# 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 $-1$. The goal of the **linear classification problem** is to determine whether there is a $d$-dimensional plane

$$x_1 \cdot c_1 + x_2 \cdot c_2 + ... + x_d \cdot c_d = 0$$

which separates the points in $P$ of the two labels.

If the plane exists, then $P$ is said to be **linearly separable**. Otherwise, $P$ is **linearly non-separable**.

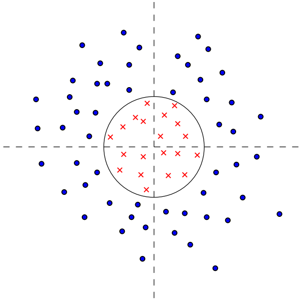
## Why the Separable Case Is Important?

So far, we have not paid much attention to non-separable datasets. All the techniques we have learned are designed for the scenario where $P$ is linearly separable.

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.

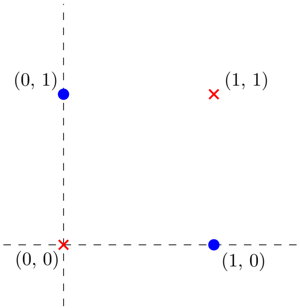


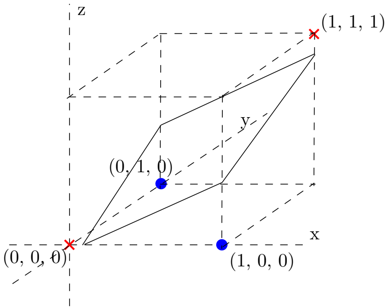
Let us map each point $p \in P$ to a point $p'$ in another space where $p'[1] = (p[1])^2$ and $p'[2] = (p[2])^2$. This gives a new dataset $P'$.

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 after the transformation from a 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.

**Think:** How do you apply the result in 2D? (Hint: just take the x-coordinates; if there are duplicates, rotate the space).

We will prove the theorem in the next two slides.

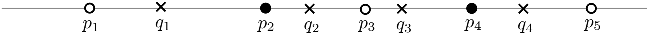
## Increasing the Dimensionality Guarantees Linearly Separability

**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 white and black points have labels $-1$ and 1, respectively.

**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:

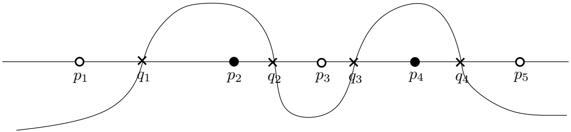



Now consider the following polynomial function

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

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). $\square$

## Issues

The conversion explained in the proof produces a new space of dimensionality $d' = n$. This motivates us to consider two issues?

- **Issue 1:** How to find a conversion with a smaller $d'$?
- **Issue 2:** 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?

## 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:

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

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:

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

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:

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

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

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

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 $\sigma$, 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?