \right) \\ &= t_k \left(\sum_{j=1}^{n} \lambda_j^* t_j \boldsymbol{\phi}(\mathbf{x}_j)^T \boldsymbol{\phi}(\mathbf{x}_k) + w_0^* \right) \\ &= t_k \left(\sum_{j=1}^{n} \lambda_j^* t_j \kappa(\mathbf{x}_j, \mathbf{x}_k) + w_0^* \right) \\ &= t_k \left(\sum_{j \in \mathcal{S}} \lambda_j^* t_j \kappa(\mathbf{x}_j, \mathbf{x}_k) + w_0^* \right) \end{aligned}$$

where $\mathcal{S}$ is the set of indices of support vectors.

Deriving coefficients

As a consequence, since $t_k = \pm 1$, in order to have a unitary product it must be

$$t_k = \sum_{j \in \mathcal{S}} \lambda_j^* t_j \kappa(\mathbf{x}_j, \mathbf{x}_k) + w_0^*$$

and

$$w_0^* = t_k - \sum_{j \in \mathcal{S}} \lambda_j^* t_j \kappa(\mathbf{x}_j, \mathbf{x}_k)$$

A more precise solution can be obtained as the mean value obtained considering all support vectors

$$w_0^* = \frac{1}{|\mathcal{S}|} \sum_{i \in \mathcal{S}} \left(t_i - \sum_{j \in \mathcal{S}} \lambda_j^* t_j \kappa(\mathbf{x}_j, \mathbf{x}_i) \right)$$

Classification through SVM

A new element $\mathbf{x}$ can be classified, given a set of base functions ϕ or a kernel function κ, by checking the sign of

$$y(\mathbf{x}) = \sum_{i=1}^{m} w_i^* \phi_i(\mathbf{x}) + w_0^* = \sum_{j=1}^{n} \lambda_j^* t_j \kappa(\mathbf{x}_j, \mathbf{x}) + w_0^*$$

As noticed, if $\mathbf{x}_i$ is not a support vector, then it must be $\lambda_i^* = 0$. Thus, the above sum can be written as

$$y(\mathbf{x}) = \sum_{j \in \mathcal{S}} \lambda_j^* t_j \kappa(\mathbf{x}_j, \mathbf{x}) + w_0^*$$

The classification performed through the dual formulation, using the kernel function, does not take into account all training set items, but only support vectors, usually a quite small subset of the training set.

Non separability in the training set

- The linear separability hypothesis for the classes is quite restrictive
- In general, a suitable set of base functions ϕ, or a suitable kernel function $\kappa(\mathbf{x}_1, \mathbf{x}_2)$, may map all training set elements onto a larger-dimensional feature space where classes turn out to be (at least approximately) linearly separable.

Non separability in the training set

- The approach described before, when applied to non linearly separable sets, does not provide acceptable solutions: it is in fact impossibile to satisfy all constraints

$$t_i(\mathbf{w}^T \phi(\mathbf{x}_i) + w_0) \geq 1 \qquad i = 1, \ldots, n$$

- These constraints must then be relaxed in order to allow them to not hold, at the cost of some increase in the objective function to be minimized
- A *slack variable* ξ_i is introduced for each constraint, to provide a measure of how much the constraint is not verified

Non separability in the training set

- This can be formalized as

$$\min_{\mathbf{w}, w_0, \boldsymbol{\xi}} \frac{1}{2} \mathbf{w}^T \mathbf{w} + C \sum_{i=1}^{n} \xi_i$$
$$t_i(\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_i) + w_0) \geq 1 - \xi_i \qquad i = 1, \ldots, n$$
$$\xi_i \geq 0 \qquad i = 1, \ldots, n$$

where $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_n)$

- By introducing suitable multipliers, the following Lagrangian can be obtained

$$
\begin{aligned}
& L(\mathbf{w},w_0,\boldsymbol{\xi},\boldsymbol{\lambda},\boldsymbol{\alpha}) \\
& \quad = \frac{1}{2}\mathbf{w}^T\mathbf{w} + C\sum_{i=1}^{n}\xi_i - \sum_{i=1}^{n}\lambda_i(y_i(\mathbf{w}^T\boldsymbol{\phi}(x_i)+w_0)-1+\xi_i) - \sum_{i=1}^{n}\alpha_i\xi_i \\
& \quad = \frac{1}{2}\sum_{i=1}^{n}w_i^2 + \sum_{i=1}^{n}(C-\alpha_i)\xi_i - \sum_{i=1}^{n}\lambda_i(t_i(\sum_{j=1}^{m}w_j\phi_j(\mathbf{x}_i))+w_0)-1+\xi_i) \\
& \quad = \frac{1}{2}\sum_{i=1}^{n}w_i^2 + \sum_{i=1}^{n}(C-\alpha_i-\lambda_i)\xi_i - \sum_{i=1}^{n}\sum_{j=1}^{m}\lambda_i t_i w_j\phi_j(\mathbf{x}_i) + w_0\sum_{i=1}^{n}\lambda_i t_i + \sum_{i=1}^{n}\lambda_i
\end{aligned}
$$

where $\alpha_i \geq 0$ and $\lambda_i \geq 0$, for $i = 1\ldots,n$.

KKT conditions

The Karush-Kuhn-Tucker conditions are now:

$$
\begin{aligned}
\frac{\partial}{\partial\mathbf{w}}L(\mathbf{w},w_0,\boldsymbol{\xi},\boldsymbol{\lambda},\boldsymbol{\alpha}) &= \mathbf{0} && && \text{null gradient} \\
\frac{\partial}{\partial w_0}L(\mathbf{w},w_0,\boldsymbol{\xi},\boldsymbol{\lambda},\boldsymbol{\alpha}) &= 0 && && \text{null gradient} \\
\frac{\partial}{\partial\boldsymbol{\xi}}L(\mathbf{w},w_0,\boldsymbol{\xi},\boldsymbol{\lambda},\boldsymbol{\alpha}) &= \mathbf{0} && && \text{null gradient} \\
t_i(\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_i)+w_0)-1+\xi_i &\geq 0 && i=1,\ldots,n && \text{constraints} \\
\xi_i &\geq 0 && i=1,\ldots,n && \text{constraints} \\
\lambda_i &\geq 0 && i=1,\ldots,n && \text{multipliers} \\
\alpha_i &\geq 0 && i=1,\ldots,n && \text{multipliers} \\
\lambda_i\left(t_i(\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_i)+w_0)-1+\xi_i\right) &= 0 && i=1,\ldots,n && \text{complementary slackness} \\
\alpha_i\xi_i &= 0 && i=1,\ldots,n && \text{complementary slackness}
\end{aligned}
$$

Deriving a dual formulation

From the null gradient conditions wrt w_i, b, ξ_j it derives

$$
\begin{aligned}
w_i &= \sum_{j=1}^{n}\lambda_j t_j\phi_i(\mathbf{x}_j) \qquad i=1,\ldots,m \\
0 &= \sum_{i=1}^{n}\lambda_i t_i \\
\lambda_i &= C-\alpha_i \leq C \qquad i=1,\ldots,n
\end{aligned}
$$

Deriving a dual formulation

By plugging the above relations into $L(\mathbf{w},w_0,\boldsymbol{\xi},\boldsymbol{\lambda},\boldsymbol{\alpha})$, the dual problem results

$$
\begin{aligned}
\max_{\boldsymbol{\lambda}}\tilde{L}(\boldsymbol{\lambda}) &= \max_{\boldsymbol{\lambda}}\left(\sum_{i=1}^{n}\lambda_i - \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\lambda_i\lambda_j t_i t_j\kappa(\mathbf{x}_i,\mathbf{x}_j)\right) \\
& 0 \leq \lambda_i \leq C \qquad i=1,\ldots,n \\
& \sum_{i=1}^{n}\lambda_i y_i = 0
\end{aligned}
$$

Observe that the only difference wrt the linearly separable case is given by constraints $0 \leq \lambda_i$ transformed into in $0 \leq \lambda_i \leq C$

Item characterization

Given a solution of the above problem, the elements of the training set can be partitioned into several subsets:

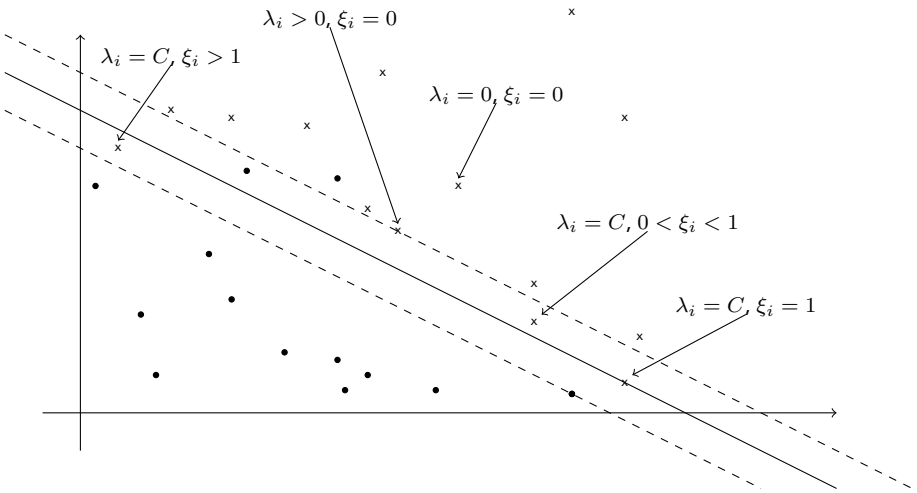
- elements correctly classified and not relevant, the ones such that $\lambda_i = 0$ and $\xi_i = 0$: such elements are in the correct halfspace, in terms of classification, and do not lie on the maximum margin hyperplanes (they are not support vectors)
- elements correctly classified and relevant, the ones such that $\lambda_i > 0$ and $0 \leq \xi_i < 1$: such elements are in the correct halfspace, in terms of classification, either on the maximum margin hyperplanes ($\xi_i = 0$) or within the margin region ($0 < \xi_i < 1$).
- elements incorrectly classified, the ones with $\lambda_i > 0$ and $\xi_i > 1$: such elements are in the wrong halfspace.

Item characterization

Let $\mathbf{x}_i$ be a training set element, then one of the following conditions holds:

1. $\xi_i = 0, \lambda_i = 0$ if $\phi(\mathbf{x}_i)$ is in the correct halfspace, outside the margin strip
2. $\xi_i = 0, 0 < \lambda_i < C$ if $\phi(\mathbf{x}_i)$ is in the correct halfspace, on the maximum margin hyperplane
3. $0 < \xi_i < 1, \lambda_i = C$ if $\phi(\mathbf{x}_i)$ is in the correct halfspace, within the margin strip
4. $\xi_i = 1, \lambda_i = C$ if $\phi(\mathbf{x}_i)$ is on the separating hyperplane
5. $\xi_i > 1, \lambda_i = C$ if $\phi(\mathbf{x}_i)$ is in the wrong halfspace

Item characterization



Classification

From the optimal solution $\boldsymbol{\lambda}^*$ of the dual problem, the coefficients $\mathbf{w}^*$ and b^* can be derived just as done in the linearly separable case.

A new element $\mathbf{x}$ can then be classified, again, through the sign of

$$y(\mathbf{x}) = \sum_{i=1}^{m} w_i^* \phi_i(\mathbf{x}) + b^*$$

or, equivalently, of

$$y(\mathbf{x}) = \sum_{i \in \mathcal{S}} \lambda_j^* t_j \kappa(\mathbf{x}_i, \mathbf{x}_j) + b^*$$

Some comments

- Training time of the standard SVM is $O(n^3)$ (solving QP)

  - Can be prohibitive for large datasets
- Lots of research has gone into speeding up the SVMs
  - Many approximate QP solvers are used to speed up SVMs
  - Online training (e.g., using stochastic gradient descent)
- Several extensions exist
  - More than 2 classes (multiclass classification)
  - Real-valued outputs (support vector regression)

Loss Functions for Linear Classification

- Linear binary classification written as a general optimization problem:

$$\underset{\mathbf{w},w_0}{\text{argmin}}\, L(\mathbf{w},w_0) = \underset{\mathbf{w},w_0}{\text{argmin}} \sum_{i=1}^{n} \mathcal{I}(t_i(\mathbf{w}^Y \boldsymbol{\phi}(\mathbf{x}_i) + w_0) < 0) + \lambda \mathcal{R}(\mathbf{w},w_0)$$

- $\mathcal{I}$ is the indicator function (1 if the condition is true, 0 otherwise)
- The objective is sum of two parts: the loss function and the regularizer
  - Want to fit training data well and also want to have simple solutions
- The above loss function is called the 0-1 loss
- Hard to optimize

Approximations to the 0-1 loss

- We use loss functions that are convex approximations to the 0-1 loss
  - These are called surrogate loss functions
- Examples of surrogate loss functions:
  - Hinge loss: max $(0, 1x)$
  - Log loss: log$(1 + e^{-x})$
  - Exponential loss: e^{-x}
  - All are convex upper bounds on the 0-1 loss
  - Minimizing a convex upper bound also pushes down the original function
  - Unlike 0-1 loss, these loss functions depend on how far the examples are from the hyperplane
- Apart from convexity, smoothness is the other desirable for loss functions
  - Smoothness allows using gradient (or stochastic gradient) descent
  - Note: hinge loss is not smooth at (1,0) but subgradient descent can be used

SVM and gradient descent

A different approach to the problem can be defined by observing that for each item $\mathbf{x}_i$ it is possible to define a cost $c(\mathbf{x}_i)$ as follows:

- if $t_i(\mathbf{w}^T\mathbf{x}_i + w_0) \geq 1$ then $\mathbf{x}_i$ is well classified and external with respect to the margin strip: the cost is $c(\mathbf{x}_i) = 0$

- else, either $\mathbf{x}_i$ is well classified and internal to the strip, or $\mathbf{x}_i$ is wrongly classified: in both cases, we consider as cost the distance of the item from the "correct" margin, $c(\mathbf{x}_i) = 1 - t_i(\mathbf{w}^T\mathbf{x}_i + w_0)$

SVM and gradient descent

The formalization of the problem in the general case

$$\begin{aligned}\min_{\mathbf{w},w_0,\boldsymbol{\xi}} \; & \frac{1}{2}\mathbf{w}^T\mathbf{w} + C\sum_{i=1}^{n}\xi_i \\ & t_i(\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_i) + w_0) \geq 1 - \xi_i \qquad i = 1,\ldots,n \\ & \xi_i \geq 0 \qquad i = 1,\ldots,n\end{aligned}$$

corresponds to the minimization of $\frac{1}{2}\mathbf{w}^T\mathbf{w}$, at the same time minimizing the sum of the costs $c(\boldsymbol{\phi}(\mathbf{x}_i))$, according to a ratio given by C.

In an equivalent way, we can then define the cost function to be minimized as

$$C(\mathbf{w}) = \frac{\alpha}{2}\mathbf{w}^T\mathbf{w} + \sum_{i=1}^{n} h(t_i(\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_i) + w_0))$$

where $h(x)$ is the *hinge* function, defined as $h(x) = 0$ if $x \geq 1$ and $h(x) = x$ otherwise.

SVM and gradient descent

The minimum of $C(\mathbf{w})$ can be derived by gradient descent, noting however that $h(x)$ is not differentiable everywhere (at $x = 0$), hence its gradient is not well defined.

In any case, it is possible to refer to the *subgradient*, which provides a lower bound to the slope of h which holds everywhere

$$\overline{\nabla}_w = -\sum_{\mathbf{x}_i \in L} t_i\boldsymbol{\phi}(\mathbf{x}_i)$$

where $x_i \in L$ iff $c(\boldsymbol{\phi}(\mathbf{x}_i)) > 0$.

The (sub)gradient descent approach derives

$$\mathbf{w}^{(r+1)} = \mathbf{w}^{(r)} - \alpha\mathbf{w}^{(r)} + \sum_{\mathbf{x}_i \in L} t_i\boldsymbol{\phi}(\mathbf{x}_i)$$

Kernel methods motivation

- Often we want to *capture nonlinear patterns* in the data
  - Nonlinear Regression: Input-output relationship may not be linear
  - Nonlinear Classification: Classes may not be separable by a linear boundary
- Linear models (e.g., linear regression, linear SVM) are not just rich enough
- Kernels: Make linear models work in nonlinear settings
  - By mapping data to higher dimensions where it exhibits linear patterns
  - Apply the linear model in the new input space
  - Mapping changing the feature representation
- Note: Such mappings can be expensive to compute in general
  - Kernels give such mappings for (almost) free
    - In most cases, the mappings need not be even computed
    - .. using the Kernel Trick!

Kernels: Formally Defined

- Recall: Each kernel k has an associated basis function ϕ
- ϕ takes input $x \in \mathcal{X}$ (input space) and maps it to $\mathcal{F}$ (feature space)
- Kernel $\kappa(\mathbf{x}_1, \mathbf{x}_2)$ takes two inputs and gives their similarity in $\mathcal{F}$ space

$$\phi : \mathcal{X} \mapsto \mathcal{F}$$
$$\kappa : \mathcal{X} \times \mathcal{X} \mapsto \mathbf{R} \qquad \kappa(\mathbf{x}_1, \mathbf{x}_2) = \phi(\mathbf{x}_1)^T \phi(\mathbf{x}_2)$$

- $\mathcal{F}$ needs to be a vector space with a dot product defined on it (Hilbert space)
- Can just any function be used as a kernel function?
  - No. It must satisfy Mercer's Condition

Mercer's Condition

- For κ to be a kernel function
  - There must exist a Hilbert Space $\mathcal{F}$ for which κ defines a dot product
  - The above is true if κ is a positive definite function

$$\int_{\mathbf{x}_1} \int_{\mathbf{x}_2} f(\mathbf{x}_1)\kappa(\mathbf{x}_1, \mathbf{x}_2)f(\mathbf{x}_2)d\mathbf{x}_1 d\mathbf{x}_2 \qquad \forall f \text{ s.t. } \int_{-\infty}^{+\infty} f(x)^2 dx < \infty$$

Constructing kernel functions

Example 1. Let $\mathbf{x}_1, \mathbf{x}_2 \in \mathbf{R}^2$: $\kappa(\mathbf{x}_1, \mathbf{x}_2) = (\mathbf{x}_1 \cdot \mathbf{x}_2)^2$ is a valid kernel function?
This can be verified by observing that

$$\begin{aligned}\kappa(\mathbf{x}_1, \mathbf{x}_2) &= (x_{11}x_{21} + x_{12}x_{22})^2 \\ &= x_{11}^2 x_{21}^2 + x_{12}^2 x_{22}^2 + 2x_{11}x_{12}x_{21}x_{22} \\ &= (x_{11}^2, x_{12}^2, x_{11}x_{12}, x_{11}x_{12}) \cdot (x_{21}^2, x_{22}^2, x_{21}x_{22}, x_{21}x_{22}) \\ &= \phi(\mathbf{x}_1) \cdot \phi(\mathbf{x}_2)\end{aligned}$$

and by defining the base functions as $\phi(\mathbf{x}) = (x_1^2, x_2^2, x_1x_2, x_1x_2)^T$.

Constructing kernel functions

- In general, if $\mathbf{x}_1, \mathbf{x}_2 \in \mathbf{R}^d$ then $\kappa(\mathbf{x}_1, \mathbf{x}_2) = (\mathbf{x}_1 \cdot \mathbf{x}_2)^2 = \phi(\mathbf{x}_1)^T \phi(\mathbf{x}_2)$, where

$$\phi(\mathbf{x}) = (x_1^2, \ldots, x_d^2, x_1x_2, \ldots, x_1x_d, x_2x_1, \ldots, x_dx_{d-1})^T$$

- the d-dimensional input space is mapped onto a space with dimension $m = d^2$
- observe that computing $\kappa(\mathbf{x}_1, \mathbf{x}_2)$ requires time $O(d)$, while deriving it from $\phi(\mathbf{x}_1)^T \phi(\mathbf{x}_2)$ requires $O(d^2)$ steps

Constructing kernel functions

The function $\kappa(\mathbf{x}_1, \mathbf{x}_2) = (\mathbf{x}_1 \cdot \mathbf{x}_2 + c)^2$ is a kernel function. In fact,

$$\begin{aligned}\kappa(\mathbf{x}_1, \mathbf{x}_2) &= (\mathbf{x}_1 \cdot \mathbf{x}_2 + c)^2 \\ &= \sum_{i=1}^{n}\sum_{j=1}^{n} x_{1i}x_{1j}x_{2i}x_{2j} + \sum_{i=1}^{n}(\sqrt{2}cx_{1i})(\sqrt{2}cx_{2i}) + c^2 \\ &= \boldsymbol{\phi}(\mathbf{x}_1)^T\boldsymbol{\phi}(\mathbf{x}_2)\end{aligned}$$

for

$$\boldsymbol{\phi}(\mathbf{x}) = (x_1^2, \ldots, x_d^2, x_1x_2, \ldots, x_1x_d, x_2x_1, \ldots, x_dx_{d-1}, \sqrt{2c}x_1, \ldots, \sqrt{2c}x_d, c)^T$$

This implies a mapping from a d-dimensional to a $(d+1)^2$-dimensional space.

Constructing kernel functions

Function $\kappa(\mathbf{x}_1, \mathbf{x}_2) = (\mathbf{x}_1 \cdot \mathbf{x}_2 + c)^t$ is a kernel function corresponding to a mapping from a d-dimensional space to a space of dimension

$$m = \sum_{i=0}^{t} d^i = \frac{d^{t+1} - 1}{d - 1}$$

corresponding to all products $x_{i_1}x_{i_2}\ldots x_{i_l}$ with $0 \leq l \leq t$.

Observe that, even if the space has dimension $O(d^t)$, evaluating the kernel function requires just time $O(d)$.

Verifying a given function is a kernel

A necessary and sufficient condition for a function $\kappa : \mathbf{R}^n \times \mathbf{R}^n \mapsto \mathbf{R}^n$ to be a kernel is that, for all sets $(\mathbf{x}_1, \ldots, \mathbf{x}_n)$, the Gram matrix $\mathbf{K}$ such that $k_{ij} = \kappa(\mathbf{x}_i, \mathbf{x}_j)$ is semidefinite positive, that is

$$\mathbf{v}^T\mathbf{K}\mathbf{v} \geq 0$$

for all vectors $\mathbf{v}$.

Techniques for constructing kernel functions

Given kernel functions $\kappa_1(\mathbf{x}_1, \mathbf{x}_2)$, $\kappa_2(\mathbf{x}_1, \mathbf{x}_2)$, the function $\kappa(\mathbf{x}_1, \mathbf{x}_2)$ is a kernel in all the following cases

- $\kappa(\mathbf{x}_1, \mathbf{x}_2) = e^{\kappa_1(\mathbf{x}_1, \mathbf{x}_2)}$
- $\kappa(\mathbf{x}_1, \mathbf{x}_2) = \kappa_1(\mathbf{x}_1, \mathbf{x}_2) + \kappa_2(\mathbf{x}_1, \mathbf{x}_2)$
- $\kappa(\mathbf{x}_1, \mathbf{x}_2) = \kappa_1(\mathbf{x}_1, \mathbf{x}_2)\kappa_2(\mathbf{x}_1, \mathbf{x}_2)$
- $\kappa(\mathbf{x}_1, \mathbf{x}_2) = c\kappa_1(\mathbf{x}_1, \mathbf{x}_2)$, for any $c > 0$
- $\kappa(\mathbf{x}_1, \mathbf{x}_2) = \mathbf{x}_1^T\mathbf{A}\mathbf{x}_2$, with $\mathbf{A}$ positive definite
- $\kappa(\mathbf{x}_1, \mathbf{x}_2) = f(\mathbf{x}_1)\kappa_1(\mathbf{x}_1, \mathbf{x}_2)g(\mathbf{x}_2)$, for any $f, g : \mathbf{R}^n \mapsto \mathbf{R}$
- $\kappa(\mathbf{x}_1, \mathbf{x}_2) = p(\kappa_1(\mathbf{x}_1, \mathbf{x}_2))$, for any polynomial $p : \mathbf{R}^q \mapsto \mathbf{R}$ with non-negative coefficients
- $\kappa(\mathbf{x}_1, \mathbf{x}_2) = \kappa_3(\boldsymbol{\phi}(\mathbf{x}_1), \boldsymbol{\phi}(\mathbf{x}_2))$, for any vector $\boldsymbol{\phi}$ of m functions $\phi_i : \mathbf{R}^n \mapsto \mathbf{R}$ and for any kernel function $\kappa_3(\mathbf{x}_1, \mathbf{x}_2)$ in $\mathbf{R}^m$

Costructing kernel functions

$\kappa(\mathbf{x}_1, \mathbf{x}_2) = (\mathbf{x}_1 \cdot \mathbf{x}_2 + c)^d$ is a kernel function. In fact,

1. $\mathbf{x}_1 \cdot \mathbf{x}_2 = \mathbf{x}_1^T\mathbf{x}_2$ is a kernel function corresponding to the base functions $\boldsymbol{\phi} = (\phi_1, \ldots, \phi_n)$, with $\phi_i(\mathbf{x}) = \mathbf{x}$
2. c is a kernel function corresponding to the base functions $\boldsymbol{\phi} = (\phi_1, \ldots, \phi_n)$, with $\phi_i(\mathbf{x}) = \frac{\sqrt{c}}{n}$
3. $\mathbf{x}_1 \cdot \mathbf{x}_2 + c$ is a kernel function since it is the sum of two kernel functions

4. $(\mathbf{x}_1 \cdot \mathbf{x}_2 + c)^d$ is a kernel function since it is a polynomial with non negative coefficients (in particular $p(z) = z^d$) of a kernel function

Costructing kernel functions

$$\kappa(\mathbf{x}_1, \mathbf{x}_2) = e^{-\frac{||\mathbf{x}_1 - \mathbf{x}_2||^2}{2\sigma^2}}$$

is a kernel function. In fact,

1. since $||\mathbf{x}_1 - \mathbf{x}_2||^2 = \mathbf{x}_1^T\mathbf{x}_1 + \mathbf{x}_2^T\mathbf{x}_2 - 2\mathbf{x}_1^T\mathbf{x}_2$, it results

$$\kappa(\mathbf{x}_1, \mathbf{x}_2) = e^{-\frac{\mathbf{x}_1^T\mathbf{x}_1}{2\sigma^2}} e^{-\frac{\mathbf{x}_2^T\mathbf{x}_2}{2\sigma^2}} e^{\frac{\mathbf{x}_1^T\mathbf{x}_2}{\sigma^2}}$$

2. $\mathbf{x}_1^T\mathbf{x}_2$ is a kernel function (see above)
3. then, $\frac{\mathbf{x}_1^T\mathbf{x}_2}{\sigma^2}$ is a kernel function, being the product of a kernel function with a constant $c = \frac{1}{\sigma^2}$
4. $e^{\frac{\mathbf{x}_1^T\mathbf{x}_2}{\sigma^2}}$ is the exponential of a kernel function, and as a consequence a kernel function itself
5. $e^{-\frac{\mathbf{x}_1^T\mathbf{x}_1}{\sigma^2}} e^{-\frac{\mathbf{x}_1^T\mathbf{x}_1}{2\sigma^2}} e^{\frac{\mathbf{x}_1^T\mathbf{x}_2}{\sigma^2}}$ is a kernel function, being the product of a kernel function with two functions $f(\mathbf{x}_1) = e^{-\frac{\mathbf{x}_1^T\mathbf{x}_1}{2\sigma^2}}$ and $g(\mathbf{x}_2) = e^{-\frac{\mathbf{x}_2^T\mathbf{x}_2}{2\sigma^2}}$

Relevant kernel functions

1. Polynomial kernel

$$\kappa(\mathbf{x}_1, \mathbf{x}_2) = (\mathbf{x}_1 \cdot \mathbf{x}_2 + 1)^d$$

2. Sigmoidal kernel

$$\kappa(\mathbf{x}_1, \mathbf{x}_2) = \tanh\left(c_1\mathbf{x}_1 \cdot \mathbf{x}_2 + c_2\right)$$

3. Gaussian kernel

$$\kappa(\mathbf{x}_1, \mathbf{x}_2) = \exp\left(-\frac{||\mathbf{x}_1 - \mathbf{x}_2||^2}{2\sigma^2}\right)$$

where $\sigma \in \mathbb{R}$

Observe that a gaussian kernel can be derived also starting from a non linear kernel function $\kappa(\mathbf{x}_1, \mathbf{x}_2)$ instead of $\mathbf{x}_1^T\mathbf{x}_2$.