

Machine Learning Lecture 8

Kernel Method

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1 Exercise 1

Dual representation

Start with Ridge Regression loss function

$$L = \frac{1}{N} \sum_{i=1}^N (\hat{y}_i - y_i)^2 + \|w\|_2^2$$

$$L = \frac{1}{N} \sum_{i=1}^N (w^T \phi(x_i) - y_i)^2 + \|w\|_2^2$$

Take derivative of L with respect to w, we have:

$$\frac{\partial L}{\partial w} = \sum_{i=1}^N (\phi(x_i)(w^T \phi(x_i) - y_i) + \lambda w$$

$$\rightarrow w = \frac{-1}{\lambda} \sum_{i=1}^N (\phi(x_i)(w^T \phi(x_i) - y_i)$$

w is a combination of inputs in featured space ($\phi(x_n) \mid 1 \leq n \leq N$)

$$w = \frac{-1}{\lambda} \sum_{i=1}^N \phi(x_i) a_i$$

$$w = \frac{-1}{\lambda} \phi^T a, \quad \phi = [\phi(x_1), \phi(x_2), \dots, \phi(x_N)]$$

$$a = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{bmatrix} = \begin{bmatrix} w^T \phi(x_1) - y_1 \\ w^T \phi(x_2) - y_2 \\ \vdots \\ w^T \phi(x_N) - y_N \end{bmatrix} \text{ and } a_i = w^T \phi(x_i) - y_i$$

The loss function in matrix form

$$\begin{aligned}
L &= \frac{1}{2} \|\phi w - y\|_2^2 + \frac{\lambda}{2} \|w\|_2^2 \\
&= \frac{1}{2}(\phi w - y)^T(\phi w - y) + \frac{\lambda}{2} w^T w \\
&= \frac{1}{2}(\phi^T w^T - y^T)(\phi w - y) + \frac{\lambda}{2} w^T w \\
&= \frac{1}{2}(\phi^T w^T \phi w - w^T \phi^T y - y^T \phi w + y^T y) + \frac{\lambda}{2} w^T w \\
&= \frac{1}{2}\phi^T w^T \phi w - y^T \phi w + \frac{1}{2}y^T y + \frac{\lambda}{2} w^T w
\end{aligned}$$

Substitute $w = \frac{-1}{\lambda} \phi^T a$

$$= \frac{1}{2\lambda^2} a^T \phi \phi^T \phi \phi^T a + \frac{1}{\lambda} y^T \phi \phi^T a + \frac{1}{2} \frac{1}{\lambda^2} a^T \phi \phi^T a$$

$$\rightarrow L(a, \phi, t) = \frac{1}{2\lambda^2} a^T \phi \phi^T \phi \phi^T a - a^T \phi \phi^T t + \frac{1}{2} t^T t + \frac{\lambda}{2} a^T \phi \phi^T a$$

Let $K = \phi \phi^T$ [K is symmetric]

$$L = \frac{1}{2} a^T K K a - a^T K t + \frac{\lambda}{2} a^T K a + \frac{1}{2} t^T t$$

** Proof that K is positive semi-definite:

$$\iff v^T K v \geq 0 \text{ with } v \in R^n$$

$$v^T K v = v^T \phi \phi^T v = \|\phi^T v\|_2^2 \geq 0$$

Take the derivative of L with respect to a:

$$\begin{aligned}
\frac{\partial L}{\partial a} &= a K K - K t + \lambda a &= 0 \\
K(K a - t + \lambda a) &= 0 \\
K a - t + \lambda a &= 0 \\
a(K + \lambda I_n) &= t \\
a &= (K + \lambda I_n)^{-1} t
\end{aligned}$$

2 Exercise 2: Prove valid kernels

2.1 Prove that $ck_1(x, x')$ is a valid kernel

Since $k_1(x, x')$ is a valid kernel, it can be written as:

$$\begin{aligned} k_1(x, x') &= \phi(x^T)\phi(x') \\ k(x, x') &= ck_1(x, x') = [\sqrt{c}\phi(x)]^T[\sqrt{c}\phi(x')] \end{aligned}$$

$\rightarrow ck_1(x, x')$ is a valid kernel

2.2 Prove that $k(x, x') = f(x)k_1(x, x')f(x')$ is a valid kernel

Since $k_1(x, x')$ is a valid kernel, it can be written as:

$$\begin{aligned} k_1(x, x') &= \phi(x^T)\phi(x') \\ k(x, x') &= f(x)k_1(x, x')f(x') = f(x)\phi(x)^T\phi(x')f(x') \\ &= (f(x)\phi(x))^T(f(x')\phi(x')) \\ \text{With } \bar{\phi}(x) &= f(x)\phi(x), k(x, x') = \bar{\phi}(x)^T\bar{\phi}(x') \end{aligned}$$

$\rightarrow f(x)k_1(x, x')f(x')$ is a valid kernel

3 Exercise 3: Compute kernel matrix

$$X = [(-3, 4), (1, 0)]$$

$$\phi(x) = [x_1, x_2, \|x\|]^T$$

$$\begin{aligned} \phi((-3, 4)) &= [-3, 4, 5]^T \\ \phi((1, 0)) &= [1, 0, 1]^T \\ \phi((-3, 4))^T\phi((-3, 4)) &= 50 \\ \phi((-3, 4))^T\phi((1, 0)) &= 2 \\ \phi((1, 0))^T\phi((1, 0)) &= 2 \end{aligned}$$

$$K = \begin{bmatrix} 50 & 2 \\ 2 & 2 \end{bmatrix}$$