Outline

- The kernel trick

- Soft-margin SVM

What do we need from the $\mathcal{Z}$ space?

$$\mathcal{L}(\boldsymbol{\alpha}) = \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} y_n y_m \, \alpha_n \alpha_m \, \mathbf{z}_n^{\mathsf{T}} \mathbf{z}_m$$

Constraints: $\alpha_n \geq 0$ for $n = 1, \cdots, N$ and $\sum_{n=1}^{N} \alpha_n y_n = 0$

$$\boxed{g(\mathbf{x}) = \operatorname{sign}\left(\mathbf{w}^{\mathsf{T}} \mathbf{z} + b\right)}$$ need $\mathbf{z}_n^{\mathsf{T}} \mathbf{z}$

where $\mathbf{w} = \sum_{\mathbf{z}_n \text{ is SV}} \alpha_n y_n \mathbf{z}_n$

and b: $y_m \left(\mathbf{w}^{\mathsf{T}} \mathbf{z}_m + b\right) = 1$ need $\mathbf{z}_n^{\mathsf{T}} \mathbf{z}_m$

Generalized inner product

Given two points $\mathbf{x}$ and $\mathbf{x}' \in \mathcal{X}$, we need $\mathbf{z}^\intercal\mathbf{z}'$

Let $\mathbf{z}^\intercal\mathbf{z}' = K(\mathbf{x}, \mathbf{x}')$ (the kernel) "inner product" of $\mathbf{x}$ and $\mathbf{x}'$

Example: $\mathbf{x} = (x_1, x_2) \longrightarrow$ 2nd-order Φ

$$\mathbf{z} = \Phi(\mathbf{x}) = (1, x_1, x_2, x_1^2, x_2^2, x_1 x_2)$$

$$K(\mathbf{x}, \mathbf{x}') = \mathbf{z}^\intercal\mathbf{z}' = 1 + x_1 {x'}_1 + x_2 {x'}_2 + x_1^2 {x'}_1^2 + x_2^2 {x'}_2^2 + x_1 {x'}_1 x_2 {x'}_2$$

The trick

Can we compute $K(\mathbf{x}, \mathbf{x}')$ **without** transforming $\mathbf{x}$ and $\mathbf{x}'$?

Example: Consider $K(\mathbf{x}, \mathbf{x}') = (1 + \mathbf{x}^{\intercal}\mathbf{x}')^2 = (1 + x_1 x'_1 + x_2 x'_2)^2$

$$= 1 + x_1^2 x'^2_1 + x_2^2 x'^2_2 + 2x_1 x'_1 + 2x_2 x'_2 + 2x_1 x'_1 x_2 x'_2$$

This is an inner product!

$$(\ 1\ ,\ x_1^2\ ,\ x_2^2\ ,\ \sqrt{2}\,x_1\ ,\ \sqrt{2}\,x_2\ ,\ \sqrt{2}\ x_1 x_2\ )$$

$$(\ 1\ ,\ x'^2_1\ ,\ x'^2_2\ ,\ \sqrt{2}x'_1\ ,\ \sqrt{2}x'_2\ ,\ \sqrt{2}x'_1 x'_2\ )$$

The polynomial kernel

$\mathcal{X} = \mathbb{R}^d$ and $\Phi : \mathcal{X} \to \mathcal{Z}$ is polynomial of order Q

The "equivalent" kernel $K(\mathbf{x}, \mathbf{x}') = (1 + \mathbf{x}^\intercal \mathbf{x}')^Q$

$$= (1 + x_1 x'_1 + x_2 x'_2 + \cdots + x_d x'_d)^Q$$

Compare for $d = 10$ and $Q = 100$

Can adjust scale: $K(\mathbf{x}, \mathbf{x}') = (a\mathbf{x}^\intercal \mathbf{x}' + b)^Q$

We only need $\mathcal{Z}$ to exist!

If $K(\mathbf{x}, \mathbf{x}')$ is an inner product in <u>some</u> space $\mathcal{Z}$, we are good.

Example: $$K(\mathbf{x}, \mathbf{x}') = \exp\left(-\gamma \left\|\mathbf{x} - \mathbf{x}'\right\|^2\right)$$

Infinite-dimensional $\mathcal{Z}$: take simple case

$$K(x, x') = \exp\left(-(x - x')^2\right)$$

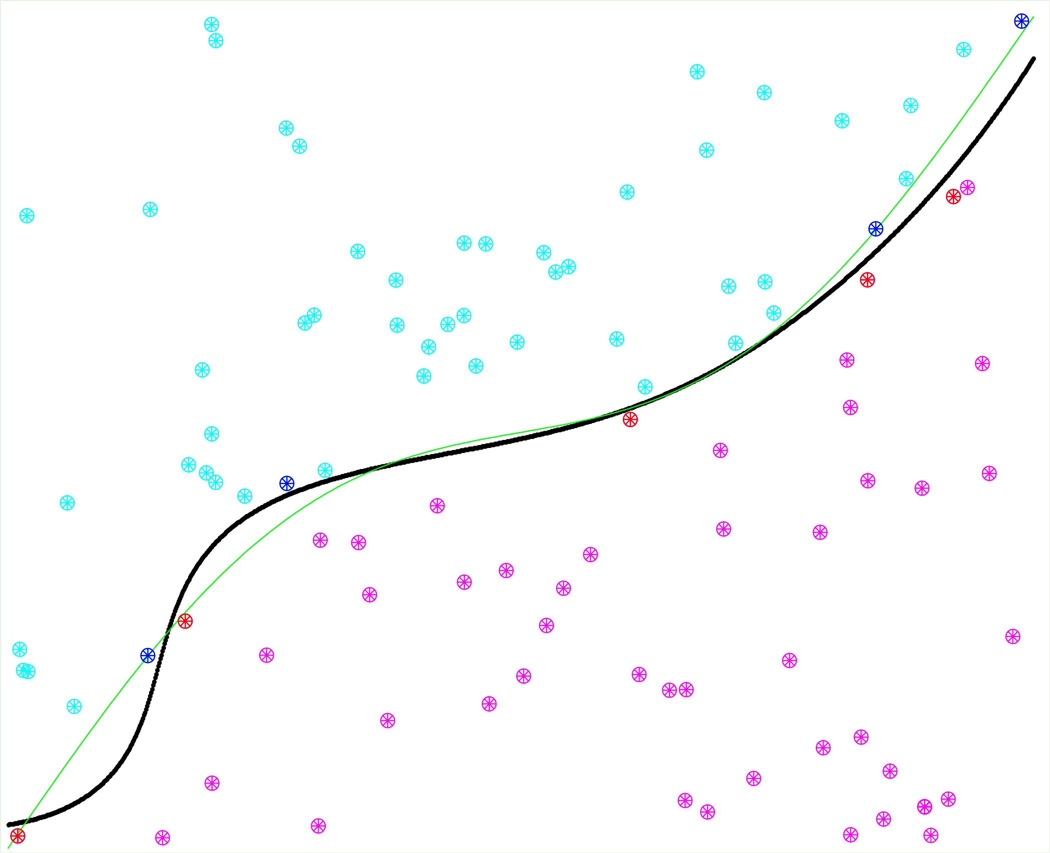
$$= \exp\left(-x^2\right) \exp\left(-{x'}^2\right) \underbrace{\sum_{k=0}^{\infty} \frac{2^k (x)^k (x')^k}{k!}}_{\exp(2xx')}$$

This kernel in action

Slightly non-separable case:

Transforming $\mathcal{X}$ into ∞-dimensional $\mathcal{Z}$

Overkill? Count the support vectors



Kernel formulation of SVM

Remember quadratic programming? The only difference now is:

$$\underbrace{\begin{bmatrix} y_1y_1\,K(\mathbf{x}_1,\mathbf{x}_1) & y_1y_2\,K(\mathbf{x}_1,\mathbf{x}_2) & \ldots & y_1y_N K(\mathbf{x}_1,\mathbf{x}_N) \\ y_2y_1\,K(\mathbf{x}_2,\mathbf{x}_1) & y_2y_2\,K(\mathbf{x}_2,\mathbf{x}_2) & \ldots & y_2y_N K(\mathbf{x}_2,\mathbf{x}_N) \\ \ldots & \ldots & \ldots & \ldots \\ y_Ny_1 K(\mathbf{x}_N,\mathbf{x}_1) & y_Ny_2 K(\mathbf{x}_N,\mathbf{x}_2) & \ldots & y_Ny_N K(\mathbf{x}_N,\mathbf{x}_N) \end{bmatrix}}_{\text{quadratic coefficients}}$$

Everything else is the same.

The final hypothesis

Express $g(\mathbf{x}) = \text{sign}\left(\mathbf{w}^{\intercal}\mathbf{z} + b\right)$ in terms of $K(-,-)$

$$\mathbf{w} = \sum_{\mathbf{z}_n \text{ is SV}} \alpha_n y_n \mathbf{z}_n \quad \Longrightarrow \quad g(\mathbf{x}) = \text{sign}\left(\sum_{\alpha_n > 0} \alpha_n y_n K(\mathbf{x}_n, \mathbf{x}) + b\right)$$

where $$b = y_m - \sum_{\alpha_n > 0} \alpha_n y_n K(\mathbf{x}_n, \mathbf{x}_m)$$

for any support vector $(\alpha_m > 0)$

How do we know that $\mathcal{Z}$ exists . . .

. . . for a given $K(\mathbf{x}, \mathbf{x}')$? valid kernel

Three approaches:

1. By construction
2. Math properties (*Mercer's condition*)
3. Who cares? ☺

Design your own kernel

$K(\mathbf{x}, \mathbf{x}')$ is a valid kernel iff

1. It is symmetric and **2.** The matrix:

$$\begin{bmatrix} K(\mathbf{x}_1, \mathbf{x}_1) & K(\mathbf{x}_1, \mathbf{x}_2) & \dots & K(\mathbf{x}_1, \mathbf{x}_N) \\ K(\mathbf{x}_2, \mathbf{x}_1) & K(\mathbf{x}_2, \mathbf{x}_2) & \dots & K(\mathbf{x}_2, \mathbf{x}_N) \\ \dots & \dots & \dots & \dots \\ K(\mathbf{x}_N, \mathbf{x}_1) & K(\mathbf{x}_N, \mathbf{x}_2) & \dots & K(\mathbf{x}_N, \mathbf{x}_N) \end{bmatrix}$$

is **positive semi-definite**

for any $\mathbf{x}_1, \cdots, \mathbf{x}_N$ (Mercer's condition)