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Exercise Nr. 6

(Deadline 30.05.2022)

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a)

trivial: show that K is symmetric

Let k_1, k_2 be kernel functions with

$$
\begin{aligned}
\phi_1 : X \to H_1, \phi_2 : X \to H_2 \\
k_1(x,y) &= \langle \Phi_1(x), \Phi_1(y) \rangle \\
k_2(x,y) &= \langle \Phi_2(x), \Phi_2(y) \rangle \\
k(x,y) &= \alpha_1 k_1 + k_2 \\
&= \alpha_1 k_1(x,y) + k_2(x,y) \\
&= \alpha_1 \langle \Phi_1(x), \Phi_1(y) \rangle + \langle \Phi_2(x), \Phi_2(y) \rangle \\
&= \langle \alpha_1 \Phi_1(x), \Phi_1(y) \rangle + \langle \Phi_2(x), \Phi_2(y) \rangle \\
&= \langle \alpha_1 \Phi_1(x) + \Phi_2(x), \Phi_1(y) + \Phi_2(y) \rangle \\
&= \alpha_1 \langle \Phi_1(x) + \Phi_2(x), \Phi_1(y) + \Phi_2(y) \rangle
\end{aligned}
$$

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Let $\phi_3 : X \to H_3$ be a Hilbert space with

$$
\begin{aligned}
H_3 = H_1 \cup H_2, \Phi_3(x) = \Phi_1(x) \cup \Phi_2(x) \\
&= \alpha_1 \langle \Phi_3(x), \Phi_3(y) \rangle
\end{aligned}
$$

✓

Defining $k' = \langle \Phi_3(x), \Phi_3(y) \rangle$

Let K' be the kernel matrix of k':

$$\Rightarrow c^T K c \overset{\geq}{\cancel{\leq}} 0 \forall c$$

$$\Rightarrow \alpha_1 c^T K' c = c^T \alpha_1 K' c \overset{\geq}{\cancel{\leq}} 0 \; \forall c$$

$$\Rightarrow \alpha_1 K' = K \text{ is the kernel matrix of k}$$

$$\Rightarrow \text{ k is kernel}$$

b)

Proof by counterexample: Let $k_1(x,y) = x^T y, k_2(x,y) = 2x^T y$

$k = k_1(x,y) - k_2(x,y) = -x^T y \Rightarrow$ not psd

$\Rightarrow$ Therefore k is not a valid kernel

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c)

1. Proof: $k = k_1 * k_2$ is a kernel with k_1, k_2 being any kernels

Let k_1, k_2 be kernel functions with

$$\phi_1 : X \to H_1, \phi_2 : X \to H_2$$

$$\begin{aligned}
k_1(x,y) &= \langle \Phi_1(x), \Phi_1(y) \rangle \\
k_2(x,y) &= \langle \Phi_2(x), \Phi_2(y) \rangle \\
k &= k_1 \cdot k_2 \\
&= \langle \Phi_1(x), \Phi_1(y) \rangle \cdot \langle \Phi_2(x), \Phi_2(y) \rangle \\
&= \sum_i (\Phi_1)_i(x) \cdot (\Phi_1)_i(y) \cdot \sum_j (\Phi_2)_j(x) \cdot (\Phi_2)_j(y) \\
&= \sum_i \sum_j (\Phi_1)_i(x) \cdot (\Phi_1)_i(y) \cdot (\Phi_2)_j(x) \cdot (\Phi_2)_j(y) \\
&= \sum_i \sum_j (\Phi_1)_i(x) \cdot (\Phi_2)_j(x) \cdot (\Phi_1)_i(y) \cdot (\Phi_2)_j(y) \\
&= \sum_i \sum_j (\Phi_3)_{ij}(x) \cdot (\Phi_3)_{ij}(y) \\
&= \langle \Phi_3(x), \Phi_3(y) \rangle
\end{aligned}$$

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With $\phi_3 : X \to H_3 : \quad (\Phi_3)_{ij}(x) = (\Phi_1)_i(x) \cdot (\Phi_2)_j(x)$

$H_3 = H_1 \times H_2$ is a Hilbert space, the norm is given by: $||(x,y)|| = \sqrt{||x||^2_{H_1} + ||y||^2_{H_2}}$

$\implies$ k is kernel

2. Proof: $\overline{k} = f(x)f(y)$ is a kernel with $f(x), f(y)$ being any functions

$$\overline{k} = f(x)f(y) = \langle f(x), f(y) \rangle$$

Nice !

if f is one-dimensional, $\overline{k}$ is a kernel as well. From above we know that the multiplication of two kernels is a kernel as well. Therefore $k = f(x) * k_1(x,y) * f(y) = k_1(x,y) * f(x)f(y) = k_1 * \overline{k}$ is a kernel.

d)

$$\begin{aligned}
k(x,y) &= \frac{k_1(x,y)}{\sqrt{k_1(x,x)k_2(y,y)}} \\
&= \frac{1}{\sqrt{k_1(x,x)}} k_1(x,y) \frac{1}{\sqrt{k_1(y,y)}} \\
&= f(x)k_1(x,y)f(y) \\
\text{with } f(x) &= \frac{1}{\sqrt{k_1(x,x)}} \\
f(y) &= \frac{1}{\sqrt{k_1(y,y)}}
\end{aligned}$$

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see c) for the proof that a k of this form is a kernel

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$\Rightarrow$ next weeks assignment

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a)

The setting can be applied to friendship connections within communities or to the travelling salesman problem with different locations on a map.

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b)

$$
\begin{aligned}
f^T L f &= \sum_{i,j} f_i f_j L_{ij} \\
&= \sum_{i,j} f_i f_j (D_{ij} - A_{ij}) \\
&= \sum_{i,j} f_i f_j D_{ij} - \sum_{i,j} f_i f_j A_{ij} \\
&= \sum_{i} D_{ii} f_i^2 - \sum_{i\sim j} f_i f_j \\
&= \frac{1}{2} \sum_{i} D_{ii} f_i^2 - \sum_{i\sim j} f_i f_j + \frac{1}{2} \sum_{j} D_{jj} f_j^2 \\
&\left(= \frac{1}{2} \sum_{i} \left[\sum_{j \text{ with: } i\sim j} f_i^2 \right] - \sum_{i\sim j} f_i f_j + \frac{1}{2} \sum_{j} \left[\sum_{i \text{ with: } i\sim j} f_j^2 \right] \right) \\
&= \frac{1}{2} \sum_{i\sim j} f_i^2 - \sum_{i\sim j} f_i f_j + \frac{1}{2} \sum_{i\sim j} f_j^2 \\
&= \frac{1}{2} x \sum_{i\sim j} (f_i^2 - 2 f_i f_j + f_j^2) \\
&= \frac{1}{2} \sum_{i\sim j} (f_i - f_j)^2 \\
&= \Omega(f)^2
\end{aligned}
$$

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c)

Well Defined

$f, g \in \mathcal{H} \implies f, g \in \mathbb{R}^n$
thus, they are unique and $\langle f, g \rangle_{\mathcal{H}} = f^T L g$ is well-defined

Linearity

$$\begin{aligned}
&\text{show:}\\
&\langle x_1 + x_2, y\rangle = \langle x_1, y\rangle + \langle x_2, y\rangle
\end{aligned}$$

$$\begin{aligned}
\langle f_1 + f_2, g\rangle_{\mathcal{H}} &= (f_1 + f_2)^T L g\\
&= \sum_{ij} (f_{1i} + f_{2i}) L_{ij} g_j\\
&= \sum_{ij} f_{1i} L_{ij} g_j + \sum_{ij} f_{2i} L_{ij} g_j\\
&= f_1^T L g + f_2^T L g\\
&= \langle f_1, g\rangle_{\mathcal{H}} + \langle f_2, g\rangle_{\mathcal{H}}
\end{aligned}$$

$$\begin{aligned}
&\text{show:}\\
&\langle \lambda x, y\rangle = \lambda \langle x, y\rangle \quad \forall \lambda \in \mathbb{R}
\end{aligned}$$

$$\begin{aligned}
\langle \lambda f, g\rangle_{\mathcal{H}} &= (\lambda f^T) L g\\
&= \lambda (f^T L g)\\
&= \lambda \langle f, g\rangle_{\mathcal{H}}
\end{aligned}$$

Symmetry

$$\begin{aligned}
&\text{show:}\\
&\langle x, y\rangle = \langle y, x\rangle
\end{aligned}$$

$$\begin{aligned}
\langle f, g\rangle_{\mathcal{H}} &= f^T L g\\
&= \sum_{ij} f_i L_{ij} g_j\\
&= \sum_{ij} g_j L_{ij} g_i\\
&= g^T L f\\
&= \langle g, f\rangle_{\mathcal{H}}
\end{aligned}$$

Pos. Def.

$$\begin{aligned}
&\text{show:}\\
&\langle x, x\rangle \geq 0
\end{aligned}$$

$$\begin{aligned}
\langle f, f\rangle_{\mathcal{H}} &= f^T L g\\
&= \Omega(f)^2 \geq 0
\end{aligned}$$

show:

$$\langle x, x \rangle = 0 \implies x = 0$$

$$\langle f, f \rangle_{\mathcal{H}} = 0$$
$$\implies \Omega(f)^2 = 0$$
$$\implies \sum_{i \sim j} (f_i - f_j)^2 = 0$$
$$\implies f_i = f_j \quad \forall i, j : i \sim j$$

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as graph is connected:

$$\implies f_i = f_j \quad \forall i, j$$

$$\text{as } \sum_{i=1}^{n} f_i = 0 :$$
$$\implies f_i = 0 \quad \forall i$$
$$\iff f = 0$$

$\implies \langle f, g \rangle_{\mathcal{H}}$ is a scalar product on $\mathcal{H}$

d)

Let $k(i, j) \in \mathbb{R}$ be the weight of the edge between the nodes i and j
Then $\Phi(i)$ is the vector of edge weights to all other nodes.