Fisher Discriminant Analysis

Statistical Machine Learning (ENGG*6600*02)

School of Engineering,
University of Guelph, ON, Canada

Course Instructor: Benyamin Ghojogh

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One-dimensional Subspace

Scatters in Two-Class Case

- Assume we have two classes, $\{\boldsymbol{x}_i^{(1)}\}_{i=1}^{n_1}$ and $\{\boldsymbol{x}_i^{(2)}\}_{i=1}^{n_2}$, where n_1 and n_2 denote the sample size of the first and second class, respectively, and $\boldsymbol{x}_i^{(j)}$ denotes the i-th instance of the j-th class.
- If the data instances of the j-th class are projected onto a one-dimensional subspace (vector $\boldsymbol{u}$) by $\boldsymbol{u}^\top \boldsymbol{x}_i^{(j)}$, the mean and the variance of the projected data are $\boldsymbol{u}^\top \boldsymbol{\mu}_j$ and $\boldsymbol{u}^\top \boldsymbol{S}_j \boldsymbol{u}$, respectively, where $\boldsymbol{\mu}_j$ and $\boldsymbol{S}_j$ are the mean and covariance matrix (scatter) of the j-th class.
- The mean of the j-th class is:

$$\mathbb{R}^d \ni \boldsymbol{\mu}_j := \frac{1}{n_j} \sum_{i=1}^{n_j} \boldsymbol{x}_i^{(j)}. \tag{1}$$

Scatters in Two-Class Case

- After projection onto the one-dimensional subspace, the distance between the means of classes is:

$$\begin{aligned}\mathbb{R} \ni d_B &:= (\boldsymbol{u}^\top \boldsymbol{\mu}_1 - \boldsymbol{u}^\top \boldsymbol{\mu}_2)^\top (\boldsymbol{u}^\top \boldsymbol{\mu}_1 - \boldsymbol{u}^\top \boldsymbol{\mu}_2) = (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)^\top \boldsymbol{u}\boldsymbol{u}^\top (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2) \\ &\overset{(a)}{=} \mathbf{tr}\big((\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)^\top \boldsymbol{u}\boldsymbol{u}^\top (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)\big) \overset{(b)}{=} \mathbf{tr}\big(\boldsymbol{u}^\top (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)^\top \boldsymbol{u}\big) \\ &\overset{(c)}{=} \boldsymbol{u}^\top (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)^\top \boldsymbol{u} \overset{(d)}{=} \boldsymbol{u}^\top \boldsymbol{S}_B\, \boldsymbol{u}, \end{aligned} \tag{2}$$

  where (a) is because $(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)^\top \boldsymbol{u}\boldsymbol{u}^\top (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)$ is a scalar, (b) is because of the cyclic property of trace, (c) is because $\boldsymbol{u}^\top (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)^\top \boldsymbol{u}$ is a scalar, and (d) is because we define:

$$\mathbb{R}^{d\times d} \ni \boldsymbol{S}_B := (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)^\top, \tag{3}$$

  as the **between-scatter** of classes.

- The Eq. (2) can also be interpreted in this way: the d_B is the variance of projection of the class means or the squared length of reconstruction of the class means.

Scatters in Two-Class Case

- We saw that the variance of projection is $\boldsymbol{u}^\top \boldsymbol{S}_j \boldsymbol{u}$ for the j-th class. If we add up the variances of projections of the two classes, we have:

$$\begin{aligned}\mathbb{R} \ni d_W &:= \boldsymbol{u}^\top \boldsymbol{S}_1 \boldsymbol{u} + \boldsymbol{u}^\top \boldsymbol{S}_2 \boldsymbol{u} = \boldsymbol{u}^\top (\boldsymbol{S}_1 + \boldsymbol{S}_2)\, \boldsymbol{u} \\ &\overset{(a)}{=} \boldsymbol{u}^\top \boldsymbol{S}_W\, \boldsymbol{u}, \end{aligned} \tag{4}$$

  where:

$$\mathbb{R}^{d \times d} \ni \boldsymbol{S}_W := \boldsymbol{S}_1 + \boldsymbol{S}_2, \tag{5}$$

  is the **within-scatter** of classes.

- The d_W is the summation of projection variance of class instances or the summation of the reconstruction length of class instances.

Scatters in Multi-Class Case: Variant 1

- Assume $\{\boldsymbol{x}_i^{(j)}\}_{i=1}^{n_j}$ are the instances of the j-th class where we have multiple classes. In this case, the **between-scatter** is defined as:

  $$\mathbb{R}^{d\times d} \ni \boldsymbol{S}_B := \sum_{j=1}^{c} (\boldsymbol{\mu}_j - \boldsymbol{\mu})(\boldsymbol{\mu}_j - \boldsymbol{\mu})^\top, \tag{6}$$

  where c is the number of classes and:

  $$\mathbb{R}^{d} \ni \boldsymbol{\mu} := \frac{1}{\sum_{k=1}^{c} n_k} \sum_{j=1}^{c} n_j\, \boldsymbol{\mu}_j = \frac{1}{n} \sum_{i=1}^{n} \boldsymbol{x}_i, \tag{7}$$

  is the weighted mean of means of classes or the total mean of data.
- It is noteworthy that some researches define the between-scatter in a weighted way:

  $$\mathbb{R}^{d\times d} \ni \boldsymbol{S}_B := \sum_{j=1}^{c} n_j (\boldsymbol{\mu}_j - \boldsymbol{\mu})(\boldsymbol{\mu}_j - \boldsymbol{\mu})^\top. \tag{8}$$

Scatters in Multi-Class Case: Variant 1

- If we extend the Eq. (5) to c number of classes, the **within-scatter** is defined as:

$$\mathbb{R}^{d \times d} \ni \boldsymbol{S}_W := \sum_{j=1}^{c} \boldsymbol{S}_j \tag{9}$$

$$= \sum_{j=1}^{c} \sum_{i=1}^{n_j} (\boldsymbol{x}_i^{(j)} - \boldsymbol{\mu}_j)(\boldsymbol{x}_i^{(j)} - \boldsymbol{\mu}_j)^\top, \tag{10}$$

  where n_j is the sample size of the j-th class.

- In this case, the d_B and d_W are:

$$\mathbb{R} \ni d_B := \boldsymbol{u}^\top \boldsymbol{S}_B \, \boldsymbol{u}, \tag{11}$$

$$\mathbb{R} \ni d_W := \boldsymbol{u}^\top \boldsymbol{S}_W \, \boldsymbol{u}, \tag{12}$$

  where $\boldsymbol{S}_B$ and $\boldsymbol{S}_W$ are Eqs. (6) and (10).

Scatters in Multi-Class Case: Variant 2

- There is another variant for multi-class case in FDA. In this variant, the within-scatter is the same as Eq. (10). The between-scatter is, however, different.
- The **total-scatter** is defined as the covariance matrix of the whole data, regardless of classes [1]:

$$\mathbb{R}^{d\times d} \ni \boldsymbol{S}_T := \frac{1}{n}\sum_{i=1}^{n}(\boldsymbol{x}_i - \boldsymbol{\mu})(\boldsymbol{x}_i - \boldsymbol{\mu})^\top, \tag{13}$$

  where the total mean $\boldsymbol{\mu}$ is the Eq. (7). We can also use the scaled total-scatter by dropping the $1/n$ factor.
- On the other hand, the total scatter is equal to the summation of the within- and between-scatters:

$$\boldsymbol{S}_T = \boldsymbol{S}_W + \boldsymbol{S}_B. \tag{14}$$

  Therefore, the between-scatter, in this variant, is obtained as:

$$\boldsymbol{S}_B := \boldsymbol{S}_T - \boldsymbol{S}_W. \tag{15}$$

Fisher Subspace: Variant 1

- In FDA, we want to maximize the projection variance (scatter) of means of classes and minimize the projection variance (scatter) of class instances. In other words, we want to maximize d_B and minimize d_W. The reason is that after projection, we want the within scatter of every class to be small and the between scatter of classes to be large; therefore, the instances of every class get close to one another and the classes get far from each other.
- The two mentioned optimization problems are:

$$\underset{\boldsymbol{u}}{\text{maximize}} \quad d_B(\boldsymbol{u}), \tag{16}$$

$$\underset{\boldsymbol{u}}{\text{minimize}} \quad d_W(\boldsymbol{u}). \tag{17}$$

- We can merge these two optimization problems as a regularized optimization problem:

$$\underset{\boldsymbol{u}}{\text{maximize}} \quad d_B(\boldsymbol{u}) - \alpha\, d_W(\boldsymbol{u}), \tag{18}$$

  where $\alpha > 0$ is the regularization parameter.
- Another way of merging Eqs. (16) and (17) is:

$$\underset{\boldsymbol{u}}{\text{maximize}} \quad f(\boldsymbol{u}) := \frac{d_B(\boldsymbol{u})}{d_W(\boldsymbol{u})} = \frac{\boldsymbol{u}^\top \boldsymbol{S}_B\, \boldsymbol{u}}{\boldsymbol{u}^\top \boldsymbol{S}_W\, \boldsymbol{u}}, \tag{19}$$

  where $f(\boldsymbol{u}) \in \mathbb{R}$ is referred to as the **Fisher criterion** [2].

Fisher Subspace: Variant 1

- The Fisher criterion is a generalized Rayleigh-Ritz quotient (recall preliminaries):

$$f(\boldsymbol{u}) = R(\boldsymbol{S}_B, \boldsymbol{S}_W; \boldsymbol{u}). \tag{20}$$

According to the preliminaries slides, the optimization in Eq. (19) is equivalent to:

$$\begin{aligned} \underset{\boldsymbol{u}}{\text{maximize}} \quad & \boldsymbol{u}^\top \boldsymbol{S}_B\, \boldsymbol{u} \\ \text{subject to} \quad & \boldsymbol{u}^\top \boldsymbol{S}_W\, \boldsymbol{u} = 1. \end{aligned} \tag{21}$$

- The Lagrangian [3] is:

$$\mathcal{L} = \boldsymbol{w}^\top \boldsymbol{S}_B\, \boldsymbol{w} - \lambda(\boldsymbol{w}^\top \boldsymbol{S}_W\, \boldsymbol{w} - 1),$$

where λ is the Lagrange multiplier. Equating the derivative of $\mathcal{L}$ to zero gives:

$$\begin{aligned} \mathbb{R}^d \ni \frac{\partial \mathcal{L}}{\partial \boldsymbol{u}} &= 2\, \boldsymbol{S}_B\, \boldsymbol{u} - 2\, \lambda\, \boldsymbol{S}_W\, \boldsymbol{u} \overset{\text{set}}{=} \boldsymbol{0} \\ \implies 2\, \boldsymbol{S}_B\, \boldsymbol{u} &= 2\, \lambda\, \boldsymbol{S}_W\, \boldsymbol{u} \implies \boldsymbol{S}_B\, \boldsymbol{u} = \lambda\, \boldsymbol{S}_W\, \boldsymbol{u}, \end{aligned} \tag{22}$$

which is a generalized eigenvalue problem $(\boldsymbol{S}_B, \boldsymbol{S}_W)$ according to [4]. The $\boldsymbol{u}$ is the eigenvector with the largest eigenvalue (because the optimization is maximization) and the λ is the corresponding eigenvalue.

- The $\boldsymbol{u}$ is referred to as the **Fisher direction** or **Fisher axis**.

Fisher Subspace: Variant 1

- One possible solution to the generalized eigenvalue problem $(\boldsymbol{S}_B, \boldsymbol{S}_W)$ is [4]:

$$\begin{aligned} \boldsymbol{S}_B\, \boldsymbol{u} = \lambda\, \boldsymbol{S}_W\, \boldsymbol{u} &\implies \boldsymbol{S}_W^{-1} \boldsymbol{S}_B\, \boldsymbol{u} = \lambda\, \boldsymbol{u} \\ &\implies \boldsymbol{u} = \mathbf{eig}(\boldsymbol{S}_W^{-1} \boldsymbol{S}_B), \end{aligned} \tag{23}$$

  where **eig**(.) denotes the eigenvector of the matrix with the largest eigenvalue. Although the solution in Eq. (23) is a little dirty [4] because $\boldsymbol{S}_w$ might be singular and not invertible, but this solution is very common for FDA.

- In some researches, the diagonal of $\boldsymbol{S}_W$ is strengthened slightly to make it full rank and invertible [4]:

$$\boldsymbol{u} = \mathbf{eig}((\boldsymbol{S}_W + \varepsilon \boldsymbol{I})^{-1} \boldsymbol{S}_B), \tag{24}$$

  where ε is a very small positive number, large enough to make $\boldsymbol{S}_W$ full rank.

Projection and Reconstruction in FDA

- The projection, projection of out-of-sample, reconstruction, and reconstruction of out-of-sample in SPCA are:

$$\widetilde{\boldsymbol{x}} = \boldsymbol{U}^\top \boldsymbol{x}, \tag{25}$$

$$\widetilde{\boldsymbol{x}}_t = \boldsymbol{U}^\top \boldsymbol{x}_t, \tag{26}$$

$$\widehat{\boldsymbol{x}} = \boldsymbol{U}\boldsymbol{U}^\top \boldsymbol{x} = \boldsymbol{U}\widetilde{\boldsymbol{x}}, \tag{27}$$

$$\widehat{\boldsymbol{x}}_t = \boldsymbol{U}\boldsymbol{U}^\top \boldsymbol{x}_t = \boldsymbol{U}\widetilde{\boldsymbol{x}}_t, \tag{28}$$

  respectively.
- In FDA, there is no need to center the data, in contrast to PCA.

Fisher Subspace: Variant 2

- Another way to find the FDA direction is to consider another version of Fisher criterion. According to Eq. (15) for $\boldsymbol{S}_B$, the Fisher criterion becomes [1]:

$$\begin{aligned} f(\boldsymbol{u}) &= \frac{\boldsymbol{u}^\top \boldsymbol{S}_B\, \boldsymbol{u}}{\boldsymbol{u}^\top \boldsymbol{S}_W\, \boldsymbol{u}} \overset{(15)}{=} \frac{\boldsymbol{u}^\top (\boldsymbol{S}_T - \boldsymbol{S}_W)\, \boldsymbol{u}}{\boldsymbol{u}^\top \boldsymbol{S}_W\, \boldsymbol{u}} \\ &= \frac{\boldsymbol{u}^\top \boldsymbol{S}_T\, \boldsymbol{u} - \boldsymbol{u}^\top \boldsymbol{S}_W\, \boldsymbol{u}}{\boldsymbol{u}^\top \boldsymbol{S}_W\, \boldsymbol{u}} = \frac{\boldsymbol{u}^\top \boldsymbol{S}_T\, \boldsymbol{u}}{\boldsymbol{u}^\top \boldsymbol{S}_W\, \boldsymbol{u}} - 1. \end{aligned} \tag{29}$$

- The -1 is a constant and is dropped in the optimization; therefore:

$$\begin{aligned} \underset{\boldsymbol{u}}{\text{maximize}} \quad & \boldsymbol{u}^\top \boldsymbol{S}_T\, \boldsymbol{u} \\ \text{subject to} \quad & \boldsymbol{u}^\top \boldsymbol{S}_W\, \boldsymbol{u} = 1, \end{aligned} \tag{30}$$

whose solution is similarly obtained as:

$$\boldsymbol{S}_T\, \boldsymbol{u} = \lambda\, \boldsymbol{S}_W\, \boldsymbol{u}, \tag{31}$$

which is a generalized eigenvalue problem $(\boldsymbol{S}_T, \boldsymbol{S}_W)$ according to [4].

Multi-dimensional Subspace

Multi-dimensional Subspace

- In case the Fisher subspace is the span of several Fisher directions, $\{\boldsymbol{u}_j\}_{j=1}^{p}$ where $\boldsymbol{u}_j \in \mathbb{R}^d$, the d_B and d_W are defined as:

$$\mathbb{R} \ni d_B := \mathbf{tr}(\boldsymbol{U}^\top \boldsymbol{S}_B\, \boldsymbol{U}), \tag{32}$$

$$\mathbb{R} \ni d_W := \mathbf{tr}(\boldsymbol{U}^\top \boldsymbol{S}_W\, \boldsymbol{U}), \tag{33}$$

where $\mathbb{R}^{d \times p} \ni \boldsymbol{U} = [\boldsymbol{u}_1, \dots, \boldsymbol{u}_p]$. In this case, maximizing the *Fisher criterion* is:

$$\underset{\boldsymbol{U}}{\text{maximize}} \quad f(\boldsymbol{U}) := \frac{d_B(\boldsymbol{U})}{d_W(\boldsymbol{U})} = \frac{\mathbf{tr}(\boldsymbol{U}^\top \boldsymbol{S}_B\, \boldsymbol{U})}{\mathbf{tr}(\boldsymbol{U}^\top \boldsymbol{S}_W\, \boldsymbol{U})}. \tag{34}$$

- The Fisher criterion $f(\boldsymbol{U})$ is a generalized Rayleigh-Ritz quotient (see preliminaries). According to preliminaries, the optimization in Eq. (34) is **approximately** equivalent to:

$$\begin{aligned} &\underset{\boldsymbol{U}}{\text{maximize}} && \mathbf{tr}(\boldsymbol{U}^\top \boldsymbol{S}_B\, \boldsymbol{U}) \\ &\text{subject to} && \boldsymbol{U}^\top \boldsymbol{S}_W\, \boldsymbol{U} = \boldsymbol{I}. \end{aligned} \tag{35}$$

- Note that it is exactly true for one projection vector $\boldsymbol{u}$ but it approximately holds for the projection matrix $\boldsymbol{U}$ having multiple projection directions.

Multi-dimensional Subspace

- The Lagrangian [3] is:

$$\mathcal{L} = \mathbf{tr}(\boldsymbol{U}^\top \boldsymbol{S}_B\, \boldsymbol{U}) - \mathbf{tr}\big(\boldsymbol{\Lambda}^\top (\boldsymbol{U}^\top \boldsymbol{S}_W\, \boldsymbol{U} - \boldsymbol{I})\big),$$

  where $\boldsymbol{\Lambda} \in \mathbb{R}^{d \times d}$ is a diagonal matrix whose diagonal entries are the Lagrange multipliers. Equating the derivative of $\mathcal{L}$ to zero gives:

$$\begin{aligned} \mathbb{R}^{d \times p} \ni \frac{\partial \mathcal{L}}{\partial \boldsymbol{U}} &= 2\, \boldsymbol{S}_B\, \boldsymbol{U} - 2\, \boldsymbol{S}_W\, \boldsymbol{U}\boldsymbol{\Lambda} \overset{\text{set}}{=} \mathbf{0} \\ \implies 2\, \boldsymbol{S}_B\, \boldsymbol{U} = 2\, \boldsymbol{S}_W\, \boldsymbol{U}\boldsymbol{\Lambda} &\implies \boldsymbol{S}_B\, \boldsymbol{U} = \boldsymbol{S}_W\, \boldsymbol{U}\boldsymbol{\Lambda}, \end{aligned} \tag{36}$$

  which is a generalized eigenvalue problem $(\boldsymbol{S}_B, \boldsymbol{S}_W)$ according to [4]. The columns of $\boldsymbol{U}$ are the eigenvectors sorted by largest to smallest eigenvalues (because the optimization is maximization) and the diagonal entries of $\boldsymbol{\Lambda}$ are the corresponding eigenvalues.

- The columns of $\boldsymbol{U}$ are referred to as the **Fisher directions** or **Fisher axes**.

Multi-dimensional Subspace

- One possible solution to the generalized eigenvalue problem $(\boldsymbol{S}_B, \boldsymbol{S}_W)$ is [4]:

$$\begin{aligned} \boldsymbol{S}_B\, \boldsymbol{U} = \boldsymbol{S}_W\, \boldsymbol{U}\boldsymbol{\Lambda} \implies \boldsymbol{S}_W^{-1}\boldsymbol{S}_B\, \boldsymbol{U} = \boldsymbol{U}\boldsymbol{\Lambda} \\ \implies \boldsymbol{U} = \textbf{eig}(\boldsymbol{S}_W^{-1}\boldsymbol{S}_B), \end{aligned} \tag{37}$$

where **eig**(.) denotes the eigenvectors of the matrix stacked column-wise. Again, we can have [4]:

$$\boldsymbol{U} = \textbf{eig}((\boldsymbol{S}_W + \varepsilon \boldsymbol{I})^{-1}\boldsymbol{S}_B). \tag{38}$$

Projection and Reconstruction in FDA

- The projection, projection of out-of-sample, reconstruction, and reconstruction of out-of-sample in SPCA are:

$$\widetilde{\boldsymbol{X}} = \boldsymbol{U}^\top \boldsymbol{X}, \tag{39}$$

$$\widetilde{\boldsymbol{X}}_t = \boldsymbol{U}^\top \boldsymbol{X}_t, \tag{40}$$

$$\widehat{\boldsymbol{X}} = \boldsymbol{U}\boldsymbol{U}^\top \boldsymbol{X} = \boldsymbol{U}\widetilde{\boldsymbol{X}}, \tag{41}$$

$$\widehat{\boldsymbol{X}}_t = \boldsymbol{U}\boldsymbol{U}^\top \boldsymbol{X}_t = \boldsymbol{U}\widetilde{\boldsymbol{X}}_t, \tag{42}$$

  respectively.
- In FDA, there is no need to center the data, in contrast to PCA.

Discussion on Dimensionality of the Fisher Subspace

Discussion on Dimensionality of the Fisher Subspace

- In general, the rank of a covariance (scatter) matrix over the d-dimensional data with sample size n is at most $\min(d, n-1)$. The d is because the covariance matrix is a $d \times d$ matrix and the n is because we iterate over n data instances for calculating the covariance matrix. The -1 is because of subtracting the mean in calculation of the covariance matrix.
- For clarification, assume we only have one instance which becomes zero after removing the mean. This makes the covariance matrix a zero matrix.
- According to Eq. (10), the rank of the $\boldsymbol{S}_W$ is at most $\min(d, n-1)$ because all the instances of all the classes are considered. Hence, the rank of $\boldsymbol{S}_W$ is also at most $\min(d, n-1)$. According to Eq. (6), the rank of the $\boldsymbol{S}_B$ is at most $\min(d, c-1)$ because we have c iterations in its calculation.
- In Eq. (37), we have $\boldsymbol{S}_W^{-1}\boldsymbol{S}_B$ whose rank is:

$$\begin{aligned}\textbf{rank}(\boldsymbol{S}_W^{-1}\boldsymbol{S}_B) &\leq \min\big(\textbf{rank}(\boldsymbol{S}_W^{-1}), \textbf{rank}(\boldsymbol{S}_B)\big) \\ &\leq \min\big(\min(d, n-1), \min(d, c-1)\big) \\ &= \min(d, n-1, c-1) \overset{(a)}{=} c-1, \end{aligned} \tag{43}$$

  where (a) is because we usually have $c < d, n$. Therefore, the rank of $\boldsymbol{S}_W^{-1}\boldsymbol{S}_B$ is limited because of the rank of $\boldsymbol{S}_B$ which is at most $c-1$.
- According to Eq. (37), the $c-1$ leading eigenvalues will be valid and the rest are zero or very small. Therefore, the p, which is the dimensionality of the Fisher subspace, is at most $c-1$. The $c-1$ leading eigenvectors are considered as the Fisher directions and the rest of eigenvectors are invalid and ignored.

Comparison of FDA and PCA Directions

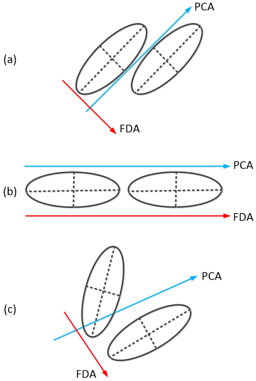
Comparison of FDA and PCA Directions

- FDA optimization:

$$\begin{aligned} \underset{\boldsymbol{U}}{\text{maximize}} \quad & \textbf{tr}(\boldsymbol{U}^\top \boldsymbol{S}_T\, \boldsymbol{U}) \\ \text{subject to} \quad & \boldsymbol{U}^\top \boldsymbol{S}_W\, \boldsymbol{U} = \boldsymbol{I}. \end{aligned} \tag{44}$$

- PCA optimization: [5]:

$$\begin{aligned} \underset{\boldsymbol{U}}{\text{maximize}} \quad & \textbf{tr}(\boldsymbol{U}^\top \boldsymbol{S}_T\, \boldsymbol{U}) \\ \text{subject to} \quad & \boldsymbol{U}^\top \boldsymbol{U} = \boldsymbol{I}. \end{aligned} \tag{45}$$



FDA $\overset{?}{\equiv}$ LDA

FDA $\overset{?}{\equiv}$ LDA

- The FDA is also referred to as **Linear Discriminant Analysis (LDA)** and **Fisher LDA (FLDA)**.
- Note that FDA is a manifold (subspace) learning method and LDA [6] is a classification method. However, LDA can be seen as a metric learning method [6] and as metric learning is a subspace learning method, there is a connection between FDA and LDA.
- We know that FDA is a projection-based subspace learning method. Consider the projection vector $\boldsymbol{u}$. The projection of data $\boldsymbol{x}$ is:

$$\boldsymbol{x} \mapsto \boldsymbol{u}^\top \boldsymbol{x}, \tag{46}$$

  which can be done for all the data instances of every class. Thus, the mean and the covariance matrix of the class are transformed as:

$$\boldsymbol{\mu} \mapsto \boldsymbol{u}^\top \boldsymbol{\mu}, \tag{47}$$

$$\boldsymbol{\Sigma} \mapsto \boldsymbol{u}^\top \boldsymbol{\Sigma}\, \boldsymbol{u}, \tag{48}$$

  respectively, because of characteristics of mean and variance.
- According to Eq. (19), the Fisher criterion is the ratio of the between-class variance, σ_b^2, and within-class variance, σ_w^2:

$$f := \frac{\sigma_b^2}{\sigma_w^2} = \frac{(\boldsymbol{u}^\top \boldsymbol{\mu}_2 - \boldsymbol{u}^\top \boldsymbol{\mu}_1)^2}{\boldsymbol{u}^\top \boldsymbol{\Sigma}_2\, \boldsymbol{u} + \boldsymbol{u}^\top \boldsymbol{\Sigma}_1\, \boldsymbol{u}} = \frac{\big(\boldsymbol{u}^\top (\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)\big)^2}{\boldsymbol{u}^\top (\boldsymbol{\Sigma}_2 + \boldsymbol{\Sigma}_1)\, \boldsymbol{u}}, \tag{49}$$

  where $\boldsymbol{\mu}_1$ and $\boldsymbol{\mu}_2$ are the means of the two classes and $\boldsymbol{\Sigma}_1$ and $\boldsymbol{\Sigma}_2$ are the covariances of the two classes.

FDA $\overset{?}{\equiv}$ LDA

- We had:

$$f := \frac{\sigma_b^2}{\sigma_w^2} = \frac{(\boldsymbol{u}^\top \boldsymbol{\mu}_2 - \boldsymbol{u}^\top \boldsymbol{\mu}_1)^2}{\boldsymbol{u}^\top \boldsymbol{\Sigma}_2\, \boldsymbol{u} + \boldsymbol{u}^\top \boldsymbol{\Sigma}_1\, \boldsymbol{u}} = \frac{\big(\boldsymbol{u}^\top (\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)\big)^2}{\boldsymbol{u}^\top (\boldsymbol{\Sigma}_2 + \boldsymbol{\Sigma}_1)\, \boldsymbol{u}}.$$

- The FDA maximizes the Fisher criterion:

$$\underset{\boldsymbol{u}}{\text{maximize}} \quad \frac{\big(\boldsymbol{u}^\top (\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)\big)^2}{\boldsymbol{u}^\top (\boldsymbol{\Sigma}_2 + \boldsymbol{\Sigma}_1)\, \boldsymbol{u}}, \tag{50}$$

which can be restated as:

$$\begin{aligned} &\underset{\boldsymbol{u}}{\text{maximize}} && \big(\boldsymbol{u}^\top (\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)\big)^2, \\ &\text{subject to} && \boldsymbol{u}^\top (\boldsymbol{\Sigma}_2 + \boldsymbol{\Sigma}_1)\, \boldsymbol{u} = 1, \end{aligned} \tag{51}$$

according to Rayleigh-Ritz quotient method [7].

- The Lagrangian [3] is:

$$\mathcal{L} = \big(\boldsymbol{u}^\top (\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)\big)^2 - \lambda\big(\boldsymbol{u}^\top (\boldsymbol{\Sigma}_2 + \boldsymbol{\Sigma}_1)\, \boldsymbol{u} - 1\big),$$

where λ is the Lagrange multiplier.

FDA $\overset{?}{\equiv}$ LDA

- Equating the derivative of $\mathcal{L}$ to zero gives:

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{u}} = 2\,(\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)(\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)^\top \boldsymbol{u} - 2\,\lambda\,(\boldsymbol{\Sigma}_2 + \boldsymbol{\Sigma}_1)\,\boldsymbol{u} \overset{\text{set}}{=} \boldsymbol{0}$$
$$\implies (\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)(\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)^\top \boldsymbol{u} = \lambda\,(\boldsymbol{\Sigma}_2 + \boldsymbol{\Sigma}_1)\,\boldsymbol{u},$$

  which is a generalized eigenvalue problem $\big((\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)(\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)^\top, (\boldsymbol{\Sigma}_2 + \boldsymbol{\Sigma}_1)\big)$ according to [4].

- The projection vector is the eigenvector of $(\boldsymbol{\Sigma}_2 + \boldsymbol{\Sigma}_1)^{-1}(\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)(\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)^\top$; therefore, we can say:

$$\boldsymbol{u} \propto (\boldsymbol{\Sigma}_2 + \boldsymbol{\Sigma}_1)^{-1}(\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)(\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)^\top. \tag{52}$$

- On the other hand, in LDA, the decision function is [6]:

$$2\,\big(\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)\big)^\top \boldsymbol{x} + \boldsymbol{\mu}_1^\top \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2^\top \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_2 + 2\ln(\frac{\pi_1}{\pi_2}) = 0, \tag{53}$$

  where π_1 and π_2 are the prior distributions of the two classes. Moreover, in LDA, the covariance matrices are assumed to be equal [6]: $\boldsymbol{\Sigma}_1 = \boldsymbol{\Sigma}_2 = \boldsymbol{\Sigma}$. Therefore, in LDA, the Eq. (52) becomes [6]:

$$\begin{aligned}\boldsymbol{u} &\propto (2\,\boldsymbol{\Sigma})^{-1}(\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)(\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)^\top \\ &\propto \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)(\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)^\top.\end{aligned} \tag{54}$$

  According to Eq. (46), we have:

$$\boldsymbol{u}^\top \boldsymbol{x} \propto \big(\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)(\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)^\top\big)^\top \boldsymbol{x}. \tag{55}$$

FDA $\overset{?}{\equiv}$ LDA

- Comparing Eq. (53) and Eq. (55):

$$2\,\big(\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_2-\boldsymbol{\mu}_1)\big)^\top \boldsymbol{x} + \boldsymbol{\mu}_1^\top \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2^\top \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_2 + 2\ln(\frac{\pi_1}{\pi_2}) = 0,$$

$$\boldsymbol{u}^\top \boldsymbol{x} \propto \big(\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_2-\boldsymbol{\mu}_1)(\boldsymbol{\mu}_2-\boldsymbol{\mu}_1)^\top\big)^\top \boldsymbol{x},$$

  shows that LDA and FDA are equivalent up to a scaling factor $\boldsymbol{\mu}_1^\top \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2^\top \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_2 + 2\pi_1/\pi_2$.
- Note that this term is multiplied as an exponential factor before taking logarithm to obtain Eq. (53), so this term is a scaling factor (see the LDA lecture or [6] for more details).
- It should be noted that in manifold (subspace) learning, the scale does not matter because all the distances can scale similarly in the subspace, without impacting the relative distances of points.
- Hence, we can say that LDA and FDA are equivalent:

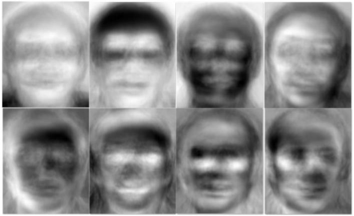
$$\text{LDA} \equiv \text{FDA}. \tag{56}$$

  Therefore, **the two subspaces of FDA and LDA are the same subspace.**
- In other words, **FDA followed by the use of Euclidean distance for classification in the subspace is equivalent to LDA.** This sheds light on why LDA and FDA are used interchangeably in the literature.
- Note that LDA assumes *one* (and not several) Gaussian for every class [6] and so does the FDA because they are equivalent. That is why FDA faces problem for multi-modal data [8].

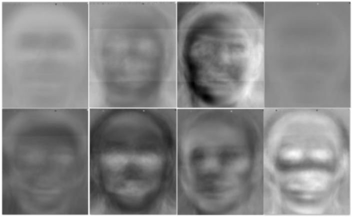
Eigenfaces vs. Fisherfaces

Eigenfaces vs. Fisherfaces

eigenfaces (1991) [9, 10] and *Fisherfaces* (1997) [11, 12, 13]



eigenfaces



Fisherfaces

Kernel Fisher Discriminant Analysis

Kernel Fisher Discriminant Analysis

- The Eq. (3) in the feature space is:

$$\mathbb{R}^{t \times t} \ni \boldsymbol{\Phi}(\boldsymbol{S}_B) := \big(\phi(\boldsymbol{\mu}_1) - \phi(\boldsymbol{\mu}_2)\big)\big(\phi(\boldsymbol{\mu}_1) - \phi(\boldsymbol{\mu}_2)\big)^\top, \tag{57}$$

  where the mean of the j-th class in the feature space is:

$$\mathbb{R}^t \ni \phi(\boldsymbol{\mu}_j) := \frac{1}{n_j} \sum_{i=1}^{n_j} \phi(\boldsymbol{x}_i^{(j)}). \tag{58}$$

- According to the **representation theory** [14], **any solution (direction)** $\phi(\boldsymbol{u}) \in \mathcal{H}$ **must lie in the span of "all" the training vectors mapped to** $\mathcal{H}$**, i.e.,** $\boldsymbol{\Phi}(\boldsymbol{X}) = [\phi(\boldsymbol{x}_1), \dots, \phi(\boldsymbol{x}_n)] \in \mathbb{R}^{t \times n}$ **(usually** $t \gg d$**).** Note that $\mathcal{H}$ denotes the Hilbert space (feature space). Therefore, we can state that:

$$\mathbb{R}^t \ni \phi(\boldsymbol{u}) = \sum_{i=1}^{n} \theta_i \, \phi(\boldsymbol{x}_i) = \boldsymbol{\Phi}(\boldsymbol{X})\, \boldsymbol{\theta}, \tag{59}$$

  where $\mathbb{R}^n \ni \boldsymbol{\theta} := [\theta_1, \dots, \theta_n]^\top$ is the unknown vector of coefficients, and $\phi(\boldsymbol{u}) \in \mathbb{R}^t$ is the pulled Fisher direction to the feature space.
- The pulled directions can be put together in $\mathbb{R}^{t \times p} \ni \boldsymbol{\Phi}(\boldsymbol{U}) := [\phi(\boldsymbol{u}_1), \dots, \phi(\boldsymbol{u}_p)]$:

$$\mathbb{R}^{t \times p} \ni \boldsymbol{\Phi}(\boldsymbol{U}) = \boldsymbol{\Phi}(\boldsymbol{X})\, \boldsymbol{\Theta}, \tag{60}$$

  where $\boldsymbol{\Theta} := [\boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_p] \in \mathbb{R}^{n \times p}$.

Kernel Fisher Discriminant Analysis

- The d_B in the feature space is:

$$\mathbb{R} \ni d_B := \phi(\boldsymbol{u})^\top \boldsymbol{\Phi}(\boldsymbol{S}_B)\, \phi(\boldsymbol{u}) \tag{61}$$

$$\overset{(a)}{=} \boldsymbol{\theta}^\top \boldsymbol{\Phi}(\boldsymbol{X})^\top \big(\phi(\boldsymbol{\mu}_1) - \phi(\boldsymbol{\mu}_2)\big)\big(\phi(\boldsymbol{\mu}_1) - \phi(\boldsymbol{\mu}_2)\big)^\top \boldsymbol{\Phi}(\boldsymbol{X})\, \boldsymbol{\theta}, \tag{62}$$

  where (a) is because of Eqs. (57). and (59).

- For the j-th class (here $j \in \{1, 2\}$), we have:

$$\boldsymbol{\theta}^\top \boldsymbol{\Phi}(\boldsymbol{X})^\top \phi(\boldsymbol{\mu}_j) \overset{(59)}{=} \sum_{i=1}^{n} \theta_i\, \phi(\boldsymbol{x}_i)^\top \phi(\boldsymbol{\mu}_j) \overset{(58)}{=} \frac{1}{n_j} \sum_{i=1}^{n} \sum_{k=1}^{n_j} \theta_i\, \phi(\boldsymbol{x}_i)^\top \phi(\boldsymbol{x}_k^{(j)})$$

$$= \frac{1}{n_j} \sum_{i=1}^{n} \sum_{k=1}^{n_j} \theta_i\, k(\boldsymbol{x}_i, \boldsymbol{x}_k^{(j)}) = \boldsymbol{\theta}^\top \boldsymbol{m}_j, \tag{63}$$

  where $\boldsymbol{m}_j \in \mathbb{R}^n$ whose i-th entry is:

$$\boldsymbol{m}_j(i) := \frac{1}{n_j} \sum_{k=1}^{n_j} k(\boldsymbol{x}_i, \boldsymbol{x}_k^{(j)}). \tag{64}$$

Kernel Fisher Discriminant Analysis

- We had:

$$d_B = \boldsymbol{\theta}^\top \boldsymbol{\Phi}(\boldsymbol{X})^\top \big(\phi(\boldsymbol{\mu}_1) - \phi(\boldsymbol{\mu}_2)\big)\big(\phi(\boldsymbol{\mu}_1) - \phi(\boldsymbol{\mu}_2)\big)^\top \boldsymbol{\Phi}(\boldsymbol{X})\,\boldsymbol{\theta},$$

$$\boldsymbol{\theta}^\top \boldsymbol{\Phi}(\boldsymbol{X})^\top \phi(\boldsymbol{\mu}_j) = \frac{1}{n_j} \sum_{i=1}^{n} \sum_{k=1}^{n_j} \theta_i\, k(\boldsymbol{x}_i, \boldsymbol{x}_k^{(j)}) = \boldsymbol{\theta}^\top \boldsymbol{m}_j,$$

$$\boldsymbol{m}_j(i) := \frac{1}{n_j} \sum_{k=1}^{n_j} k(\boldsymbol{x}_i, \boldsymbol{x}_k^{(j)}).$$

- Hence, Eq. (62) becomes:

$$d_B \overset{(63)}{=} \boldsymbol{\theta}^\top (\boldsymbol{m}_1 - \boldsymbol{m}_2)(\boldsymbol{m}_1 - \boldsymbol{m}_2)^\top \boldsymbol{\theta} = \boldsymbol{\theta}^\top \boldsymbol{M}\boldsymbol{\theta}, \tag{65}$$

where:

$$\mathbb{R}^{n \times n} \ni \boldsymbol{M} := (\boldsymbol{m}_1 - \boldsymbol{m}_2)(\boldsymbol{m}_1 - \boldsymbol{m}_2)^\top, \tag{66}$$

is the **between-scatter** in kernel FDA. Hence, the Eq. (62) becomes:

$$d_B = \phi(\boldsymbol{u})^\top \boldsymbol{\Phi}(\boldsymbol{S}_B)\,\phi(\boldsymbol{u}) = \boldsymbol{\theta}^\top \boldsymbol{M}\boldsymbol{\theta}. \tag{67}$$

Kernel Fisher Discriminant Analysis

- The Eq. (10) in the feature space is:

$$\mathbb{R}^{t\times t} \ni \boldsymbol{\Phi}(\boldsymbol{S}_W) := \sum_{j=1}^{c}\sum_{i=1}^{n_j}\big(\phi(\boldsymbol{x}_i^{(j)}) - \phi(\boldsymbol{\mu}_j)\big)\big(\phi(\boldsymbol{x}_i^{(j)}) - \phi(\boldsymbol{\mu}_j)\big)^\top. \tag{68}$$

- The d_W in the feature space is:

$$\begin{aligned}
&\mathbb{R} \ni d_W := \phi(\boldsymbol{u})^\top \boldsymbol{\Phi}(\boldsymbol{S}_W)\,\phi(\boldsymbol{u}) \\
&\overset{(a)}{=} \Big(\sum_{\ell=1}^{n}\theta_\ell\,\phi(\boldsymbol{x}_\ell)^\top\Big)\Big(\sum_{j=1}^{c}\sum_{i=1}^{n_j}\big(\phi(\boldsymbol{x}_i^{(j)}) - \phi(\boldsymbol{\mu}_j)\big)\big(\phi(\boldsymbol{x}_i^{(j)}) - \phi(\boldsymbol{\mu}_j)\big)^\top\Big)\Big(\sum_{k=1}^{n}\theta_k\,\phi(\boldsymbol{x}_k)\Big) \\
&= \sum_{j=1}^{c}\sum_{\ell=1}^{n}\sum_{i=1}^{n_j}\sum_{k=1}^{n}\Big(\theta_\ell\,\phi(\boldsymbol{x}_\ell)^\top\big(\phi(\boldsymbol{x}_i^{(j)}) - \phi(\boldsymbol{\mu}_j)\big)\big(\phi(\boldsymbol{x}_i^{(j)}) - \phi(\boldsymbol{\mu}_j)\big)^\top\theta_k\,\phi(\boldsymbol{x}_k)\Big) \\
&\overset{(58)}{=} \sum_{j=1}^{c}\sum_{\ell=1}^{n}\sum_{i=1}^{n_j}\sum_{k=1}^{n}\Big(\theta_\ell\,\phi(\boldsymbol{x}_\ell)^\top\big(\phi(\boldsymbol{x}_i^{(j)}) - \frac{1}{n_j}\sum_{e=1}^{n_j}\phi(\boldsymbol{x}_e^{(j)})\big) \\
&\qquad\qquad \big(\phi(\boldsymbol{x}_i^{(j)}) - \frac{1}{n_j}\sum_{z=1}^{n_j}\phi(\boldsymbol{x}_z^{(j)})\big)^\top\theta_k\,\phi(\boldsymbol{x}_k)\Big)
\end{aligned}$$

Kernel Fisher Discriminant Analysis

$$= \sum_{j=1}^{c} \sum_{\ell=1}^{n} \sum_{i=1}^{n_j} \sum_{k=1}^{n} \Big(\theta_\ell\, k(\boldsymbol{x}_\ell, \boldsymbol{x}_i^{(j)}) - \frac{1}{n_j} \sum_{e=1}^{n_j} \theta_\ell\, k(\boldsymbol{x}_\ell, \boldsymbol{x}_e^{(j)})\Big)$$

$$\Big(\theta_k\, k(\boldsymbol{x}_i^{(j)}, \boldsymbol{x}_k) - \frac{1}{n_j} \sum_{z=1}^{n_j} \theta_k\, k(\boldsymbol{x}_z^{(j)}, \boldsymbol{x}_k)\Big)$$

$$\overset{(b)}{=} \sum_{j=1}^{c} \sum_{\ell=1}^{n} \sum_{i=1}^{n_j} \sum_{k=1}^{n} \Big(\theta_\ell\, k(\boldsymbol{x}_\ell, \boldsymbol{x}_i^{(j)}) - \frac{1}{n_j} \sum_{e=1}^{n_j} \theta_\ell\, k(\boldsymbol{x}_\ell, \boldsymbol{x}_e^{(j)})\Big) \Big(\theta_k\, k(\boldsymbol{x}_k, \boldsymbol{x}_i^{(j)}) - \frac{1}{n_j} \sum_{z=1}^{n_j} \theta_k\, k(\boldsymbol{x}_k, \boldsymbol{x}_z^{(j)})\Big)$$

$$= \sum_{j=1}^{c} \sum_{\ell=1}^{n} \sum_{i=1}^{n_j} \sum_{k=1}^{n} \Big(\theta_\ell\, \theta_k\, k(\boldsymbol{x}_\ell, \boldsymbol{x}_i^{(j)})\, k(\boldsymbol{x}_k, \boldsymbol{x}_i^{(j)}) - \frac{2\,\theta_\ell\, \theta_k}{n_j} \sum_{z=1}^{n_j} k(\boldsymbol{x}_\ell, \boldsymbol{x}_i^{(j)})\, k(\boldsymbol{x}_k, \boldsymbol{x}_z^{(j)})$$

$$+ \frac{\theta_\ell\, \theta_k}{n_j^2} \sum_{e=1}^{n_j} \sum_{z=1}^{n_j} k(\boldsymbol{x}_\ell, \boldsymbol{x}_e^{(j)})\, k(\boldsymbol{x}_k, \boldsymbol{x}_z^{(j)})\Big)$$

$$= \sum_{j=1}^{c} \sum_{\ell=1}^{n} \sum_{i=1}^{n_j} \sum_{k=1}^{n} \Big(\theta_\ell\, \theta_k\, k(\boldsymbol{x}_\ell, \boldsymbol{x}_i^{(j)})\, k(\boldsymbol{x}_k, \boldsymbol{x}_i^{(j)}) - \frac{\theta_\ell\, \theta_k}{n_j} \sum_{z=1}^{n_j} k(\boldsymbol{x}_\ell, \boldsymbol{x}_i^{(j)})\, k(\boldsymbol{x}_k, \boldsymbol{x}_z^{(j)})\Big)$$

Kernel Fisher Discriminant Analysis

$$
\begin{aligned}
&= \sum_{j=1}^{c}\sum_{\ell=1}^{n}\sum_{i=1}^{n_j}\sum_{k=1}^{n}\Big(\theta_\ell\,\theta_k\,k(\boldsymbol{x}_\ell,\boldsymbol{x}_i^{(j)})\,k(\boldsymbol{x}_k,\boldsymbol{x}_i^{(j)}) - \frac{\theta_\ell\,\theta_k}{n_j}\sum_{z=1}^{n_j} k(\boldsymbol{x}_\ell,\boldsymbol{x}_i^{(j)})\,k(\boldsymbol{x}_k,\boldsymbol{x}_z^{(j)})\Big) \\
&= \sum_{j=1}^{c}\Bigg(\sum_{\ell=1}^{n}\sum_{i=1}^{n_j}\sum_{k=1}^{n}\Big(\theta_\ell\,\theta_k\,k(\boldsymbol{x}_\ell,\boldsymbol{x}_i^{(j)})\,k(\boldsymbol{x}_k,\boldsymbol{x}_i^{(j)})\Big) \\
&\qquad\qquad - \sum_{\ell=1}^{n}\sum_{i=1}^{n_j}\sum_{k=1}^{n}\Big(\frac{\theta_\ell\,\theta_k}{n_j}\sum_{z=1}^{n_j} k(\boldsymbol{x}_\ell,\boldsymbol{x}_i^{(j)})\,k(\boldsymbol{x}_k,\boldsymbol{x}_z^{(j)})\Big)\Bigg) \\
&\overset{(c)}{=} \sum_{j=1}^{c}(\boldsymbol{\theta}^\top\boldsymbol{K}_j\boldsymbol{K}_j^\top\boldsymbol{\theta} - \boldsymbol{\theta}^\top\boldsymbol{K}_j\frac{1}{n_j}\boldsymbol{1}\boldsymbol{1}^\top\boldsymbol{K}_j^\top\boldsymbol{\theta}) = \sum_{j=1}^{c}\boldsymbol{\theta}^\top\boldsymbol{K}_j(\boldsymbol{I} - \frac{1}{n_j}\boldsymbol{1}\boldsymbol{1}^\top)\boldsymbol{K}_j^\top\boldsymbol{\theta} \\
&\overset{(d)}{=} \sum_{j=1}^{c}\boldsymbol{\theta}^\top\boldsymbol{K}_j\boldsymbol{H}_j\boldsymbol{K}_j^\top\boldsymbol{\theta} = \boldsymbol{\theta}^\top\Big(\sum_{j=1}^{c}\boldsymbol{K}_j\boldsymbol{H}_j\boldsymbol{K}_j^\top\Big)\boldsymbol{\theta},
\end{aligned}
$$

where (a) is because of Eqs. (68) and (59), (b) is because $k(\boldsymbol{x}_1,\boldsymbol{x}_2) = k(\boldsymbol{x}_2,\boldsymbol{x}_1) \in \mathbb{R}$, and (c) is because $\boldsymbol{K}_j \in \mathbb{R}^{n\times n_j}$ is the kernel matrix of the whole training data and the training data of the j-th class. The (a,b)-th element of $\boldsymbol{K}_j$ is:

$$
\boldsymbol{K}_j(a,b) := k(\boldsymbol{x}_a,\boldsymbol{x}_b^{(j)}). \tag{69}
$$

Kernel Fisher Discriminant Analysis

- The (d) is because:

$$\mathbb{R}^{n_j \times n_j} \ni \boldsymbol{H}_j := \boldsymbol{I} - \frac{1}{n_j}\boldsymbol{1}\boldsymbol{1}^\top, \tag{70}$$

  is the **centering matrix**.
- We define:

$$\mathbb{R}^{n \times n} \ni \boldsymbol{N} := \sum_{j=1}^{c} \boldsymbol{K}_j \boldsymbol{H}_j \boldsymbol{K}_j^\top, \tag{71}$$

  as the **within-scatter** in kernel FDA. Hence, the d_W becomes:

$$d_W = \phi(\boldsymbol{u})^\top \boldsymbol{\Phi}(\boldsymbol{S}_W)\, \phi(\boldsymbol{u}) = \boldsymbol{\theta}^\top \boldsymbol{N} \boldsymbol{\theta}. \tag{72}$$

- The **kernel Fisher criterion** is:

$$f(\boldsymbol{\theta}) := \frac{d_B(\boldsymbol{\theta})}{d_W(\boldsymbol{\theta})} = \frac{\phi(\boldsymbol{u})^\top \boldsymbol{\Phi}(\boldsymbol{S}_B)\, \phi(\boldsymbol{u})}{\phi(\boldsymbol{u})^\top \boldsymbol{\Phi}(\boldsymbol{S}_W)\, \phi(\boldsymbol{u})} = \frac{\boldsymbol{\theta}^\top \boldsymbol{M} \boldsymbol{\theta}}{\boldsymbol{\theta}^\top \boldsymbol{N} \boldsymbol{\theta}}, \tag{73}$$

  where the $\boldsymbol{\theta} \in \mathbb{R}^n$ is the **kernel Fisher direction**.
- Similar to the solution of Eq. (19), the solution to maximization of Eq. (73) is:

$$\boldsymbol{M}\boldsymbol{\theta} = \lambda\, \boldsymbol{N}\boldsymbol{\theta}, \tag{74}$$

  which is a generalized eigenvalue problem $(\boldsymbol{M}, \boldsymbol{N})$ according to [4]. The $\boldsymbol{\theta}$ is the eigenvector with the largest eigenvalue (because the optimization is maximization) and the λ is the corresponding eigenvalue. The $\boldsymbol{\theta}$ is the **kernel Fisher direction** or **kernel Fisher axis**.

Kernel Fisher Discriminant Analysis

- Again, one possible solution to the generalized eigenvalue problem $(\boldsymbol{M}, \boldsymbol{N})$ is [4]:

$$\boldsymbol{\theta} = \textbf{eig}(\boldsymbol{N}^{-1}\boldsymbol{M}), \tag{75}$$

or [4]:

$$\boldsymbol{\theta} = \textbf{eig}((\boldsymbol{N} + \varepsilon\boldsymbol{I})^{-1}\boldsymbol{M}), \tag{76}$$

where **eig**(.) denotes the eigenvector of the matrix with the largest eigenvalue.

- The projection and reconstruction of the training data point $\boldsymbol{x}_i$ and the out-of-sample data point $\boldsymbol{x}_t$ are:

$$\mathbb{R} \ni \phi(\widetilde{\boldsymbol{x}}_i) = \boldsymbol{\phi}(\boldsymbol{u})^\top \boldsymbol{\phi}(\boldsymbol{x}_i) \overset{(59)}{=} \boldsymbol{\theta}^\top \boldsymbol{\Phi}(\boldsymbol{X})^\top \boldsymbol{\phi}(\boldsymbol{x}_i) = \boldsymbol{\theta}^\top \boldsymbol{k}(\boldsymbol{X}, \boldsymbol{x}_i), \tag{77}$$

$$\mathbb{R}^t \ni \boldsymbol{\phi}(\widehat{\boldsymbol{x}}_i) = \boldsymbol{\phi}(\boldsymbol{u})\boldsymbol{\phi}(\boldsymbol{u})^\top \boldsymbol{\phi}(\boldsymbol{x}_i) \overset{(59)}{=} \boldsymbol{\Phi}(\boldsymbol{X})\, \boldsymbol{\theta}\boldsymbol{\theta}^\top \boldsymbol{k}(\boldsymbol{X}, \boldsymbol{x}_i), \tag{78}$$

$$\mathbb{R} \ni \phi(\widetilde{\boldsymbol{x}}_t) = \boldsymbol{\theta}^\top \boldsymbol{k}(\boldsymbol{X}, \boldsymbol{x}_t), \tag{79}$$

$$\mathbb{R}^t \ni \boldsymbol{\phi}(\widehat{\boldsymbol{x}}_t) = \boldsymbol{\Phi}(\boldsymbol{X})\, \boldsymbol{\theta}\boldsymbol{\theta}^\top \boldsymbol{k}(\boldsymbol{X}, \boldsymbol{x}_t). \tag{80}$$

- However, in reconstruction expressions, the $\boldsymbol{\Phi}(\boldsymbol{X})$ is not necessarily available; therefore, in kernel FDA, similar to kernel PCA [5], **reconstruction cannot be done.**
- For the whole training and out-of-sample data, the projections are:

$$\mathbb{R}^{1\times n} \ni \boldsymbol{\Phi}(\widetilde{\boldsymbol{X}}) = \boldsymbol{\theta}^\top \boldsymbol{K}(\boldsymbol{X}, \boldsymbol{X}), \tag{81}$$

$$\mathbb{R}^{1\times n_t} \ni \boldsymbol{\Phi}(\widetilde{\boldsymbol{X}}_t) = \boldsymbol{\theta}^\top \boldsymbol{K}(\boldsymbol{X}, \boldsymbol{X}_t). \tag{82}$$

Kernel Fisher Discriminant Analysis

- In multi-dimensional kernel Fisher subspace, the within- and between-scatters are the same but the Fisher criterion is different. According to Eq. (60), the d_B and d_W are:

$$d_B = \mathbf{tr}\big(\phi(\boldsymbol{U})^\top \boldsymbol{\Phi}(\boldsymbol{S}_B)\, \phi(\boldsymbol{U})\big) = \mathbf{tr}(\boldsymbol{\Theta}^\top \boldsymbol{M}\boldsymbol{\Theta}), \tag{83}$$

$$d_W = \mathbf{tr}\big(\phi(\boldsymbol{U})^\top \boldsymbol{\Phi}(\boldsymbol{S}_W)\, \phi(\boldsymbol{U})\big) = \mathbf{tr}(\boldsymbol{\Theta}^\top \boldsymbol{N}\boldsymbol{\Theta}), \tag{84}$$

  where $\mathbb{R}^{n\times p} \ni \boldsymbol{\Theta} = [\boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_p]$ and $\boldsymbol{M} \in \mathbb{R}^{n\times n}$ and $\boldsymbol{N} \in \mathbb{R}^{n\times n}$ are the between- and within-scatters, respectively, determined for either two-class or multi-class case.

- The Fisher criterion becomes:

$$f(\boldsymbol{\Theta}) := \frac{d_B(\boldsymbol{\Theta})}{d_W(\boldsymbol{\Theta})} = \frac{\mathbf{tr}\big(\phi(\boldsymbol{U})^\top \boldsymbol{\Phi}(\boldsymbol{S}_B)\, \phi(\boldsymbol{U})\big)}{\mathbf{tr}\big(\phi(\boldsymbol{U})^\top \boldsymbol{\Phi}(\boldsymbol{S}_W)\, \phi(\boldsymbol{U})\big)} = \frac{\mathbf{tr}(\boldsymbol{\Theta}^\top \boldsymbol{M}\boldsymbol{\Theta})}{\mathbf{tr}(\boldsymbol{\Theta}^\top \boldsymbol{N}\boldsymbol{\Theta})}, \tag{85}$$

  where the columns of $\boldsymbol{\Theta}$ are the *kernel Fisher directions*.

- Similar to Eq. (34), the solution to maximization of this criterion is:

$$\boldsymbol{M}\boldsymbol{\Theta} = \boldsymbol{N}\boldsymbol{\Theta}\boldsymbol{\Lambda}, \tag{86}$$

  which is the generalized eigenvalue problem $(\boldsymbol{M}, \boldsymbol{N})$ according to [4]. The columns of $\boldsymbol{\Theta}$ are the eigenvectors sorted from the largest to smallest eigenvalues (because the optimization is maximization) and the diagonal entries of $\boldsymbol{\Lambda}$ are the corresponding eigenvalues.

Kernel Fisher Discriminant Analysis

- As mentioned before, in kernel FDA, we do not have reconstruction.
- The projection of the training data point $\boldsymbol{x}_i$ and the out-of-sample data point $\boldsymbol{x}_t$ are:

$$\mathbb{R}^p \ni \phi(\widetilde{\boldsymbol{x}}_i) = \boldsymbol{\Phi}(\boldsymbol{U})^\top \phi(\boldsymbol{x}_i) \overset{(60)}{=} \boldsymbol{\Theta}^\top \boldsymbol{\Phi}(\boldsymbol{X})^\top \phi(\boldsymbol{x}_i) = \boldsymbol{\Theta}^\top \boldsymbol{k}(\boldsymbol{X}, \boldsymbol{x}_i), \tag{87}$$

$$\mathbb{R}^p \ni \phi(\widetilde{\boldsymbol{x}}_t) = \boldsymbol{\Theta}^\top \boldsymbol{k}(\boldsymbol{X}, \boldsymbol{x}_t). \tag{88}$$

- For the whole training and out-of-sample data, the projections are:

$$\mathbb{R}^{p \times n} \ni \boldsymbol{\Phi}(\widetilde{\boldsymbol{X}}) = \boldsymbol{\Theta}^\top \boldsymbol{K}(\boldsymbol{X}, \boldsymbol{X}), \tag{89}$$

$$\mathbb{R}^{p \times n_t} \ni \boldsymbol{\Phi}(\widetilde{\boldsymbol{X}}_t) = \boldsymbol{\Theta}^\top \boldsymbol{K}(\boldsymbol{X}, \boldsymbol{X}_t). \tag{90}$$

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- The code of FDA in my GitHub page (in Python language): `https://github.com/bghojogh/Fisher-Discriminant-Analysis`
- FDA/LDA in sklearn: `https://scikit-learn.org/stable/modules/generated/sklearn.discriminant_analysis.LinearDiscriminantAnalysis.html`

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