

check if kernels are valid?

Let $K(x, z)$ be a kernel where $x, z \in \mathbb{R}^n$ and are

feature vectors. i.e. $x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}_{n \times 1}$ $z = \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{bmatrix}_{n \times 1}$

$K(x, z)$ must be expressed in

$\phi^T(x) \phi(z)$ or $\langle \phi(x), \phi(z) \rangle$

i.e. $K(x, z) = \phi^T(x) \cdot \phi(z) = \langle \phi(x), \phi(z) \rangle$
 $K(x, z) \in \mathbb{R}$

Tutorial Problems.

Polynomial kernel

1) Check if $K(x, z) = (x^T z)^2$ is a valid kernel?
 Soln. Let $x, z \in \mathbb{R}^n$

$$\begin{aligned} K(x, z) &= \left([x_1, x_2, x_3, \dots, x_n] \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{bmatrix} \right)^2 \\ &= \left(\sum_{i=1}^n x_i z_i \right)^2 = \left(\sum_{i=1}^n x_i z_i \right) \left(\sum_{j=1}^n x_j z_j \right) \\ &= (x_1 z_1 + x_2 z_2 + \dots + x_n z_n) (x_1 z_1 + \dots + x_n z_n) \\ &= \sum_{i=1}^n \sum_{j=1}^n x_i z_i x_j z_j = \sum_{i=1}^n \sum_{j=1}^n x_i x_j z_i z_j \end{aligned}$$

$$\phi(x) = \begin{bmatrix} x_1 x_1 \\ x_1 x_2 \\ x_1 x_3 \\ \vdots \\ x_2 x_1 \\ x_2 x_2 \\ \vdots \\ x_3 x_1 \\ x_3 x_2 \\ \vdots \\ x_3 x_3 \end{bmatrix}$$

$$\phi(z) = \begin{bmatrix} z_1 z_1 \\ z_1 z_2 \\ z_1 z_3 \\ \vdots \\ z_2 z_1 \\ z_2 z_2 \\ \vdots \\ z_3 z_1 \\ z_3 z_2 \\ \vdots \\ z_3 z_3 \end{bmatrix}$$

$$K(x, z) = \phi^T(x) \phi(z)$$

2. check if $K(x, z) = (x^T z + c)^2$ is valid kernel?
 $x, z \in \mathbb{R}^n$

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

$$= (x^T z)^2 + c^2 + 2c x^T z$$

$$= \sum_{i=1}^n \sum_{j=1}^n x_i x_j z_i z_j + c^2 + 2c \sum_{i=1}^n x_i z_i$$

$$= \sum_{i=1}^n \sum_{j=1}^n x_i x_j z_i z_j + c \cdot c + \sum_{i=1}^n \sqrt{2c} x_i \sqrt{2c} z_i$$

$$\phi(x) = \begin{bmatrix} x_1 x_1 \\ x_1 x_2 \\ x_1 x_3 \\ 1 \\ \\ x_3 x_3 \\ \sqrt{2c} x_1 \\ \sqrt{2c} x_2 \\ \sqrt{2c} x_3 \\ c \end{bmatrix}$$

$$= \phi^T(x) \phi(z) + c \cdot c + \sum_{i=1}^n \sqrt{2c} x_i \sqrt{2c} z_i$$

Prove Gaussian kernel $k(x, z) = \exp\left(-\frac{\|x-z\|^2}{2\sigma^2}\right)$ is a valid kernel?

Let $x, z \in \mathbb{R}^n$

$$k(x, z) = \exp\left(-\frac{\|x-z\|^2}{2\sigma^2}\right)$$

using $e^{a+b} = e^a \cdot e^b$

$$k(x, z) = \exp\left(-\frac{\|x\|^2 + \|z\|^2 - 2\|x\|\|z\|}{2\sigma^2}\right)$$

$$= \exp\left(-\frac{x^T x + z^T z - 2x^T z}{2\sigma^2}\right)$$

$$= e^{-\frac{x^T x}{2\sigma^2}} \cdot e^{-\frac{z^T z}{2\sigma^2}} \cdot e^{\frac{x^T z}{\sigma^2}}$$

it can be assumed as linear kernels, scaled by $\frac{1}{2\sigma^2}$ and exponent applied.

Date: 28.5.2018

Mercer Theorem for Validating Kernels?

Statement: Let $K(x, z)$ be given. Then K is a valid (Mercer) kernel (i.e. $\exists \phi$ s.t. $K(x, z) = \phi^T(x) \phi(z)$) if and only if for all $\{x^{(1)}, x^{(2)}, \dots, x^{(m)}\}$, $m < \infty$ the kernel matrix $K \in \mathbb{R}^{m \times m}$ is symmetric positive semi-definite.

Proof: To prove: A valid kernel matrix is positive-semi-definite.
 Let $K(x, z)$ be a valid kernel.
 s.t. $\exists \phi$ s.t. $K(x, z) = \phi^T(x) \phi(z) = \langle \phi(x), \phi(z) \rangle$
 For set of points i.e. training examples $\{x^{(1)}, x^{(2)}, \dots, x^{(m)}\}$
 for any pair of points/training examples $x^{(i)}, x^{(j)}$ we can define $K(x^{(i)}, x^{(j)})$. So, we can have such $m \times m$ kernels.



Kernel matrix \uparrow

$$K = \begin{bmatrix} K(x^{(1)}, x^{(1)}) & K(x^{(1)}, x^{(2)}) & \dots & K(x^{(1)}, x^{(m)}) \\ K(x^{(2)}, x^{(1)}) & K(x^{(2)}, x^{(2)}) & \dots & K(x^{(2)}, x^{(m)}) \\ \vdots & \vdots & \ddots & \vdots \\ K(x^{(m)}, x^{(1)}) & K(x^{(m)}, x^{(2)}) & \dots & K(x^{(m)}, x^{(m)}) \end{bmatrix}$$

$m \times m$

$K_{ij} = K(x^{(i)}, x^{(j)}) = \langle \phi(x^{(i)}), \phi(x^{(j)}) \rangle = \phi^T(x^{(i)}) \phi(x^{(j)})$
 \uparrow (i, j)th element

define some $z_i \in \mathbb{R}^m$

writes $Z^T K Z$

$$Z^T K Z = \sum_{i=1}^m \sum_{j=1}^m Z_i^T K Z_j$$

$$= \sum_{i=1}^m \sum_{j=1}^m \phi(x_i)^T \phi(x_j) Z_i^T Z_j$$

$$= \sum_{i=1}^m \sum_{j=1}^m Z_i^T \sum_{k=1}^m \phi(x_i)_k \phi(x_j)_k Z_j$$

$$= \sum_{k=1}^m \sum_{i=1}^m \sum_{j=1}^m Z_i (\phi(x_i)_k) (\phi(x_j)_k) Z_j$$

$$= \sum_{k=1}^m \sum_{i=1}^m Z_i (\phi(x_i)_k)^2 \geq 0$$

Sum of squares $\therefore K \succeq 0$

Positive semi-definite.