Introduction to Machine Learning

Kernel Methods

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Outline

Contents

1 Kernel Methods

1.1 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 **E,F,G,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:

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

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 $\mathbf{X}^\top = \mathbf{G}$:

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

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

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

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

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

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

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

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

- Prediction:

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

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

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

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

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

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

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

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

- Measure **similarity** between $\mathbf{x}_i$ and $\mathbf{x}_j$
- Should follow *Mercer's Condition*
  - **Kernel/Gram matrix must be positive semi-definite**
- k should be *symmetric*

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

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

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

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

2.2 Constructing New Kernels Using Building Blocks

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

3 Kernels

- **Radial Basis Function** or **Gaussian Kernel**

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

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

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

3.1 RBF Kernel

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

- 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 RBF/Gaussian kernel, one can note that:

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

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

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

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 Extension to Non-Vector Data Examples

- What if $\mathbf{x} \notin \Re^D$?
- 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**
- Domain-defined measure of similarity

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

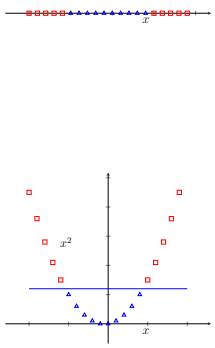
Example 2. **Multi-attribute Categorical Vectors:** Number of matching values

- **String Kernel**
- **Pyramid Kernels**

4 More About Kernels

4.1 Motivation

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



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

4.2 Radial Basis Function or Gaussian Kernel

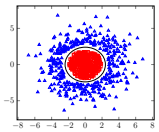
- The *squared dot product* kernel ($\mathbf{x_i}, \mathbf{x_j} \in \Re^2$):

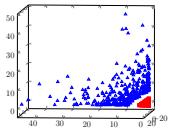
$$k(\mathbf{x_i}, \mathbf{x_j}) = \mathbf{x_i}^\top \mathbf{x_j} \triangleq \boldsymbol{\phi}(\mathbf{x_i})^\top \boldsymbol{\phi}(\mathbf{x_j})$$

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

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

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





- Assume $\gamma = 1$ and $\mathbf{x} \in \Re$ (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 Maclaurin Series Expansion*

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

One can note above that since computing the RBF/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

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

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

- 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"

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

References