

Introduction to Machine Learning

Kernel Methods

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1 Kernel Methods

1.1 Extension to Non-Vector Data Examples

- What if $\mathbf{x} \notin \mathbb{R}^D$?

- Does $\mathbf{w}^\top \mathbf{x}$ make sense?
- How to adapt?
 1. Extract features from \mathbf{x}
 2. Is not always possible
- Sometimes it is easier/natural to compare two objects.
 - A similarity function or **kernel**
 - Nonparametric method
- Domain-defined measure of similarity

Example 1. Strings: Length of longest common subsequence, inverse of edit distance

Example 2. Multi-attribute Categorical Vectors: Number of matching values

1.2 Kernel Regression

- Ridge regression estimate:

$$\mathbf{w} = (\lambda I_D + \mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$$

- Prediction at \mathbf{x}^* :

$$y^* = \mathbf{w}^\top \mathbf{x}^* = ((\lambda I_D + \mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y})^\top \mathbf{x}^*$$

- Still needs training and test examples as D length vectors
- Rearranging above (Sherman-Morrison-Woodbury formula or *Matrix Inversion Lemma* [See Murphy p120, Matrix Cookbook])

$$y^* = \mathbf{y}^\top (\lambda I_N + \mathbf{X} \mathbf{X}^\top)^{-1} \mathbf{X} \mathbf{x}^*$$

The above mentioned “rearrangement” can be obtained using the *Matrix Inversion Lemma*, which in general term states for matrices $\mathbf{E}, \mathbf{F}, \mathbf{G}, \mathbf{H}$:

$$(\mathbf{E} - \mathbf{F}\mathbf{H}^{-1}\mathbf{G})^{-1}\mathbf{F}\mathbf{H}^{-1} = \mathbf{E}^{-1}\mathbf{F}(\mathbf{H} - \mathbf{G}\mathbf{E}^{-1}\mathbf{F})^{-1}$$

Setting $\mathbf{H} = \mathbf{I}$ and $\mathbf{E} = -a\mathbf{I}$, where a is a scalar value, we get:

$$(a\mathbf{I} + \mathbf{F}\mathbf{G})^{-1}\mathbf{F} = \mathbf{F}(a\mathbf{I} + \mathbf{G}\mathbf{F})^{-1} \quad (1)$$

Consider the prediction equation for ridge regression (we use the fact that $(\lambda\mathbf{I}_D + \mathbf{X}^\top\mathbf{X})$ is a square and symmetric matrix):

$$\begin{aligned} y^* &= ((\lambda\mathbf{I}_D + \mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y})^\top \mathbf{x}^* \\ &= \mathbf{y}^\top \mathbf{X}(\lambda\mathbf{I}_D + \mathbf{X}^\top\mathbf{X})^{-1} \mathbf{x}^* \end{aligned}$$

Using the result in (1) with $a = \lambda$, $\mathbf{F} = \mathbf{X}$, and $\mathbf{X}^\top = \mathbf{G}$:

$$y^* = \mathbf{y}^\top (\lambda\mathbf{I}_N + \mathbf{X}\mathbf{X}^\top)^{-1} \mathbf{X}\mathbf{x}^*$$

$\mathbf{X}\mathbf{X}^\top$?

$$\mathbf{X}\mathbf{X}^\top = \begin{pmatrix} \langle \mathbf{x}_1, \mathbf{x}_1 \rangle & \langle \mathbf{x}_1, \mathbf{x}_2 \rangle & \cdots & \langle \mathbf{x}_1, \mathbf{x}_N \rangle \\ \langle \mathbf{x}_2, \mathbf{x}_1 \rangle & \langle \mathbf{x}_2, \mathbf{x}_2 \rangle & \cdots & \langle \mathbf{x}_2, \mathbf{x}_N \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle \mathbf{x}_N, \mathbf{x}_1 \rangle & \langle \mathbf{x}_N, \mathbf{x}_2 \rangle & \cdots & \langle \mathbf{x}_N, \mathbf{x}_N \rangle \end{pmatrix}$$

$\mathbf{X}\mathbf{x}^*$?

$$\mathbf{X}\mathbf{x}^* = \begin{pmatrix} \langle \mathbf{x}_1, \mathbf{x}^* \rangle \\ \langle \mathbf{x}_2, \mathbf{x}^* \rangle \\ \vdots \\ \langle \mathbf{x}_N, \mathbf{x}^* \rangle \end{pmatrix}$$

- Consider a set of P functions that can be applied on input example \mathbf{x}

$$\boldsymbol{\phi} = \{\phi_1, \phi_2, \dots, \phi_P\}$$

$$\boldsymbol{\Phi} = \begin{pmatrix} \phi_1(\mathbf{x}_1) & \phi_2(\mathbf{x}_1) & \cdots & \phi_P(\mathbf{x}_1) \\ \phi_1(\mathbf{x}_2) & \phi_2(\mathbf{x}_2) & \cdots & \phi_P(\mathbf{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(\mathbf{x}_N) & \phi_2(\mathbf{x}_N) & \cdots & \phi_P(\mathbf{x}_N) \end{pmatrix}$$

- Prediction:

$$y^* = \mathbf{y}^\top (\lambda \mathbf{I}_N + \Phi \Phi^\top)^{-1} \Phi \phi(\mathbf{x}^*)$$

- Each entry in $\Phi \Phi^\top$ is $\langle \phi(\mathbf{x}), \phi(\mathbf{x}') \rangle$

We have already seen one such non-linear transformation in which one attribute is expanded to $\{1, x, x^2, x^3, \dots, x^d\}$.

2 Kernel Trick

- Replace dot product $\langle \mathbf{x}_i, \mathbf{x}_j \rangle$ with a function $k(\mathbf{x}_i, \mathbf{x}_j)$
- Replace $\mathbf{X}\mathbf{X}^\top$ with \mathbf{K}

$$K[i][j] = k(\mathbf{x}_i, \mathbf{x}_j)$$

- \mathbf{K} - *Gram Matrix*
- k - kernel function
 - Similarity between two data objects

Kernel Regression

$$y^* = \mathbf{y}^\top (\lambda \mathbf{I}_N + \mathbf{K})^{-1} \mathbf{k}(\mathbf{X}, \mathbf{x}^*)$$

2.1 Choosing Kernel Functions

- Already know the simplest kernel function:

$$k(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i^\top \mathbf{x}_j$$

Approach 1: Start with basis functions

$$k(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i)^\top \phi(\mathbf{x}_j)$$

Approach 2: Direct design (good for non-vector inputs)

- Measure **similarity** between \mathbf{x}_i and \mathbf{x}_j
- **Gram matrix must be positive semi-definite**

- k should be *symmetric*

For instance, consider the following kernel function for two-dimensional inputs, ($\mathbf{x} = (x_1, x_2)$):

$$\begin{aligned}
 k(\mathbf{x}, \mathbf{z}) &= (\mathbf{x}^\top \mathbf{z})^2 \\
 &= x_1^2 z_1^2 + 2x_1 z_1 x_2 z_2 + x_2^2 z_2^2 \\
 &= (x_1^2, \sqrt{2}x_1 x_2, x_2^2)^\top (x_z^2, \sqrt{2}z_1 z_2, z_2^2) \\
 &= \phi(\mathbf{x})^\top \phi(\mathbf{z})
 \end{aligned}$$

where the feature mapping $\phi(\mathbf{x})$ is defined as:

$$\phi(\mathbf{x}) = (x_1^2, \sqrt{2}x_1 x_2, x_2^2)^\top$$

2.2 Constructing New Kernels Using Building Blocks

$$\begin{aligned}
 k(\mathbf{x}_i, \mathbf{x}_j) &= ck_1(\mathbf{x}_i, \mathbf{x}_j) \\
 k(\mathbf{x}_i, \mathbf{x}_j) &= f(\mathbf{x})k_1(\mathbf{x}_i, \mathbf{x}_j)f(\mathbf{x}_j) \\
 k(\mathbf{x}_i, \mathbf{x}_j) &= q(k_1(\mathbf{x}_i, \mathbf{x}_j)) \text{ } q \text{ is a polynomial} \\
 k(\mathbf{x}_i, \mathbf{x}_j) &= \exp(k_1(\mathbf{x}_i, \mathbf{x}_j)) \\
 k(\mathbf{x}_i, \mathbf{x}_j) &= k_1(\mathbf{x}_i, \mathbf{x}_j) + k_2(\mathbf{x}_i, \mathbf{x}_j) \\
 k(\mathbf{x}_i, \mathbf{x}_j) &= k_1(\mathbf{x}_i, \mathbf{x}_j)k_2(\mathbf{x}_i, \mathbf{x}_j)
 \end{aligned}$$

3 Kernels

- If \mathbf{K} is positive definite - **Mercer Kernel**
- **Radial Basis Function** or **Gaussian Kernel**

$$k(\mathbf{x}_i, \mathbf{x}_j) = \exp\left(-\frac{1}{2\sigma^2}\|\mathbf{x}_i - \mathbf{x}_j\|^2\right)$$

- **Cosine Similarity**

$$k(\mathbf{x}_i, \mathbf{x}_j) = \frac{\mathbf{x}_i^\top \mathbf{x}_j}{\|\mathbf{x}_i\| \|\mathbf{x}_j\|}$$

One can start with a Mercer kernel and show through the **Mercer's theorem** how it can be expressed as an inner product. Since \mathbf{K} is positive definite we can compute an eigenvector decomposition:

$$\mathbf{K} = \mathbf{U}^\top \mathbf{\Lambda} \mathbf{U}$$

Each element of \mathbf{K} can be rewritten as:

$$\mathbf{K}_{ij} = (\mathbf{\Lambda}^{\frac{1}{2}} \mathbf{U}_{:,i})^\top (\mathbf{\Lambda}^{\frac{1}{2}} \mathbf{U}_{:,j})$$

Let $\phi(\mathbf{x}_i) = \mathbf{\Lambda}^{\frac{1}{2}} \mathbf{U}_{:,i}$. Then we can write:

$$\mathbf{K}_{ij} = \phi(\mathbf{x}_i)^\top \phi(\mathbf{x}_j)$$

3.1 RBF Kernel

$$k(\mathbf{x}_i, \mathbf{x}_j) = \exp\left(-\frac{1}{2\sigma^2} \|\mathbf{x}_i - \mathbf{x}_j\|^2\right)$$

- Mapping inputs to an infinite dimensional space

Whenever presented with a “potential” kernel function, one needs to ensure that it is indeed a valid kernel. This can be done in two ways, one through functional analysis and second by decomposing the function into a valid combination of valid kernel functions. For instance, for the Gaussian kernel, one can note that:

$$\|\mathbf{x}_i - \mathbf{x}_j\|^2 = \mathbf{x}_i^\top \mathbf{x}_i + (\mathbf{x}_j)^\top \mathbf{x}_j - 2\mathbf{x}_i^\top \mathbf{x}_j$$

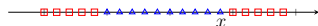
Which means that the Gaussian kernel function can be written as:

$$k(\mathbf{x}_i, \mathbf{x}_j) = \exp\left(\frac{\mathbf{x}_i^\top \mathbf{x}_i}{2\sigma^2}\right) \exp\left(\frac{\mathbf{x}_i^\top \mathbf{x}_j}{2\sigma^2}\right) \exp\left(\frac{(\mathbf{x}_j)^\top \mathbf{x}_j}{2\sigma^2}\right)$$

All three individual exponents are valid covariance functions and hence the product of these is also a valid covariance function.

3.2 Probabilistic Kernel Functions

- Allows using generative distributions in discriminative settings



- Uses class-independent probability distribution for input \mathbf{x}

$$k(\mathbf{x}_i, \mathbf{x}_j) = p(\mathbf{x}_i|\boldsymbol{\theta})p(\mathbf{x}_j|\boldsymbol{\theta})$$

- Two inputs are more similar if both have high probabilities

Bayesian Kernel

$$k(\mathbf{x}_i, \mathbf{x}_j) = \int p(\mathbf{x}_i|\boldsymbol{\theta})p(\mathbf{x}_j|\boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta}$$

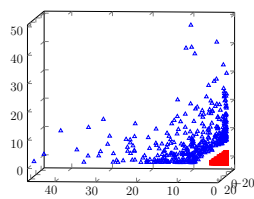
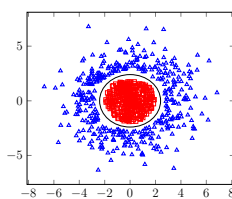
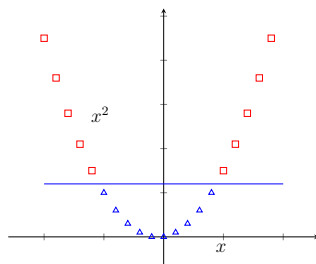
3.3 Kernels for Other Types of Data

- String Kernel
- Pyramid Kernels

4 More About Kernels

4.1 Motivation

- $x \in \Re$
- No linear separator
- Map $x \rightarrow \{x, x^2\}$
- Separable in 2D space



- $\mathbf{x} \in \mathbb{R}^2$
- No linear separator
- Map $\mathbf{x} \rightarrow \{x_1^2, \sqrt{2}x_1x_2, x_2^2\}$
- A circle as the decision boundary

4.2 Gaussian Kernel

- The *squared dot product* kernel ($\mathbf{x}_i, \mathbf{x}_j \in \mathbb{R}^2$):

$$k(\mathbf{x}_i, \mathbf{x}_j) \triangleq \phi(\mathbf{x}_i)^\top \phi(\mathbf{x}_j)$$

$$\phi(\mathbf{x}_i) = \{x_{i1}^2, \sqrt{2}x_{i1}x_{i2}, x_{i2}^2\}$$

- What about the Gaussian kernel (radial basis function)?

$$k(\mathbf{x}_i, \mathbf{x}_j) = \exp\left(-\frac{1}{2\sigma^2} \|\mathbf{x}_i - \mathbf{x}_j\|^2\right)$$

- Assume $\sigma = 1$ and $\mathbf{x} \in \mathfrak{R}$ (denoted as x)

$$\begin{aligned} k(x_i, x_j) &= \exp(-x_i^2) \exp(-x_j^2) \exp(2x_i x_j) \\ &= \exp(-x_i^2) \exp(-x_j^2) \sum_{k=0}^{\infty} \frac{2^k x_i^k x_j^k}{k!} \\ &= \sum_{k=0}^{\infty} \left(\frac{2^{k/2}}{\sqrt{k!}} x_i^k \exp(-x_i^2) \right) \left(\frac{2^{k/2}}{\sqrt{k!}} x_j^k \exp(-x_j^2) \right) \end{aligned}$$

- Using Taylor Series Expansion

$$k(x_i, x_j) = \begin{pmatrix} 1 \\ 2^{1/2} x_i^1 \exp(-x_i^2) \\ \frac{2^{2/2}}{2} x_i^2 \exp(-x_i^2) \\ \vdots \end{pmatrix}^\top \times \begin{pmatrix} 1 \\ 2^{1/2} x_j^1 \exp(-x_j^2) \\ \frac{2^{2/2}}{2} x_j^2 \exp(-x_j^2) \\ \vdots \end{pmatrix}$$

One can note above that since computing the Gaussian kernel is same as taking a dot product of two vectors of infinite length, it is equivalent to mapping the input features into an infinite dimensional space.

5 Kernel Machines

- We can use kernel function to *generate* new features
- Evaluate kernel function for each input and a set of K centroids

$$\phi(\mathbf{x}) = [k(\mathbf{x}, \boldsymbol{\mu}_1), k(\mathbf{x}, \boldsymbol{\mu}_2), \dots, k(\mathbf{x}, \boldsymbol{\mu}_K)]$$

$$y = \mathbf{w}^\top \phi(\mathbf{x}), \quad y \sim \text{Ber}(\mathbf{w}^\top \phi(\mathbf{x}))$$

- If k is a Gaussian kernel \Rightarrow Radial Basis Function Network (RBF)
- How to choose $\boldsymbol{\mu}_i$?
 - Clustering
 - Random selection

5.1 Generalizing RBF

- Another option: Use every input example as a “centroid”

$$\phi(\mathbf{x}) = [k(\mathbf{x}, \mathbf{x}_1), k(\mathbf{x}, \mathbf{x}_2), \dots, k(\mathbf{x}, \mathbf{x}_N)]$$

References

- Murphy book Chapter 17.1

References