- Kernel Methods
- SVMs

$\theta^T x$ ← input

$\phi : \mathbb{R}^d \to \mathbb{R}^p$ feature map

attributes features

$\phi(x)$: "features"

p: very high $p > n$ or ∞

LMS using gradient descent

Loop {

$$\theta := \theta + \alpha \sum_{i=1}^{n} \left(y^{(i)} - \underbrace{\theta^T}_{\mathbb{R}^p} \underbrace{\phi(x^{(i)})}_{\mathbb{R}^p} \right) \phi(x^{(i)})$$

}

$O(np)$ time

Key observation:

$$\theta = \sum_{i=1}^{n} \beta_i \phi(x^{(i)}) \quad \text{for some } \underbrace{\beta_1 \dots \beta_n}_{\beta \in \mathbb{R}^n} \in \mathbb{R}$$

New algo: update β

p parameters ⟶ n parameters

$$\beta_i := \beta_i + \alpha \left(y^{(i)} - \underbrace{\sum_{j=1}^{n}}_{n} \beta_j \underbrace{\langle \phi(x^{(j)}), \phi(x^{(i)}) \rangle}_{p} \right)$$

① Precompute $\langle \phi(x^{(i)}), \phi(x^{(j)}) \rangle$

$$\langle a, b \rangle = \sum_{i=1}^{p} a_i b_i$$

② $\langle \phi(x^{(i)}), \phi(x^{(j)}) \rangle$ can be computed faster than by explicitly computing $\phi(\ )$

Cubic polynomials

$$\phi(x) = \begin{bmatrix} 1 \\ x_i \\ x_i x_j \\ x_i x_j x_k \end{bmatrix} \quad \begin{matrix} 1 \\ \} d \\ \} d^2 \\ \} d^3 \end{matrix}$$

$$\langle \phi(x), \phi(z) \rangle = \begin{bmatrix} 1 & \cdots & x_i & \cdots & x_i x_j & \cdots & x_i x_j x_k & \cdots \end{bmatrix} \begin{bmatrix} 1 \\ \vdots \\ z_i \\ \vdots \\ z_i z_j \\ \vdots \\ z_i z_j z_k \\ \vdots \end{bmatrix}$$

$$= 1 + \sum_{i=1}^{d} x_i z_i + \sum_{i,j=1}^{d} x_i x_j z_i z_j + \sum_{i,j,k=1}^{d} x_i x_j x_k z_i z_j z_k$$

$$\sum_{i,j=1}^{d} u_i w_j = \left(\sum_{i=1}^{d} u_i \right) \left(\sum_{j=1}^{d} w_j \right)$$

$u_i \rightarrow x_i z_i \quad w_j \rightarrow x_j z_j$

$$= \left(\sum_{i=1}^{d} x_i z_i \right) \left(\sum_{j=1}^{d} x_j z_j \right) = \langle x, z \rangle^2$$

$O(d)$ time

$$= \left(\sum_{i=1}^{d} x_i z_i \right) \left(\sum_{j=1}^{d} x_j z_j \right) \left(\sum_{k=1}^{d} x_k z_k \right)$$

$$= \langle x, z \rangle^3 \qquad O(d) \text{ time}$$

$$\langle \phi(x), \phi(z) \rangle = 1 + \langle x, z \rangle + \langle x, z \rangle^2 + \langle x, z \rangle^3$$

$O(d)$ time

$p = 1 + d + d^2 + d^3 = \Theta(d^3)$

$K(x, z) = \langle \phi(x), \phi(z) \rangle$

$K(\cdot, \cdot)$ is Kernel function

$K : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$

Compute $K(x^{(i)}, x^{(j)})$ $\forall\ i, j$

n^2 entries ~~$O(n^2 p)$~~ $O(n^2 d)$ time

$\beta = 0$

Loop { $\beta_i := \beta_i + \alpha\left(y^{(i)} - \sum_{j=1}^{n} \beta_j \langle \phi(x^{(i)}), \phi(x^{(j)}) \rangle\right)$

$= \beta_i + \alpha\left(y^{(i)} - \sum_{j=1}^{n} \beta_j K(x^{(i)}, x^{(j)})\right)$

}

$K \in \mathbb{R}^{n \times n}$ Kernel matrix

$K_{ij} = K(x^{(i)}, x^{(j)})$

$\beta := \beta + \alpha(\vec{y} - K\beta)$ $O(n^2)$ time

Test time: given x, predict $\theta^T \phi(x)$

$\theta^T \phi(x) = \left(\sum_{i=1}^{n} \beta_i \phi(x^{(i)})\right)^T \phi(x)$

$= \sum_{i=1}^{n} \beta_i \langle \phi(x^{(i)}), \phi(x) \rangle = \sum_{i=1}^{n} \beta_i \cdot K(x^{(i)}, x)$

linear in # examples, independent of p

Training: Preprocessing: $O(n^2 d)$

training: $O(n^2) \times$ # iterations

Test time: $O(nd)$ assuming $K(\cdot,\cdot)$ can be computed in $O(d)$ time

Deeper Observation

- the only thing needed is $K(\cdot,\cdot)$

function $K(\cdot,\cdot)$ is valid (Kernel fn)

if $\exists\ \phi$ s.t. $K(x, z) = \langle \phi(x), \phi(z) \rangle$

Design some $K(\cdot,\cdot)$

Verify validity (by math)

run algo

Other algos can be "kernelized"

perceptron, logistic regression

- algo for linear $\theta^T x$
- replace x by $\phi(x)$
- rewrite algo s.t. it only depends on $\langle \phi(x), \phi(z) \rangle$

Kernel fns:

$$K(x,z) = 1 + x^Tz + (x^Tz)^2 + (x^Tz)^3$$

$$K(x,z) = (x^Tz)^2$$

$$K(x,z) = (x^Tz + c)^2 \qquad \phi(x) = \begin{bmatrix} c \\ \sqrt{2c}\, x_i \\ \vdots \\ x_i x_j \end{bmatrix}$$

Polynomial kernel $K(x,z) = (x^Tz + c)^K$ $\sim \binom{d+K}{K}$ monomials

$$K(x,z) = \exp\left(-\frac{\|x-z\|^2}{2\sigma^2}\right) = \langle \phi(x), \phi(z) \rangle$$

ϕ : ∞ dimensional

Valid Kernel?

Necessary condn

n examples $x^{(1)} \ldots x^{(n)}$

Kernel matrix $K_{ij} = K(x^{(i)}, x^{(j)})$

Claim: Kernel matrix is positive semidefinite

$$K \succeq 0$$

$$z^T K z \geq 0 \qquad \forall z \in \mathbb{R}^n$$

$K(\cdot,\cdot)$ valid if $\exists \phi$ s.t. $K_{ij} = \langle \phi(x^{(i)}), \phi(x^{(j)}) \rangle$

$$z^T K z = \sum_{i=1}^{n} \sum_{j=1}^{n} z_i K_{ij} z_j$$

$$= \sum_{i=1}^{n} \sum_{j=1}^{n} z_i \langle \phi(x^{(i)}), \phi(x^{(j)}) \rangle z_j$$

$$= \left\langle \sum_{i=1}^{n} z_i \phi(x^{(i)}) , \sum_{j=1}^{n} z_j \phi(x^{(j)}) \right\rangle$$

$$\geq 0$$

also sufficient

Theorem (Mercer, 1909)

$K: \mathbb{R}^d \times \mathbb{R}^d \longrightarrow \mathbb{R}$ is a valid kernel fn

if for any $n < \infty$ and any $x^{(1)} \ldots x^{(n)} \in \mathbb{R}^d$

the kernel matrix $K_{ij} := K(x^{(i)}, x^{(j)})$

is positive semidefinite

$\Longrightarrow$

$\Longleftarrow$

eg. Protein sequence classification

20 amino acids

A, B, C ...

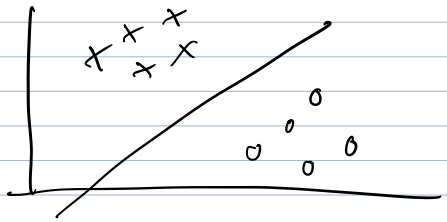
A B A C B D A ...

$\phi(x) =$ [0 AAAA, 2 AAAB, ...]

20^4 dimensional vector

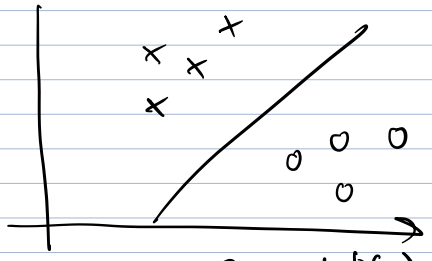
$\langle \phi(x), \phi(z) \rangle$ can be computed via dynamic programming

SVM: support vector machines



$\{x : w^T x + b = 0\}$

Space of X



Space of $\phi(x)$

$y^{(i)} \in \{-1, +1\}$

$\{x : w^T x + b = 0\}$

$\{x : w^T \phi(x) + b = 0\}$

linear in kernel space

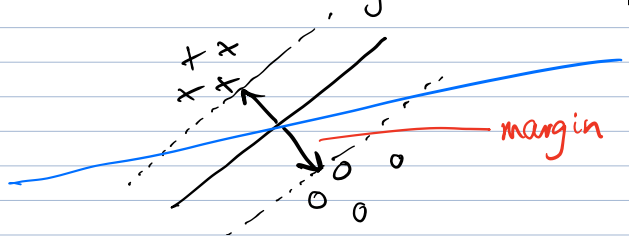
$\phi(x) = x$

Find w, b s.t.

If $y^{(i)} = 1$, $w^T x^{(i)} + b > 0$ ①

$y^{(i)} = -1$, $w^T x^{(i)} + b < 0$ ②

Choose (w, b) that give the most separation



Amongst all (w, b) pairs that satisfy ①, ②

$$\max_{w,b} \left[\min_i \text{dist}\left(x^{(i)}, \text{decision boundary}\right) \right]$$

① , ② $\Rightarrow$ $y^{(i)}(w^T x^{(i)} + b) > 0 \quad \forall\, i$

Fact: $\text{dist}\left(x^{(i)}, \text{boundary}\right) = \dfrac{|w^T x^{(i)} + b|}{\|w\|_2}$

$$= \frac{y^{(i)}(w^T x^{(i)} + b)}{\|w\|_2}$$

$$\max_{w,b} \quad \min_{i \in \{1 \dots n\}} \quad \frac{y^{(i)}(w^T x^{(i)} + b)}{\|w\|_2}$$

$\theta^T x \equiv w^T x + b$

scaling invariant $(w, b) \longrightarrow (10w, 10b)$

$$\Longleftrightarrow \min \frac{1}{2}\|w\|_2^2$$

$$\text{s.t. } y^{(i)}(w^T x^{(i)} + b) \geq 1 \quad \forall\, i$$

Facts (non trivial) (need KKT cond^n)

① Optimal sol^n w^*, b^* satisfies

$$w^* = \sum_{i=1}^{n} \alpha_i\, x^{(i)} y^{(i)} \qquad \alpha_i \geq 0 \qquad \alpha_i \in \mathbb{R}$$

② $\alpha = (\alpha_1 \dots \alpha_n)$ is optimal sol^n of program

$$W(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} y^{(i)} y^{(j)} \alpha_i \alpha_j \langle x^{(i)}, x^{(j)} \rangle$$

$K(x^{(i)}, x^{(j)})$

$$\text{s.t. } \alpha_i \geq 0$$

$$\sum_{i=1}^{n} \alpha_i y^{(i)} = 0$$

$$w^* = \sum_{i=1}^{n} \alpha_i \phi(x^{(i)}) y^{(i)}$$

test time: $w^{*T} \phi(x) = \sum_{i=1}^{n} \alpha_i \langle \phi(x^{(i)}), \phi(x) \rangle y^{(i)}$

$$= \sum_{i=1}^{n} \alpha_i K(x^{(i)}, x)\, y^{(i)}$$

Random Features, Random Kitchen Sinks

Rahimi, Recht [NeurIPS 2007]

Fast Food [ICML 2013]

Le, Sarlos, Jordan