- Kernel Methods
- SVMs

$\theta^T x$

$\uparrow$ input

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

attributes features

$\phi(x)$: "features"

p : very high $p > n$ p ∞

LMS using gradient descent

Loop {

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

}

each iteration: $O(np)$ time

Key observation:

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

$\theta \in \mathbb{R}^p$

New algo : update β

$$\theta = \sum_{i=1}^{n} \underbrace{\left(\beta_i + \alpha\left(y^{(i)} - \theta^T \phi(x^{(i)})\right)\right)}_{\text{new } \beta_i} \phi(x^{(i)})$$

p parameters $\longrightarrow$ n parameters

$$\beta_i := \beta_i + \alpha\left(y^{(i)} - \theta^T \phi(x^{(i)})\right)$$

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

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

Precompute

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

$\langle a, b \rangle = \sum_{i=1}^{p} a_i b_i$ $\qquad a = (a_1 \ldots a_p)$, $b = (b_1 \ldots b_p)$

② $\langle \phi(x^{(i)}), \phi(x^{(j)}) \rangle$ can often be computed much faster without explicitly computing $\phi(\ )$

eg. cubic polynomials

$$\phi(x) = \begin{bmatrix} 1 \\ \vdots \\ x_i \\ \vdots \\ x_i x_j \\ \vdots \\ x_i x_j x_k \\ \vdots \end{bmatrix} \begin{array}{l} \\ \\ \}\, d \\ \\ \}\, d^2 \\ \\ \}\, d^3 \\ \\ \end{array}$$

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

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

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

$$u_i \to x_i z_i, \quad w_j \to x_j z_j$$

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

$O(d)$ 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 $\quad (p = 1 + d + d^2 + d^3 = \theta(d^3))$

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

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

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

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

n^2 entries $\cancel{O(n^2 p)}$ $O(n^2 d)$ time

$\beta = 0$

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

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

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

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

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

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

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

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

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 you need 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 also 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:

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

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

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

polynomial kernel $K(x,z) = (x^T z + c)^k$ $\sim \binom{d+k}{k}$ 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 cond^n

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

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

Claim: Kernel matrix is positive semidefinite

$K \succeq 0$

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

also sufficient

Theorem (Mercer, 1909)

$K: \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is a valid kernel f^n

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

eg. Protein sequence classification

20 amino acids

A, B, C . . .

$\phi(x)$

AAAA

AAAB

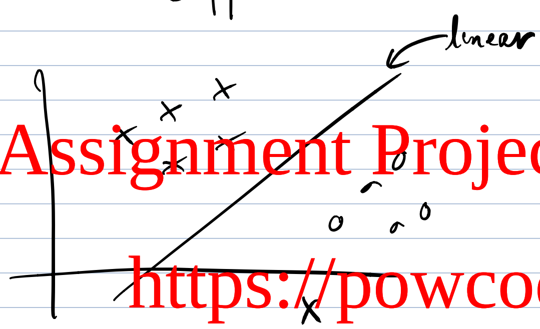
$\vdots$

$20^4 = 160{,}000$

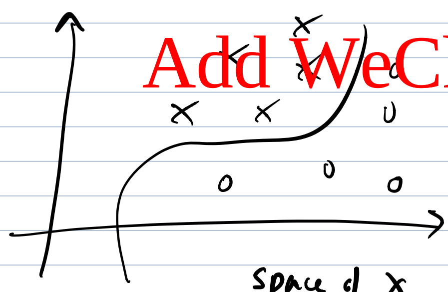
AAAA $\begin{bmatrix} \\ 0 \\ 2 \\ 1 \end{bmatrix}$

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

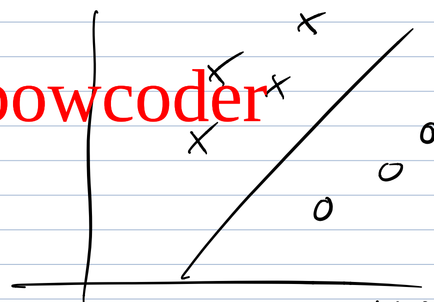
SVM : support vector machines



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



space of X



space of $\phi(x)$

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

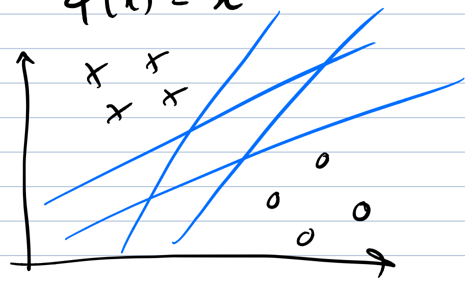
$\{x : w^T x + b = 0\}$

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

linear in Kernel space

Find w, b

$\phi(x) = x$

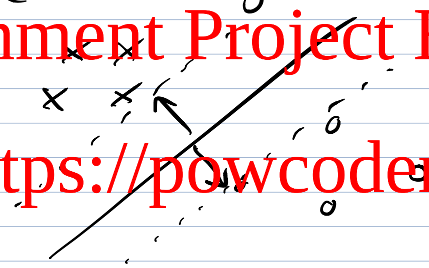


Find w, b s.t.

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

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

Choose the (w, b) that gives the most separation



Among all (w, b) satisfy ①, ②

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

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

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

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

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

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

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

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

Facts (non trivial) (need KKT condⁿ)

① Optimal solⁿ w^*, b^* satisfies

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

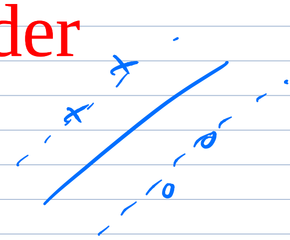
② α is optimal solⁿ of program

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

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

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

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



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

test time:

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

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