(1) Linear discriminant analysis (LDA):

Suppose we have two-classes and assume we have m-dimensional samples $\{\mathbf{x}^1, \mathbf{x}^2, \cdots, \mathbf{x}^{N_i}\}$ belong to class ω_i, where $i \in \{1, 2\}$.

The aim is to obtain a transformation of $\mathbf{x}$ to y through projecting the samples in $\mathbf{x}$ onto a line with a scalar y:

$$y = \mathbf{w}^T \mathbf{x}$$

where $\mathbf{w}$ is a projection vector.

(a) Show that an objective function to maximize for LDA can be represented as follows:

$$J(w) \triangleq \frac{|\tilde{\mu}_1 - \tilde{\mu}_2|^2}{\tilde{s}_1^2 + \tilde{s}_2^2} = \frac{w^T S_B w}{w^T S_W w},$$

$$\bar{s_i}^2 = \sum_{y \in w_i} (y - \bar{\mu}_i)^2 = \sum_{x \in w_i} (w^T x - w^T \mu_i)^2$$

$$= \sum_{x \in w_i} w^T (x - \mu_i)(x - \mu_i)^T w = w^T \left(\sum_{x \in w_i} (x - \mu_i)(x - \mu_i)^T \right) w = w^T S_i w$$

$$\Rightarrow \bar{s_i}^2 = w^T S_i w$$

so, denominator term $\bar{s_1}^2 + \bar{s_2}^2 = w^T S_1 w + w^T S_2 w = w^T (S_1 + S_2) w$

$= w^T S_W w \quad \ldots \boxed{1}$

numerator term $|\bar{\mu}_1 - \bar{\mu}_2|^2 = (\bar{\mu}_1 - \bar{\mu}_2)^2 = (w^T \mu_1 - w^T \mu_2)^2$

$= w^T ((\mu_1 - \mu_2)(\mu_1 - \mu_2)^T) w = w^T S_B w \ldots \boxed{2}$

so from $\boxed{1}$ and $\boxed{2}$

$$J(w) \triangleq \frac{|\bar{\mu}_1 - \bar{\mu}_2|^2}{\bar{s_1}^2 + \bar{s_2}^2} = \frac{w^T S_B w}{w^T S_W w} \quad \blacksquare$$

(b) Show that the solution of the LDA can be given as the eigenvector of the following term:

$$\mathbf{S_X} = \mathbf{S_W^{-1} S_B}$$

solution of the LDA $\Rightarrow$ maximize $J(w)$ To find maximum of $J(w)$,

$$\frac{d}{dw} J(w) = \frac{d}{dw} \left(\frac{w^T S_B w}{w^T S_W w} \right) = 0$$

$$\Rightarrow (w^T S_W w) \frac{d}{dw} (w^T S_B w) - (w^T S_B w) \frac{d}{dw} (w^T S_W w) = 0$$

$$\Rightarrow (w^T S_W w)\, 2 S_B w - (w^T S_B w)\, 2 S_W w = 0$$

divide with $2 w^T S_W w$

$$\Rightarrow S_B W - \frac{W^T S_B W}{W^T S_W W} S_W W = 0$$

$$\Rightarrow S_B W - J(W) S_W W = 0$$

$$\Rightarrow S_W^{-1} S_B W - J(W) W = 0$$

$$\therefore S_X = S_W^{-1} S_B$$

(2) Kernel principal component analysis (KPCA):

Suppose that the mean of the d-dimensional data in the kernal feature space is:

$$\mu = \frac{1}{n}\sum_{i=1}^{n}\phi(x_i) = 0$$

And, the covariance is :

$$C = \frac{1}{n}\sum_{i=1}^{n}\phi(x_i)\phi(x_i)^T$$

Thus, eigen-decomposition is as follows:

$$C\nu = \lambda\nu$$

(a) Show that the j^{th} eigenvector can be expressed as a linear combination of features:

$$\nu_j = \sum_{i=1}^{n}\alpha_{ji}\phi(x_i),$$

where α_{ji} is a coefficient.

$$C\nu = \frac{1}{n}\sum_{1}^{n}\phi(x_i)\phi(x_i)^T \nu = \lambda \nu$$

$$\Rightarrow \nu = \frac{1}{\lambda n}\sum_{1}^{n}\phi(x_i)\phi(x_i)^T\nu = \frac{1}{\lambda n}\sum_{1}^{n}\underbrace{(\phi(x_i)\cdot\nu)}_{\text{scalar}}\phi(x_i)^T$$

$\therefore \nu = \sum_{1}^{n} a_i \phi(x_i)$ if ν is j^{th} eigenvector,

$$\nu_j = \sum_{1}^{n} a_{ji}\phi(x_i)$$

(b) Show that the coefficient α_{ji} is obtained from the eigenvector of the kernel matrix:

$$K\alpha_j = n\lambda_j\alpha_j,$$

where $K_{ij} = K(x_i, x_j) = \phi(x_i)^T\phi(x_j)$

By Substituting $\nu = \sum_{1}^{n} a_i\phi(x_i)$ to

$$\frac{1}{n}\sum_{1}^{n}\phi(x_i)\phi(x_i)^T\nu = \lambda\nu$$

$$\frac{1}{n}\sum_{i=1}^{n}\phi(x_i)\phi(x_i)^T\left(\sum_{l=1}^{n} a_{jl}\phi(x_l)\right) = \lambda_j \sum_{l=1}^{n} a_{jl}\,\phi(x_l)$$

$$\Rightarrow \quad \frac{1}{n}\sum_{i=1}^{n}\phi(x_i)\left(\sum_{l=1}^{n} a_{jl}K(x_i,x_l)\right) = \lambda_j\sum_{l=1}^{n} a_{jl}\,\phi(x_l)$$

Multiply $\phi(x_k)$

$$\Rightarrow \frac{1}{n}\sum_{i=1}^{n}\phi(x_k)^T\phi(x_i)\left(\sum_{l=1}^{n} a_{jl}K(x_i,x_l)\right) = \lambda_j\sum_{l=1}^{n} a_{jl}\,\phi(x_k)^T\phi(x_l)$$

$$\Rightarrow \quad K^2 a_j = n\lambda_j K a_j \quad \Rightarrow \quad K a_j = n\lambda_j a_j$$

(c) Show that the zero-meaned kernel matrix is represented as follows:

$$\tilde{K} = K - 2\mathbf{1_{1/n}K} + \mathbf{1_{1/n}K1_{1/n}},$$

where $\mathbf{1_{1/n}}$ is a matrix with all elements $1/n$.

$$\tilde{K}(x_i,x_j) = \tilde{\phi}(x_i)^T\,\tilde{\phi}(x_j) = \left(\phi(x_i)-\frac{1}{n}\sum_{k=1}^{n}\phi(x_k)\right)^T\left(\phi(x_j)-\frac{1}{n}\sum_{k=1}^{n}\phi(x_k)\right)$$

$$= K(x_i,x_j) - \frac{1}{n}\sum_{k=1}^{n}K(x_i,x_k) - \frac{1}{n}\sum_{k=1}^{n}K(x_j,x_k) + \frac{1}{n^2}\sum_{l,k=1}^{n}K(x_l,x_k)$$

in a matrix form, $= K - 2\,1_{1/n}K + 1_{1/n}K\,1_{1/n}$ $\blacksquare$

(d) Show that any data point, $\boldsymbol{x}$ can be represented as:

$$y_j = \sum_{i=1}^{n}\alpha_{ji}K(\boldsymbol{x},\boldsymbol{x_i}), j = 1,\cdots,d$$