Exercise Nr. 6
(Deadline 30.05.2022)

1

a)

$$
\begin{aligned}
\text{Let } k_1, k_2 \text{ be kernel functions with} \\
\phi_1 : X \to H_1, \phi_2 : X \to H_2 \\
k_1(x,y) &= \langle \Phi_1(x), \Phi_1(y) \rangle \\
k_2(x,y) &= \langle \Phi_2(x), \Phi_2(y) \rangle \\
k(x,y) &= \alpha_1 k_1 + k_2 \\
&= \alpha_1 k_1(x,y) + k_2(x,y) \\
&= \alpha_1 \langle \Phi_1(x), \Phi_1(y) \rangle + \langle \Phi_2(x), \Phi_2(y) \rangle \\
&= \langle \alpha_1 \Phi_1(x), \Phi_1(y) \rangle + \langle \Phi_2(x), \Phi_2(y) \rangle \\
&= \langle \alpha_1 \Phi_1(x) + \Phi_2(x), \Phi_1(y) + \Phi_2(y) \rangle \\
&= \alpha_1 \langle \Phi_1(x) + \Phi_2(x), \Phi_1(y) + \Phi_2(y) \rangle \\
\text{Let } \phi_3 : X \to H_3 \text{ be a Hilbert space with} \\
H_3 = H_1 \cup H_2, \Phi_3(x) = \Phi_1(x) \cup \Phi_2(x) \\
&= \alpha_1 \langle \Phi_3(x), \Phi_3(y) \rangle
\end{aligned}
$$

$$
\begin{gathered}
\text{Defining } k' = \langle \Phi_3(x), \Phi_3(y) \rangle \\
\text{Let K' be the kernel matrix of k':} \\
\Rightarrow c^T K c \leq 0 \forall c \\
\Rightarrow \alpha_1 c^T K' c = c^T \alpha_1 K' c \leq 0 \ \forall c \\
\Rightarrow \alpha_1 K' = K \text{ is the kernel matrix of k} \\
\Rightarrow \text{ k is kernel}
\end{gathered}
$$

b)

$$
\begin{aligned}
\text{Proof by counterexample: Let } k_1(x,y) = x^T y, k_2(x,y) = 2x^T y \\
k = k_1(x,y) - k_2(x,y) = -x^T y \Rightarrow \text{ not psd} \\
\Rightarrow \text{Therefore k is not a valid kernel}
\end{aligned}
$$

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

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

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

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: $||(x,y)|| = \sqrt{||x||_{H_1}^2 + ||y||_{H_2}^2}$

$\implies$ k is kernel

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

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

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)

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

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

2

$\Rightarrow$ next weeks assignment

3

a)

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

b)

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

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

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

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

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

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

Symmetry

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

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

Pos. Def.

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

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

$$\text{show:}$$
$$\langle x, x \rangle = 0 \implies x = 0$$

$$\begin{aligned}
\langle f, f \rangle_{\mathcal{H}} &= 0 \\
\implies \Omega(f)^2 &= 0 \\
\implies \sum_{i \sim j} (f_i - f_j)^2 &= 0 \\
\implies f_i &= f_j \quad \forall i, j : i \sim j \\
\text{as graph is connected:} & \\
\implies f_i &= f_j \quad \forall i, j \\
\text{as } \sum_{i=1}^{n} f_i = 0: & \\
\implies f_i &= 0 \quad \forall i \\
\iff f &= 0
\end{aligned}$$

$\implies \langle f, g \rangle_{\mathcal{H}}$ 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.