Sparse kernel machines

Maximum margin classifiers

Consider $K=2$ classification using a linear model: $y(\vec{x}) = \vec{w}^T \vec{\varphi}(\vec{x}) + b$

Training dataset: $\vec{x}_1, \ldots, \vec{x}_N$

$t_1, \ldots, t_N \quad t_n \in \{-1, 1\}$

Thus new data points are classified by the sign of $y(\vec{x})$.

Consider a linearly separable dataset:

$\exists$ one or more set $\{\vec{w}, b\}$ s.t.

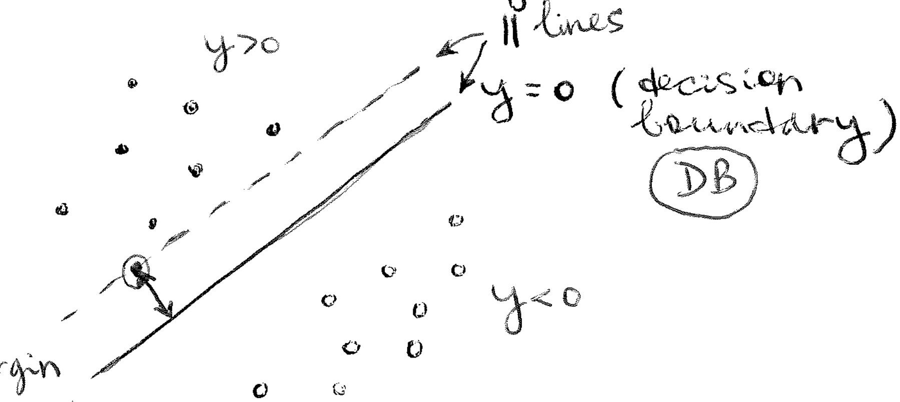
$$\begin{cases} y(\vec{x}_n) > 0 & \text{for all points with } t_n = 1 \\ y(\vec{x}_n) < 0 & \text{for all points with } t_n = -1 \end{cases}$$

$\Rightarrow$ always have $t_n y(\vec{x}_n) > 0$
$n = 1, \ldots, N$

There may be many $\{\vec{w}, b\}$, as was clear with e.g. the perceptron algorithm.

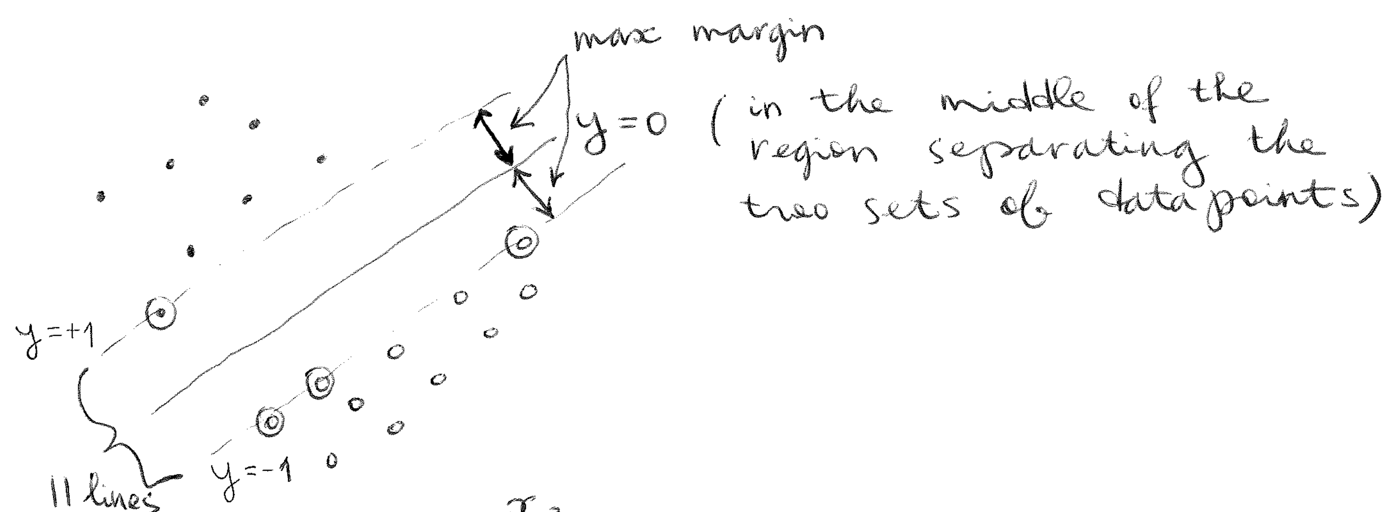
Which one is the best?

Consider an example:

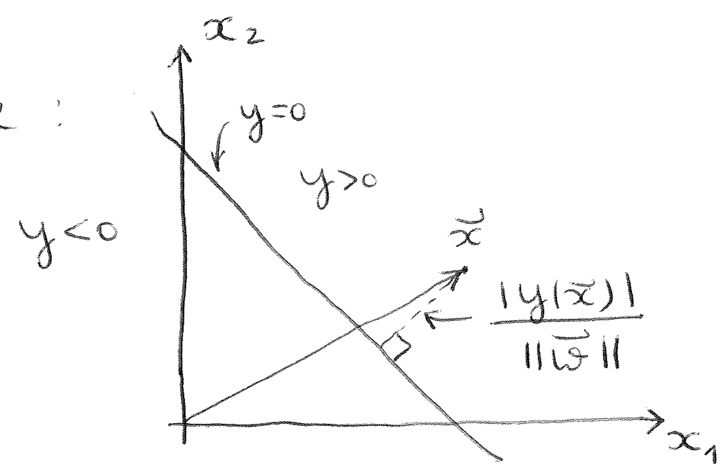


margin (perpendicular distance from the closest datapoint to $y=0$)

<u>Idea</u>: choose $\{\vec{w}, b\}$ which maximize the margin.



Recall:



Thus the distance from $\vec{x}_n$ to $y=0$ is given by:

$$\frac{t_n y(\vec{x}_n)}{\|\vec{w}\|} = \frac{t_n(\vec{w}^T \vec{\varphi}(\vec{x}_n) + b)}{\|\vec{w}\|}.$$

$t_n y(\vec{x}_n) > 0, \ \forall n$

The max margin solution is given by

$$\underset{\vec{w}, b}{\arg\max} \left\{ \frac{1}{\|\vec{w}\|} \underbrace{\min_n [t_n(\vec{w}^T \vec{\varphi}(\vec{x}_n) + b)]}_{\text{finds } \vec{x}_n \text{ closest to DB}} \right\} \quad (*)$$

Note that (*) is inv under $\begin{cases} \vec{w} \to k\vec{w} \\ b \to kb \end{cases} \forall k > 0$

Use this freedom to choose
$t_n(\vec{w}^T \vec{\varphi}(\vec{x}_n) + b) = 1$ for the <u>closest</u> $\vec{x}_n$.

Then $\underbrace{t_n(\vec{w}^T \vec{\varphi}(\vec{x}_n) + b) \geq 1}_{\text{canonical representation of the decision hyperplane}}, \ \forall n \quad (**)$

$\vec{x}_n$'s for which the LHS $= 1$ are called <u>active</u> (there is at least one), while all other $\vec{x}_n$'s are called <u>inactive</u>. Then (*) becomes

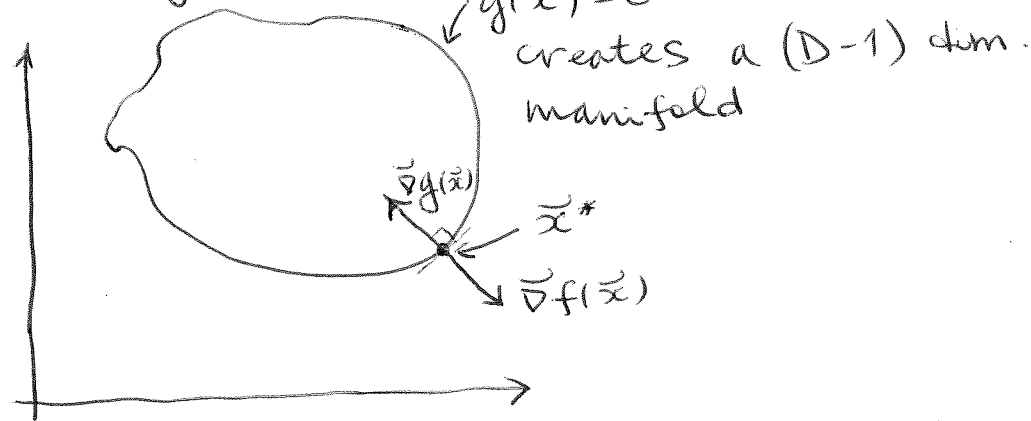
$$\underset{\vec{w}, b}{\arg\max} \left\{ \frac{1}{\|\vec{w}\|} \right\} \Rightarrow \underset{\vec{w}, b}{\arg\min} \left\{ \frac{1}{2} \|\vec{w}\|^2 \right\}$$

It's a quadratic programming problem: minimize a quadratic function subject to linear constraints (**)

This is best approached using Lagrange multipliers.

Lagrange multipliers

Consider $\vec{x} = \overline{x_1, \ldots, x_D}$ subject to a constraint $g(\vec{x}) = 0$



We want to maximize $f(\vec{x})$ subject to $g(\vec{x}) = 0$.

Consider $\underbrace{g(\vec{x} + \vec{\xi})}_{\text{both points lie on the surface}} \simeq g(\vec{x}) + \vec{\xi}^{\,T} \cdot \vec{\nabla} g(\vec{x})$ ← small

both points lie on the surface : $g(\vec{x}+\vec{\xi}) = g(\vec{x}) = 0$

as $\|\vec{\xi}\| \to 0$, $\vec{\xi}^{\,T} \cdot \vec{\nabla} g(\vec{x}) = 0 \Rightarrow$ $\vec{\xi}$ is parallel to the surface in this limit, so $\vec{\nabla} g(\vec{x})$ is $\perp$ surface.

We seek $\vec{x}^*$ on the surface s.t. $f(\vec{x})$ is maximized. At $\vec{x}^*$, $\vec{\nabla} f(\vec{x}) \perp$ surface, otherwise we could move along the gradient & maximize $f(\vec{x})$ further.

Thus $\vec\nabla g \uparrow\downarrow \vec\nabla f$ or $\vec\nabla g \uparrow\uparrow \vec\nabla f$. In both cases,

$$\vec\nabla f + \underbrace{\lambda}_{\text{Lagrange multiplier}} \vec\nabla g = 0 \quad (***) \quad \text{for some } \lambda \neq 0$$

Introduce $L(\vec x, \lambda) = f(\vec x) + \lambda g(\vec x)$, then

$\vec\nabla L = 0$ gives $(***)$ and

$\dfrac{\partial L}{\partial \lambda} = 0 \Rightarrow g(\vec x) = 0$, original constraint

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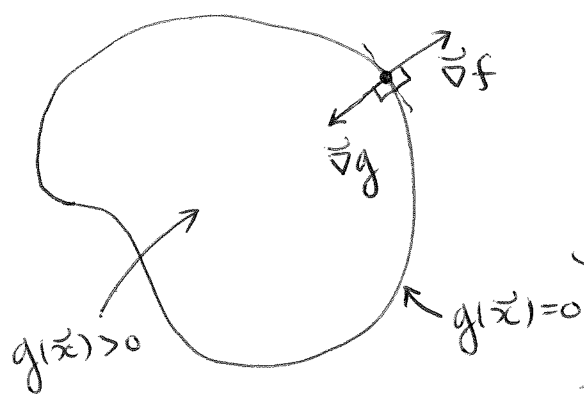
Now, consider $g(\vec x) \geq 0$ ← inequality constraint

If $g(\vec x) > 0 \Rightarrow \vec\nabla f(\vec x) = 0$, or $\vec\nabla L = 0$ with $\lambda = 0$
"constraint inactive"

If $g(\vec x) = 0 \Rightarrow \vec\nabla f + \lambda \vec\nabla g = 0$ as before, for some $\lambda \neq 0$.
"constraint active"



boundary

Note that $\vec\nabla f$ should point away from the $g(\vec x) > 0$ region since otherwise we could improve on it by stepping inside the region

So either $f(\vec x)$ is maximized inside the region **or** on the boundary. In the latter case, $\vec\nabla f$ points *away* from the region.

Note that $\vec\nabla g$ points inward since $g(\vec x) > 0$ inside the boundary

This means that

$$\vec{\nabla} f = -\lambda \vec{\nabla} g \quad \text{for some } \underline{\underline{\lambda > 0}}$$

In either case, $\lambda g(\vec{x}) = 0$.

Thus, maximizing $f(\vec{x})$ subject to $g(\vec{x}) \geq 0$ is the same as finding $\begin{cases} \frac{\partial L}{\partial \lambda} = 0, \\ \vec{\nabla} L = 0 \end{cases}$, subject to

$$\begin{cases} g(\vec{x}) \geq 0, \\ \lambda \geq 0, \\ \lambda g(\vec{x}) = 0 \end{cases} \quad \text{KKT conditions}$$

If we want to $\underline{\text{minimize}}$ $f(\vec{x})$ subject to $g(\vec{x}) \geq 0$, we minimize

$$L(\vec{x}, \lambda) = f(\vec{x}) - \lambda g(\vec{x}) \ : \ \begin{cases} \vec{\nabla} L = 0 \\ \frac{\partial L}{\partial \lambda} = 0 \end{cases}$$

subject to $\lambda \geq 0$

To solve the constrained quadratic programming problem, we introduce

$$\underbrace{\mathcal{L}(\vec{w}, b, \vec{a})}_{\text{need to minimize}} = \frac{1}{2}\|\vec{w}\|^2 - \sum_{n=1}^{N} a_n \{t_n(\vec{w}^T \cdot \vec{\varphi}(\vec{x}_n) + b) - 1\},$$

where $\vec{a} = (a_1, \dots, a_N)$ & $a_n \geq 0, \forall n$ are Lagrange multipliers.

$$\begin{cases} \dfrac{\partial \mathcal{L}}{\partial \vec{w}} = 0 \Rightarrow \vec{w} = \sum_n a_n t_n \vec{\varphi}(\vec{x}_n), \\ \dfrac{\partial \mathcal{L}}{\partial b} = 0 \Rightarrow \sum_n a_n t_n = 0. \end{cases}$$

Then $\mathcal{L} \to \tilde{\mathcal{L}}(\vec{a}) = \sum_n a_n + \frac{1}{2}\sum_{n,m} a_n t_n a_m t_m \times$

$$\times\, \vec{\varphi}^T(\vec{x}_n)\cdot\vec{\varphi}(\vec{x}_m) - \sum_{n,m} a_n t_n a_m t_m \vec{\varphi}^T(\vec{x}_m)\cdot\vec{\varphi}(\vec{x}_n) -$$

$$- b \sum_n \cancel{a_n t_n} = \sum_n a_n - \frac{1}{2}\sum_{n,m} a_n a_m t_n t_m \underbrace{\vec{\varphi}^T(\vec{x}_n)\cdot\vec{\varphi}(\vec{x}_m)}_{\equiv\, k(\vec{x}_n, \vec{x}_m)},$$

subject to $\begin{cases} a_n \geq 0, \quad \forall n \\ \sum_n a_n t_n = 0 \end{cases}$

We need to maximize $\tilde{\mathcal{L}}(\vec{a})$.

minimizing $\tilde{\mathcal{L}}(\vec{a})$ is trivially accomplished by $a_n \to +\infty, \forall n$

To classify new datapoints, need to evaluate the sign of

$$y(\vec{x}) = \vec{w}^T \cdot \vec{\varphi}(\vec{x}) + b = \sum_n a_n t_n \vec{\varphi}^T(\vec{x}_n)\cdot\vec{\varphi}(\vec{x}) + b =$$

$$= \sum_n a_n t_n k(\vec{x}_n, \vec{x}) + b \qquad (*)$$

The KKT conditions are:

$$\begin{cases} a_n \geq 0, \\ t_n y(\vec{x}_n) - 1 \geq 0, \\ a_n \{t_n y(\vec{x}_n) - 1\} = 0 \end{cases} \Rightarrow \quad \text{for each } n, \quad a_n = 0 \text{ OR } t_n y(\vec{x}_n) = 1.$$

If $a_n = 0$, $(*)$ is unaffected, so only the points for which $t_n y(\vec{x}_n) = 1$ matter. These are called <u>support vectors</u>, and lie on the max margin hyperplanes.

If we have $\vec{a}$ by solving the quadratic programming problem, we can find b:

$$t_n \Big(\sum_{\substack{m \in S \\ \uparrow}} a_m t_m k(\vec{x}_n, \vec{x}_m) + b \Big) = 1, \quad \forall n \in S$$

set of support vectors of size N_S

$t_n = t_n^{-1}$: $b = t_n - \sum_{m \in S} a_m t_m k(\vec{x}_n, \vec{x}_m)$

Average over all $n \in S$ for numerical stability:

$$b = \frac{1}{N_S} \sum_{n \in S} \Big[t_n - \sum_{m \in S} a_m t_m k(\vec{x}_n, \vec{x}_m) \Big]$$

Finally, $\vec{w} = \sum_{n \in S} a_n t_n \vec{\varphi}(\vec{x}_n)$.

The max margin classifier can be described by an ~~error~~ function (to be minimized)

corresponds to $(**)$ on p. 3

$$\sum_{n=1}^{N} E_\infty (y(\vec{x}_n) t_n - 1) + \lambda \|\vec{w}\|^2, \quad \text{where}$$

$$E_\infty(z) = \begin{cases} 0, & z \geq 0 \\ \infty, & z < 0 \end{cases}$$

$\lambda > 0$, otherwise its precise value is not important.

Note that max margin classifiers (SVMs) can draw non-linear boundaries in the $\vec{x}$-space, due to use of non-linear kernels (cf. Fig. 7.2 in Bishop).

Overlapping class distributions

So far, we've assumed linear separability in some (potentially unknown explicitly) feature space $\vec{\varphi}(\vec{x})$. We need to modify the SVM to allow for training point misclassification in order to relax this assumption.

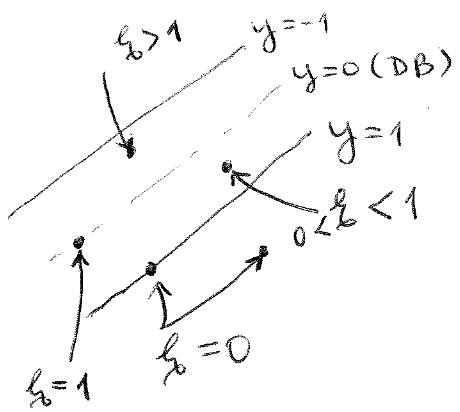
Introduce slack variables:

$$\xi_n > 0 \qquad n = 1, \dots, N$$

s.t. $\xi_n = 0$ for all points on or inside the correct margin boundary &

$\underbrace{\xi_n = |t_n - y(\vec{x}_n)|}_{\text{linear penalty}}$ for ~~misclassified~~ all points $\underbrace{\text{on the wrong side of the margin boundary}}$

Points on DB have $\xi_n = 1$, and all points with $\xi_n > 1$ are misclassified:



Now, $\underbrace{t_n\, y(\vec{x}_n) \geq 1, \ \forall n}_{\text{hard margin constraint}}$

is replaced with

$$\underbrace{\begin{gathered} t_n\, y(\vec{x}_n) \geq 1 - \xi_n, \ \forall n \\ \xi_n \geq 0 \end{gathered}}_{\text{soft margin constraint}}$$