Linear Classification: The Kernel Method

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Recall the core problem of linear classification:

Let P be a set of points in $\mathbb{R}^d$, each of which carries a label 1 or -1. P is **linearly separable**, namely, there is a d-dimensional vector $\boldsymbol{w}$ such that for each $\boldsymbol{p} \in P$:

- $\boldsymbol{w} \cdot \boldsymbol{p} > 0$ if $\boldsymbol{p}$ has label 1;
- $\boldsymbol{w} \cdot \boldsymbol{p} < 0$ if $\boldsymbol{p}$ has label -1.

The plane $\boldsymbol{w} \cdot \boldsymbol{x} = 0$ is a **separation plane** of P.

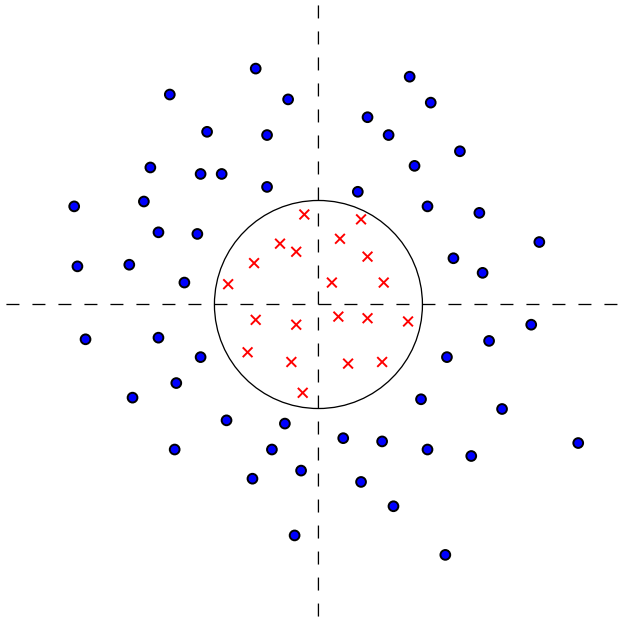
Goal: Find a separation plane of P.

Why the Separable Case Is Important?

So far, we have not paid much attention to **non-separable** datasets. This lecture will give a good reason for this. We will learn a technique — called the **kernel method** — that maps a dataset into another space of higher dimensionality. By applying the method appropriately, we can always guarantee linear separability.

Motivation

Consider the non-separable **circle dataset** P below, where a point p has label 1 if $(p[1])^2 + (p[2])^2 \leq 1$, or -1 otherwise.

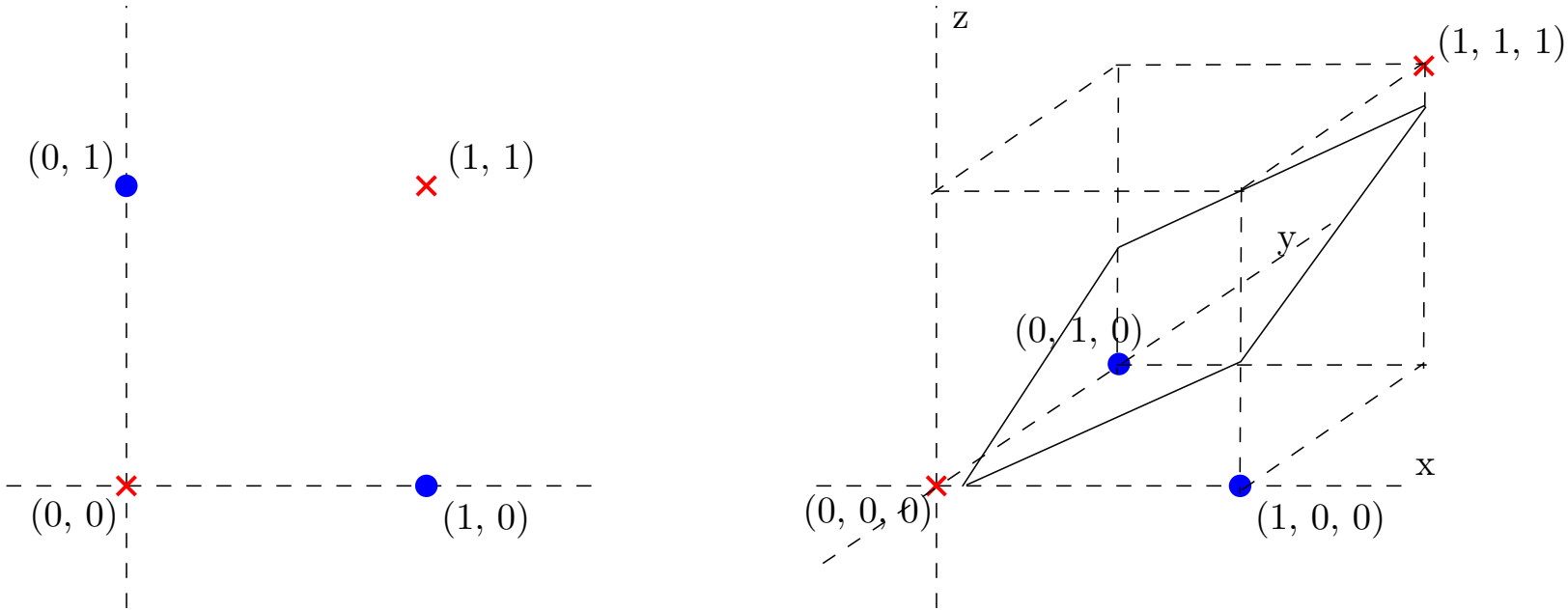


Let us map each point $p \in P$ to a point p' in another space where $p'[1] = (p[1])^2$ and $p'[2] = (p[2])^2$. This gives a new dataset P'.

Clearly the points in P' of the two labels are separated by a linear plane $p'[1] + p'[2] = 1$.

Motivation

The left figure below is another non-separable dataset P (known as the **XOR dataset**).



The right figure shows the 4 points obtained by transforming each 2D point (x, y) to a 3D point (x, y, xy). The new dataset is linearly separable.

Increasing the Dimensionality Guarantees Linearly Separability

Theorem: Let P be an arbitrary set of n points in 1D space, each of which has label 1 or -1. If we map each point $x \in P$ to an n-dimensional point $(1, x, x^2, ..., x^{n-1})$, the set of points obtained is always linearly separable.

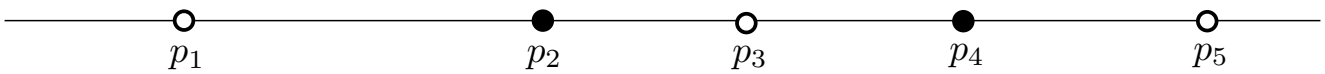
We will prove the theorem in the next two slides.

Increasing the Dimensionality Guarantees Linearly Separability

Proof: Denote the points in P as $p_1, p_2, ..., p_n$ in ascending order. We will consider that n is an odd number (the opposite case left to you). Without loss of generality, assume that p_i has label -1 when $i \in [1, n]$ is an odd integer, and 1 otherwise.

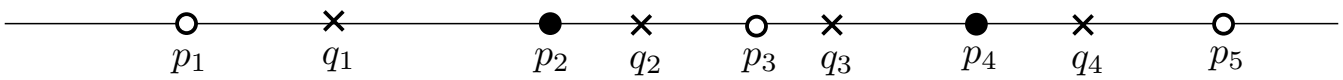
> Here, the labels of the points are "interleaving" (i.e., -1, 1, -1, 1, ...). After you have understood the proof, think how to extend it a non-interleaving P.

The following shows an example where $n = 5$, and the white and black points have labels -1 and 1, respectively.



Increasing the Dimensionality Guarantees Linearly Separability

Proof (cont.): Between p_i and p_{i+1} $(1 \leq i \leq n-1)$, pick an arbitrary point q_i. The figure below shows an example:

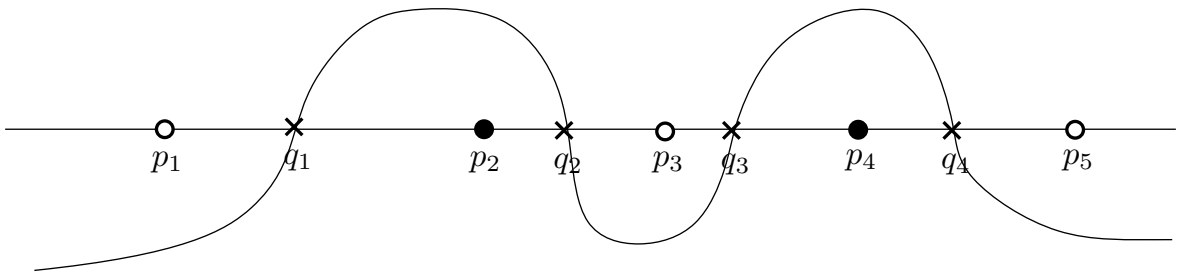


Now consider the following polynomial function

$$f(x) \quad = \quad -(x-q_1)(x-q_2)...(x-q_{n-1}).$$

It must hold that: for every label-(-1) point p, $f(p) < 0$, while for every label-1 point, $f(p) > 0$.

The figure below shows what happens when $n = 5$:



Increasing the Dimensionality Guarantees Linearly Separability

Proof (cont.): Function $f(x)$ can be expanded into the following form:

$$f(x) = c_0 + c_1 x + c_2 x^2 + ... + c_{n-1} x^{n-1}.$$

Therefore, if we convert each point $x \in P$ to a point $(1, x, x^2, ..., x^{n-1})$, the resulting set of n-dimensional points must be separable by a plane passing the origin (of the n-dimensional space). □

Issue: Efficiency

The conversion explained in the proof produces a new space of dimensionality $d' = n$. When d' is large, computation in the converted space can be very expensive (in fact, even enumerating all the coordinates of point takes $\Theta(d')$ time). Is it possible improve the efficiency?

This is where kernel functions come into the picture.

Kernel Function

A **kernel function** K is a function from $\mathbb{R}^d \times \mathbb{R}^d$ to $\mathbb{R}$ with the following property: there is a mapping $\phi : \mathbb{R}^d \to \mathbb{R}^{d'}$ such that, given any two points $p, q \in \mathbb{R}^d$, $K(p, q)$ equals the dot product of $\phi(p)$ and $\phi(q)$.

We will refer to the space $\mathbb{R}^{d'}$ (where $\phi(p)$ is) as the **kernel space**.

We will see two common kernel functions next. Henceforth, a point $p = (p[1], p[2], ..., p[d])$ in $\mathbb{R}^d$ will interchangeably be regarded as a vector $\boldsymbol{p}$. For example, the dot product of two points p, q — written as $\boldsymbol{p} \cdot \boldsymbol{q}$ — equals $\sum_{i=1}^{d} p[i]q[i]$.

Polynomial Kernel

Let p and q be two points in $\mathbb{R}^d$. A **polynomial kernel** has the form:

$$K(\boldsymbol{p}, \boldsymbol{q}) \quad = \quad (\boldsymbol{p} \cdot \boldsymbol{q} + 1)^c$$

for some integer degree $c \geq 1$.

Example

Consider that $d = 2$ and $c = 2$. We can expand the Kernel function as:

$$\begin{aligned} K(\boldsymbol{p}, \boldsymbol{q}) &= (\boldsymbol{p} \cdot \boldsymbol{q} + 1)^2 = (p[1]q[1] + p[2]q[2] + 1)^2 \\ &= 1 + (p[1])^2(q[1])^2 + (p[2])^2(q[2])^2 + \\ &\quad 2(p[1]p[2])(q[1]q[2]) + 2p[1]q[1] + 2p[2]q[2]. \end{aligned}$$

We can regard the above as the dot product of $\phi(p)$ and $\phi(q)$, where $\phi(p)$ is a 6 dimensional point:

$$\phi(p) = (1, p[1]^2, p[2]^2, \sqrt{2}p[1]p[2], \sqrt{2}p[1], \sqrt{2}p[2]).$$

In other words, the converted space has a dimensionality of $d' = 6$.

In general, a polynomial kernel with degree c converts d-dimensional space to $\binom{d+c}{c}$ dimensional space.

Gaussian Kernel (a.k.a. RBF Kernel)

Let p and q be two points in $\mathbb{R}^d$. A **Gaussian kernel** has the form:

$$K(\boldsymbol{p}, \boldsymbol{q}) \quad = \quad \exp\left(-\frac{dist(\boldsymbol{p}, \boldsymbol{q})^2}{2\sigma^2}\right)$$

for a real value $\sigma > 0$ called the **bandwidth**. Note that $dist(\boldsymbol{p}, \boldsymbol{q})$ is the Euclidean distance between p and q, namely,
$dist(\boldsymbol{p}, \boldsymbol{q})^2 = \sum_{i=1}^{d}(p[i] - q[i])^2$.

In general, a Gaussian kernel converts d-dimensional space to another space with infinite dimensionality! We will illustrate this in the next slide for $d = 1$.

Gaussian Kernel (a.k.a. RBF Kernel)

We know from Taylor expansion $e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + ...$
When $d = 1$, $dist(p,q)^2 = p^2 - 2pq + q^2$. Hence:

$$\exp\left(-\frac{dist(p,q)^2}{2\sigma^2}\right) = \exp\left(-\frac{p^2 - 2pq + q^2}{2\sigma^2}\right) =$$

$$\exp\left(-\frac{p^2 + q^2}{2\sigma^2}\right)\exp(\frac{pq}{\sigma^2}) = \frac{1}{e^{\frac{p^2}{2\sigma^2}}}\frac{1}{e^{\frac{q^2}{2\sigma^2}}}\exp(\frac{pq}{\sigma^2})$$

$$= \frac{1}{e^{\frac{p^2}{2\sigma^2}}}\frac{1}{e^{\frac{q^2}{2\sigma^2}}}\left(1 + \frac{pq}{\sigma^2} + \frac{(p/\sigma)^2(q/\sigma)^2}{2!} + \frac{(p/\sigma)^3(q/\sigma)^3}{3!} + ...\right)$$

It is now clear that $\phi(p)$ has the following coordinates:

$$\left(\frac{1}{e^{\frac{p^2}{2\sigma^2}}}, \frac{p/\sigma}{e^{\frac{p^2}{2\sigma^2}}}, \frac{(p/\sigma)^2}{\sqrt{2!}\cdot e^{\frac{p^2}{2\sigma^2}}}, \frac{(p/\sigma)^3}{\sqrt{3!}\cdot e^{\frac{p^2}{2\sigma^2}}}, ...\right)$$

Gaussian Kernel (a.k.a. RBF Kernel)

Theorem: Regardless of the choice of σ, a Gaussian kernel is capable of separating any finite set of points.

The proof will be left as an exercise (with hints).

Finding a Separation Plane in the Converted Space

A Kernel function $K(.,.)$ allows us to convert the original d-dimensional dataset P into another d'-dimensional dataset $P' = \{\phi(p) \mid p \in P\}$ where typically $d' \gg d$. But how do we find a separation plane in the kernel space $\mathbb{R}^{d'}$?

One (naive) idea is to materialize P', but this requires figuring out the details of $\phi(.)$. As shown earlier, this is either cumbersome (e.g., polynomial kernel) or impossible (e.g., Gaussian kernel).

It turns out that we can achieve the purpose without working in the d'-dimensional space at all. Our weapon is, once again, Perceptron!

Recall:

Perceptron

The algorithm starts with $\boldsymbol{w} = (0, 0, ..., 0)$, and then runs in iterations.

In each iteration, it checks whether any point in $p \in P$ violates our requirement according to $\boldsymbol{w}$. If so, the algorithm adjusts $\boldsymbol{w}$ as follows:

- If p has label 1, then $\boldsymbol{w} \leftarrow \boldsymbol{w} + \boldsymbol{p}$.
- If p has label -1, then $\boldsymbol{w} \leftarrow \boldsymbol{w} - \boldsymbol{p}$.

The algorithm finishes if the iteration finds all points of P on the right side of the plane.

In the converted space $\mathbb{R}^{d'}$, it should be modified as:

Perceptron

The algorithm starts with $\boldsymbol{w} = (\underbrace{0, 0, ..., 0}_{d'})$, and then runs in iterations.

In each iteration, it simply checks whether any point in $\phi(p) \in P'$ violates our requirement according to $\boldsymbol{w}$. If so, the algorithm adjusts $\boldsymbol{w}$ as follows:

- If $\phi(p)$ has label 1, then $\boldsymbol{w} \leftarrow \boldsymbol{w} + \phi(p)$.
- If $\phi(p)$ has label -1, then $\boldsymbol{w} \leftarrow \boldsymbol{w} - \phi(p)$.

The algorithm finishes if the iteration finds all points of P' on the right side of the plane.

Next we will show how to implement the algorithm using the Kernel function $K(.,.)$.

Perceptron

For point $p \in P$, denote by t_p the number of times that p has been used to adjust $\boldsymbol{w}$ ($t_p = 0$ if p has never been used before). Let P_{-1} (or P_1) be the set of label-(-1) (or label-1, resp.) points in P.

Hence, the current $\boldsymbol{w}$ is:

$$\boldsymbol{w} = \sum_{p \in P_1} t_p \phi(p) - \sum_{p \in P_{-1}} t_p \phi(p).$$

Perceptron

The key step to implement is this: given an arbitrary point $q \in \mathbb{R}^d$, we want to compute the dot product between $\boldsymbol{w}$ and $\phi(q)$ in the d'-dimensional space. Using the Kernel function $K(.,.)$, we have:

$$\begin{aligned}
\boldsymbol{w} \cdot \phi(q) &= \left(\sum_{p \in P_1} t_p \phi(p) - \sum_{p \in P_{-1}} t_p \phi(p) \right) \phi(q) \\
&= \left(\sum_{p \in P_1} t_p (\phi(p) \cdot \phi(q)) \right) - \left(\sum_{p \in P_{-1}} t_p (\phi(p) \cdot \phi(q)) \right) \\
&= \sum_{p \in P_1} t_p \cdot K(p,q) - \sum_{p \in P_{-1}} t_p \cdot K(p,q).
\end{aligned}$$

Therefore, by maintaining t_p for every $p \in P$, we never need to compute any dot-products in the converted d'-dimensional space.

We finish this lecture with a question for you:

Think: How to apply the margin-based generalization theorem on the set P' of points obtained by the kernel method?