3. *Positive Semi-definiteness:* Recall that a n-by-n real symmetric matrix K is called positive semi-definite (*p.s.d.* or $K \succeq 0$) iff for every $x \in \mathbb{R}^n$, $x^T K x \geq 0$.

   (a) Show that $K \succeq 0$ if and only if its eigenvalues are all nonnegative.

   (b) Show that $d_{ij} = K_{ii} + K_{jj} - 2K_{ij}$ is a squared distance function, *i.e.* there exists vectors $u_i, v_j \in \mathbb{R}^n$ $(1 \leq i, j \leq n)$ such that $d_{ij} = \|u_i - u_j\|^2$.

   (c) Let $\alpha \in \mathbb{R}^n$ be a signed measure s.t. $\sum_i \alpha_i = 1$ (or $e^T\alpha = 1$) and $H_\alpha = I - e\alpha^T$ be the Householder centering matrix. Show that $B_\alpha = -\frac{1}{2} H_\alpha D H_\alpha^T \succeq 0$ for matrix $D = [d_{ij}]$.

   (d) If $A \succeq 0$ and $B \succeq 0$ $(A, B \in \mathbb{R}^{n \times n})$, show that $A + B = [A_{ij} + B_{ij}]_{ij} \succeq 0$ (elementwise sum), and $A \circ B = [A_{ij} B_{ij}]_{ij} \succeq 0$ (Hadamard product or elementwise product).

proof

(a). "$\Rightarrow$" given K is p.s.d.

λ and u is the eigenvalue and eigenvector of K. $Ku = \lambda u$ $(u \neq 0)$

$\therefore u^T K u = u^T \lambda u = \lambda u^T u \geq 0$

since $u^T u = \|u\|^2 \geq 0$ $\Rightarrow$ $\lambda \geq 0$.

"$\Leftarrow$" given $\lambda \geq 0$, K is real and symmetric

$\therefore \exists$ orthogonal matrix Q, $Q^T K Q = \Lambda$, Λ is diagonal matrix.

$= \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix}$

$\therefore K = Q \Lambda Q^T = Q \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix} Q^T$

for $\forall x \in \mathbb{R}^n$ $x^T K x = x^T Q \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix} Q^T x = (Q^T x)^T \Lambda (Q^T x)$

Let $Q^T x = \begin{pmatrix} P_1 \\ \vdots \\ P_n \end{pmatrix}$

$x^T K x = \lambda_1 P_1^2 + \cdots + \lambda_n P_n^2 \geq 0$ $\Rightarrow$ $K \geq 0$

(b). $d_{ij} = \|u_i - v_j\|^2 = (u_i - v_j)^T (u_i - v_j) = u_i^T u_i - u_i^T v_j - v_j u_i^T + v_j^T v_j$

$= u_i^T u_i + v_j^T v_j - 2 u_i^T v_j$

notice $K = Q \Lambda Q^T = Q \Lambda^{\frac{1}{2}} \Lambda^{\frac{1}{2}} Q^T = (\Lambda^{\frac{1}{2}} Q^T)^T \Lambda^{\frac{1}{2}} Q^T = B^T B$

Let $u_i = B e_i$ $v_j = B e_j$

we have $K_{ii} + K_{jj} - 2K_{ij} = \|u_i - v_j\|^2$

(c) $d_{ij} = K_{ii} + K_{jj} - 2K_{ij}$

$\Rightarrow D = \text{diag}(K) e^T + e\, \text{diag}^T(K) - 2K$ $\quad \text{diag}(K) = \begin{pmatrix} K_{11} \\ K_{22} \\ \vdots \\ K_{nn} \end{pmatrix}$

for $\forall x \neq 0$, $x^T B_\alpha x = -\frac{1}{2} x^T H_\alpha D H_\alpha^T x = -\frac{1}{2} (H_\alpha^T x)^T D H_\alpha^T x$

$= -\frac{1}{2} (H_\alpha^T x)^T [\, diag(k) e^T + e\, diag^T(k) - 2K \,] H_\alpha^T x$

consider $H_\alpha^T x = (I - \alpha e^T) x$

$\because (H_\alpha^T x)^T diag(k) e^T H_\alpha^T x = x^T (I - e\alpha^T)\, diag(k)\, e^T (I - \alpha e^T) x$

$= x^T (I - e\alpha^T)\, diag(k)\, (e^T - e^T) x = 0$

$(H_\alpha^T x)^T e\, diag^T(k) H_\alpha^T x = x^T (I - e\alpha^T)\, e\, diag^T(k)\, (I - \alpha e^T) x = 0$

$\therefore x^T B_\alpha x = (H_\alpha^T x)^T K H_\alpha^T x \geq 0$ since $K \geq 0$

(d). for $\forall x \in R^n$ $x^T (A+B) x = x^T A x + x^T B x \geq 0 \Rightarrow A+B \geq 0$.

$x^T A \circ B x = x^T\, diag(A D_x B^T) \geq 0$

4. *Distance:* Suppose that $d : \mathbb{R}^p \times \mathbb{R}^p \to \mathbb{R}$ is a distance function.

(a) Is d^2 a distance function? Prove or give a counter example.

(b) Is $\sqrt{d}$ a distance function? Prove or give a counter example.

Proof (a) Let $d(x,y) = |x-y|$ $d^2(x,y) = |x-y|^2$

Let $x=0$ $y=2$ $z=5$

$d^2(x,z) = 25 > d^2(x,y) + d^2(y,z) = 4 + 9 = 13$

$\therefore d^2$ is not a distance function.

(b) $\sqrt{d}$ is a distance function.

because $\sqrt{d}$ can be written in the form of Schoenberg Transformation.