Course: Math 6397 Spring 2015
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1. Let S be a set of finite or infinite objects, and $s, t \in S$. A function $k : S \times S \to \mathbb{R}$ is called a positive definite kernel, provided $k(s,t) \in \mathbb{R}$, $k(s,t) = k(t,s)$ and

$$\sum_{i=1}^{n}\sum_{i=1}^{n} c_i c_j k(s_i, t_j) \geq 0$$

for arbitrary $n > 0$, any choice of n objects $s_i, \cdots, t_j \in S$, and any arbitrary value of $c_i, c_j \in \mathbb{R}$. For $s_1, \cdots, s_N \in S$, define $M_{ij} := k(s_i, s_j), M = (M_{ij})_{N\times N}$, we want M to be semi positive definite matrix which means the eigenvalues of M should not be negative. Following, we will show three groups of kernels, including: linear kernel, polynomial kernel and Gaussian kernel, which can be used to define matrix M.

2. Use following Thm to define a positive definite kernel

Thm: Any positive definite kernel k on a space S can be defined by constructing

$$k(s,t) =< \phi(s), \phi(t) >$$

from a self reproducing Hilbert space $\mathbb{H}$ and a mapping $\phi : S \to \mathbb{H}$ with $\phi(s) \in \mathbb{H}$.

3. Hilbert space $\mathbb{H}$ construction

3.1 Given a positive definite kernel $k(s,t)$, we define a self reproducing Hilbert space $\mathbb{H}$ which is a vector space of functions on S, but not all functions defined on S belong to $\mathbb{H}$. We define functions $\phi_s$ indexed by $s \in S$,

$$\phi_s(t) = k(s,t), \forall t \in S.$$

3.2 Let N be an arbitrary number. Take N arbitrary objects $(s_1, s_2, \cdots, s_N) \in S$, and define N functions $\phi_{s_1}, \phi_{s_2}, \cdots, \phi_{s_N}$ as above. Then by considering finite linear combination of these N functions $\phi_{s_1}\lambda_1 + \phi_{s_2}\lambda_2 + \cdots + \phi_{s_N}\lambda_N$ with $\lambda_i \in \mathbb{R}$, we obtain a vector space of all linear combinations of the family of functions $\phi_s$.

3.3 Based on our vector space, we define a scaler product on it to have a Pre-Hilbert space.

Know kernel k is positive definite. Consider two functions $f$ and $g$ in $\mathbb{H}$, given by

$$f = \sum_{j=1}^{N} \lambda_j \phi_{s_j}$$

and

$$g = \sum_{k=1}^{R} \mu_k \phi_{t_k}$$

for any $s$ and $t$ in $S$, define the scalar product of $\phi_s$ and $\phi_t$ by setting

$$< \phi_s, \phi_t >= k(s,t),$$

then $< f,g >= \sum_{j=1}^{N}\sum_{k=1}^{R}\lambda_j\mu_k < \phi_{s_j},\phi_{t_k} >= \sum_{j=1}^{N}\sum_{k=1}^{R}\lambda_j\mu_k k(s_j,t_k)$.

and if $f = g$, $< f,f >= \|f\|^2 = \sum_{j=1}^{N}\sum_{j=1}^{N}\lambda_j\lambda_j < \phi_{s_j},\phi_{s_j} >= \sum_{j=1}^{N}\sum_{j=1}^{N}\lambda_j\lambda_j k(s_j,s_j)$ which is non negative since $M$ is semi positive definite.

3.4 Last, let V be the vector space of finite linear combination of functions $\phi_x \in \mathbb{H}$ equipped with the scalar product $< \phi_s,\phi_t >= k(s,t)$ and the extension just given to linear combinations of the functions $\phi_x$. By taking completion of this pre-Hilbert space, we define a self-producing Hilbert space. And this Hilbert space is the smallest space containing V.

- Remark 1:Completion means the following: The space $\mathbb{H}$ contains the functions $f$ which are the sum of series such as $f = \lambda_1\phi_{s_1} + \lambda_2\phi_{s_2} + \cdots + \lambda_k\phi_{s_k} + \cdots$ with $\|f\|^2 = \sum_{j=1}^{\infty}\sum_{j=1}^{\infty}\lambda_j\lambda_j < \phi_{s_j},\phi_{s_j} >< \infty$.
- Remark 2:We could also write $\phi_s(t) = k(s,t), \forall t$ as $\phi_s = k(s,\cdot)$, thus $< k(s,\cdot), k(t,\cdot) >_{\mathcal{H}} = k(s,t)$.
- Remark 3: Kernel are often presented as measure of similarity. Function $v \to \phi_v = k(v,t), \forall t$ is a list of similarity between $v$ and the other objects. Often, we know how to define similarity between two objects.

4. Hilbert space construction examples

Assume a object $s \in \mathbb{R}^p$ with $p$ attributes, and $s$ is defined by $v(s) = (v_1, v_2, \cdots, v_p)$. Kernel $k$ is defined as $k(s,t) = k(v(s), v(t))$, following are three kernel types

4.1 Linear kernel

$$k(v,w) =< v,w >_{\mathbb{R}^p} = v_1w_1 + v_1w_1 + \cdots + v_pw_p$$
$$k(v,v) = \|v\|^2 = (v_1)^2 + (v_2)^2 + \cdots + (v_p)^2$$

Take $v \in S \sim \mathbb{R}^p$, define $\phi_v(t) = k(v,t) =< v,t >$ for $\forall t \in S$, then arbitrary N linear combination

$$f = \sum_{j=1}^{N}\lambda_j\phi_{v_j}$$

implies $f(t) =< u,t >_{\mathbb{R}^p} \in \mathbb{H}$ where $u = \sum_{j=1}^{N}\lambda_j v_j$ and this self producing Hilbert space is the dual space of $\mathbb{R}^p$ with scaler product

$$< \phi_v,\phi_w >= k(v,w)$$

.

4.2 Polynomial kernel

$S = \mathbb{R}^p$. Let $k(v,w) = (1+ < v,w >_{\mathbb{R}^p})^2$. Fix $v \in S$, define $\phi_v(t) = (1+ < v,t >)^2$ for $\forall t \in S$.

Example: $p = 3$, thus $\phi_v(t) = (1 + v_1t_1 + v_2t_2 + v_3t_3)^2$ which is a polynomial of degree two with respect to t.

For arbitrary large N, take arbitrary objects $v_1, v_2, \cdots, v_N \subseteq S$, the finite linear combination

$$\lambda_1\phi_{v_1} + \lambda_2\phi_{v_2} + \cdots + \lambda_N\phi_{v_N} \in \mathbb{H}$$

is a polynomial of degree 2 with respect to t with dimension 10 when assume $p = 2$. Thus $\mathbb{H}$ is the space of all polynomial of degree of 2.

In $\mathbb{H}$, the scalar product is defined as

$$< \phi_v, \phi_w >_{\mathbb{H}} = (1 + < v, w >)^2$$

and

$$< \phi_v, \phi_v >_{\mathbb{H}} = (1 + < v, v >_{\mathbb{R}^3})^2 = \|v\|^2$$

Generally speaking, if $k(v, w) = (1 + < v, w >_{\mathbb{R}^k})^R$, then $\mathbb{H}$ is the Hilbert space of all polynomials of degree R.

4.3 Gaussian kernel

Define kernel k as

$$k(v, w) = \exp(\frac{-\|v - w\|^2}{\sigma^2})$$

Fixed $v \in S$, define

$$\phi_v(t) = \exp(\frac{-\|v - t\|^2}{\sigma^2})$$

for $\forall t \in S$, which is a radial function,then $\mathbb{H}$ is the infinite dimensional complete Hilbert space generated by linear combination of radial functions, which consist essentially of converging series of radial functions equipped with the scalar product

$$< \phi_v, \phi_w >_{\mathbb{H}} = exp(\frac{-\|v - w\|^2}{\sigma^2})$$

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Remark: mapping $\phi$ replace finite dimension vector with infinite dimension vector in $\mathbb{H}$.