

PCA and LDA

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Why Dimension Reduction

- Many applications produce high-dimensional vectors
 - In face recognition, if an image has size 360×260 pixels, the dimension is 93600.
 - In hand-writing digit recognition, if a digit occupies 28×28 pixels, the dimension is 784.
 - In speaker recognition, the dim can be as high as 61440 per utterance.
- High-dim feature vectors can easily cause the curse-of-dimensionality problem.
- **Redundancy**: Some of the elements in the feature vectors are strongly correlated, meaning that knowing one element will also know some other elements.
- **Irrelevancy**: Some elements in the feature vectors are irrelevant to the classification task.

Dimension Reduction

- Given a feature vector $\mathbf{x} \in \mathbb{R}^D$, dimensionality reduction aims to find a low dimensional representation $\mathbf{h} \in \mathbb{R}^M$ that can approximately explain \mathbf{x} :

$$\mathbf{x} \approx f(\mathbf{h}, \boldsymbol{\theta}) \quad (1)$$

where $f(\cdot, \cdot)$ is a function that takes the hidden variable \mathbf{h} and a set of parameters $\boldsymbol{\theta}$ and $M \leq D$.

- Typically, we choose the function family $f(\cdot, \cdot)$ and then learn \mathbf{h} and $\boldsymbol{\theta}$ from training data.
- Least squares criterion:** Given N training vectors $\mathcal{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$, $\mathbf{x}_i \in \mathbb{R}^D$, we find the parameters $\boldsymbol{\theta}$ and latent variables \mathbf{h}_i 's that minimize the sum of squared error:

$$\hat{\boldsymbol{\theta}}, \{\hat{\mathbf{h}}_i\}_{i=1}^N = \operatorname{argmin}_{\boldsymbol{\theta}, \{\mathbf{h}_i\}_{i=1}^N} \left\{ \sum_{i=1}^N [\mathbf{x}_i - f(\mathbf{h}_i, \boldsymbol{\theta})]^\top [\mathbf{x}_i - f(\mathbf{h}_i, \boldsymbol{\theta})] \right\} \quad (2)$$

Dimension Reduction: Reduce to 1-Dim

- Approximate vector \mathbf{x}_i by a scalar value h_i plus the global mean $\boldsymbol{\mu}$:

$$\mathbf{x}_i \approx \boldsymbol{\phi} h_i + \boldsymbol{\mu}, \text{ where } \boldsymbol{\mu} = \frac{1}{N} \sum_{i=1}^N \mathbf{x}_i, \quad \boldsymbol{\phi} \in \mathbb{R}^{D \times 1}$$

- Assuming $\boldsymbol{\mu} = \mathbf{0}$ or vectors have been mean-subtracted, i.e., $\mathbf{x}_i \leftarrow \mathbf{x}_i - \boldsymbol{\mu} \forall i$, we have

$$\mathbf{x}_i \approx \boldsymbol{\phi} h_i$$

- The least squares criterion becomes:

$$\begin{aligned} \hat{\boldsymbol{\phi}}, \{\hat{h}_i\}_{i=1}^N &= \operatorname{argmin}_{\boldsymbol{\phi}, \{h_i\}_{i=1}^N} E(\boldsymbol{\phi}, \{h_i\}) \\ &= \operatorname{argmin}_{\boldsymbol{\phi}, \{h_i\}_{i=1}^N} \left\{ \sum_{i=1}^N [\mathbf{x}_i - \boldsymbol{\phi} h_i]^\top [\mathbf{x}_i - \boldsymbol{\phi} h_i] \right\} \end{aligned} \quad (3)$$

Dimension Reduction: Reduce to 1-Dim

- Eq. 3 has a problem in that it does not have a unique solution. If we multiply ϕ by any constant α and divide h_i 's by the same constant we get the same cost, i.e., $\alpha\phi \cdot \frac{h_i}{\alpha} = \phi h_i$.
- We make the solution unique by constraining $\|\phi\|^2 = 1$ using a Lagrange multiplier:

$$\begin{aligned} L(\phi, \{h_i\}) &= E(\phi, \{h_i\}) + \lambda(\phi^T \phi - 1) \\ &= \sum_{i=1}^N (\mathbf{x}_i - \phi h_i)^T (\mathbf{x}_i - \phi h_i) + \lambda(\phi^T \phi - 1) \\ &= \sum_{i=1}^N \mathbf{x}_i^T \mathbf{x}_i - 2h_i \phi^T \mathbf{x}_i + h_i^2 + \lambda(\phi^T \phi - 1) \end{aligned}$$

Dimension Reduction: Reduce to 1-Dim

- Setting $\frac{\partial L}{\partial \phi} = \mathbf{0}$ and $\frac{\partial L}{\partial h_i} = 0$, we obtain:

$$\sum_i \mathbf{x}_i \hat{h}_i = \lambda \hat{\phi} \quad \text{and} \quad \hat{\phi}^\top \mathbf{x}_i = \hat{h}_i = \mathbf{x}_i^\top \hat{\phi}$$

- Hence,

$$\begin{aligned} \sum_i \mathbf{x}_i (\mathbf{x}_i^\top \hat{\phi}) &= \left(\sum_i \mathbf{x}_i \mathbf{x}_i^\top \right) \hat{\phi} = \lambda \hat{\phi} \\ \implies \mathbf{S} \hat{\phi} &= \lambda \hat{\phi} \end{aligned}$$

where \mathbf{S} is the covariance matrix of training data.¹

- Therefore, $\hat{\phi}$ is the first eigenvector of \mathbf{S} .

¹Note that \mathbf{x}_i 's have been mean subtracted.

Dimension Reduction: Reduce to 1-Dim

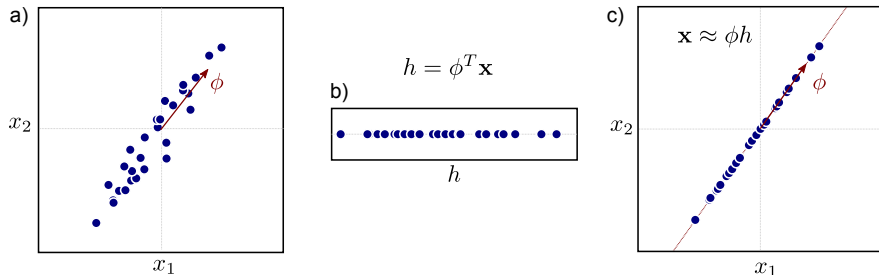
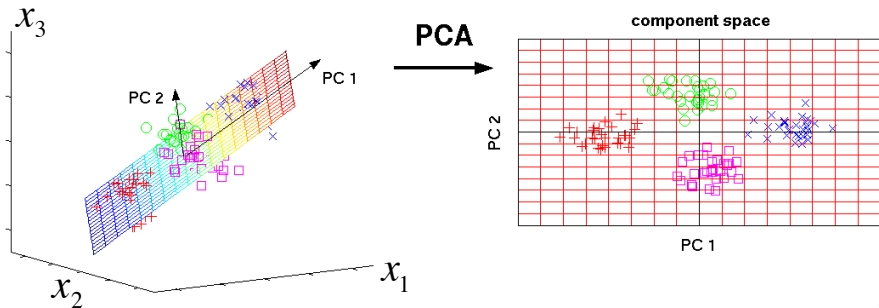


Figure 13.19 Reduction to a single dimension. a) Original data and direction ϕ of maximum variance. b) The data are projected onto ϕ to produce a one dimensional representation. c) To reconstruct the data, we re-multiply by ϕ . Most of the original variation is retained. PCA extends this model to project high dimensional data onto the K orthogonal dimensions with the most variance, to produce a K dimensional representation.

Dimension Reduction: 3D to 2D



Principle Component Analysis

- In PCA, the hidden variables $\{\mathbf{h}_i\}$ are multi-dimensional and ϕ becomes a rectangular matrix $\Phi = [\phi_1 \ \phi_2 \ \cdots \ \phi_M]$, where $M \leq D$.
- Each components of \mathbf{h}_i weights one column of matrix Φ so that data is approximated as

$$\mathbf{x}_i \approx \Phi \mathbf{h}_i, \quad i = 1, \dots, N$$

- The cost function is²

$$\begin{aligned} \hat{\Phi}, \{\hat{\mathbf{h}}_i\}_{i=1}^N &= \underset{\Phi, \{\mathbf{h}_i\}_{i=1}^N}{\operatorname{argmin}} E(\Phi, \{\mathbf{h}_i\}_{i=1}^N) \\ &= \underset{\Phi, \{\mathbf{h}_i\}_{i=1}^N}{\operatorname{argmin}} \left\{ \sum_{i=1}^N [\mathbf{x}_i - \Phi \mathbf{h}_i]^\top [\mathbf{x}_i - \Phi \mathbf{h}_i] \right\} \end{aligned} \quad (4)$$

²Note that we have defined $\theta \equiv \Phi$ in Eq. 2.

Principle Component Analysis

- To solve the non-uniqueness problem in Eq. 4, we enforce $\phi_d^\top \phi_d = 1$, $d = 1, \dots, M$, using a set of Lagrange multipliers $\{\lambda_d\}_{d=1}^M$:

$$\begin{aligned} L(\Phi, \{\mathbf{h}_i\}) &= \sum_{i=1}^N (\mathbf{x}_i - \Phi \mathbf{h}_i)^\top (\mathbf{x}_i - \Phi \mathbf{h}_i) + \sum_{d=1}^M \lambda_d (\phi_d^\top \phi_d - 1) \\ &= \sum_{i=1}^N (\mathbf{x}_i - \Phi \mathbf{h}_i)^\top (\mathbf{x}_i - \Phi \mathbf{h}_i) + \text{tr}\{\Phi \Lambda_M \Phi^\top - \Lambda\} \\ &= \sum_{i=1}^N \mathbf{x}_i^\top \mathbf{x}_i - 2 \mathbf{h}_i^\top \Phi^\top \mathbf{x}_i + \mathbf{h}_i^\top \mathbf{h}_i + \text{tr}\{\Phi \Lambda_M \Phi^\top - \Lambda\} \end{aligned} \quad (5)$$

where $\mathbf{h}_i \in \mathbb{R}^M$, $\Lambda = \text{diag}\{\lambda_1, \dots, \lambda_M, 0, \dots, 0\} \in \mathbb{R}^{D \times D}$,
 $\Lambda_M = \text{diag}\{\lambda_1, \dots, \lambda_M\} \in \mathbb{R}^{M \times M}$, and
 $\Phi = [\phi_1 \ \phi_2 \ \dots \ \phi_M] \in \mathbb{R}^{D \times M}$.

Principle Component Analysis

- Setting $\frac{\partial L}{\partial \Phi} = \mathbf{0}$ and $\frac{\partial L}{\partial \mathbf{h}_i} = \mathbf{0}$, we obtain:

$$\sum_i \mathbf{x}_i \hat{\mathbf{h}}_i^\top = \hat{\Phi} \Lambda_M \quad \text{and} \quad \hat{\Phi}^\top \mathbf{x}_i = \hat{\mathbf{h}}_i \implies \hat{\mathbf{h}}_i^\top = \mathbf{x}_i^\top \hat{\Phi}$$

where we have used:

$$\frac{\partial}{\partial \mathbf{X}} \text{tr}\{\mathbf{X} \mathbf{B} \mathbf{X}^\top\} = \mathbf{X} \mathbf{B}^\top + \mathbf{X} \mathbf{B} \quad \text{and} \quad \frac{\partial \mathbf{a}^\top \mathbf{X}^\top \mathbf{b}}{\partial \mathbf{X}} = \mathbf{b} \mathbf{a}^\top.$$

- Therefore,

$$\sum_i \mathbf{x}_i \mathbf{x}_i^\top \hat{\Phi} = \hat{\Phi} \Lambda_M \implies \mathbf{S} \hat{\Phi} = \hat{\Phi} \Lambda_M \quad (6)$$

- So, $\hat{\Phi}$ comprises the M eigenvectors of \mathbf{S} .

Interpretation of Λ_M

- Denote \mathbf{X} as a $D \times N$ centered data matrix whose n -th column is given by $(\mathbf{x}_n - \frac{1}{N} \sum_{i=1}^N \mathbf{x}_i)$.
- The projected data matrix is given by

$$\mathbf{Y} = \hat{\Phi}^T \mathbf{X}$$

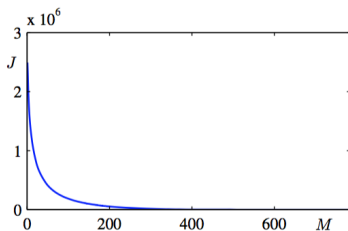
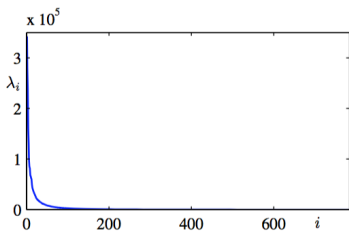
- The covariance matrix of the projected data is

$$\begin{aligned} \mathbf{Y}\mathbf{Y}^T &= (\hat{\Phi}^T \mathbf{X}) (\hat{\Phi}^T \mathbf{X})^T \\ &= \hat{\Phi}^T \mathbf{X} \mathbf{X}^T \hat{\Phi} \\ &= \hat{\Phi}^T \hat{\Phi} \Lambda_M \quad (\text{see the eigen-equation in Eq. 6}) \\ &= \Lambda_M \end{aligned}$$

- Therefore, the eigenvalues represent the variances of individual elements of the projected vectors.

Interpretation of Λ_M

- The eigenvalues are typically arranged in descending order:
 $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_D$.
- This means that the first few principal components capture most of the variances.
- If we project \mathbf{x} to M -dimensional space (i.e., keeping the first M PCs), the loss in variances is $J = \sum_{i=M+1}^D \lambda_i$.
- The variance “explained” by the first M PCs is $\sum_{i=1}^M \lambda_i$.



PCA on High-Dimensional Data

- When, the dimension D of \mathbf{x}_i is very high, computing \mathbf{S} and its eigenvectors directly are impractical.
- However, the rank of \mathbf{S} is limited by the number of training examples: If there are N training examples, there will be at most $N - 1$ eigenvectors with non-zero eigenvalues. If $N \ll D$, the principal components can be computed more easily.
- Let \mathbf{X} be a data matrix comprising the mean-subtracted \mathbf{x}_i 's in its columns. Then, $\mathbf{S} = \mathbf{X}\mathbf{X}^T$ and the eigen-decomposition of \mathbf{S} is given by

$$\mathbf{S}\phi_i = \mathbf{X}\mathbf{X}^T\phi_i = \lambda_i\phi_i$$

- Instead of performing eigen-decomposition of $\mathbf{X}\mathbf{X}^T$, we perform eigen-decomposition of

$$\mathbf{X}^T\mathbf{X}\psi_i = \lambda_i\psi_i \tag{7}$$

Principle Component Analysis

- Pre-multiplying both side of Eq. 7 by \mathbf{X} , we obtain

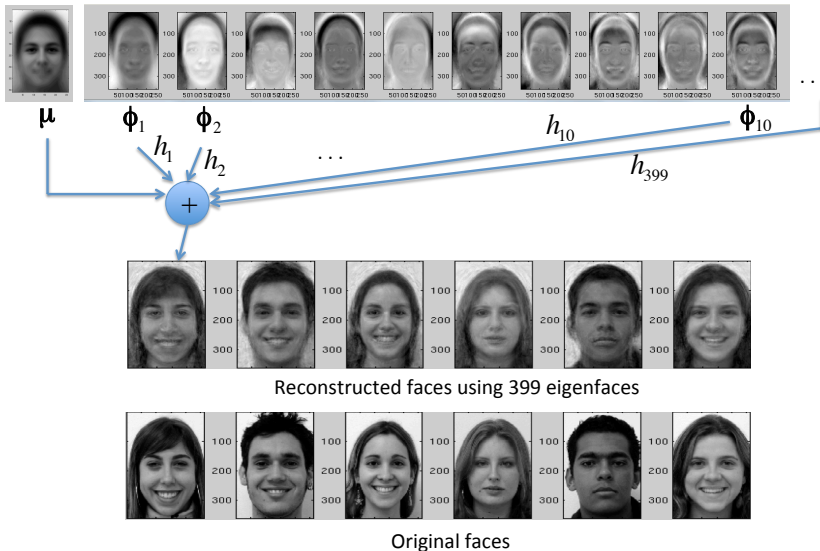
$$\mathbf{X}\mathbf{X}^T(\mathbf{X}\psi_i) = \lambda_i(\mathbf{X}\psi_i)$$

- This means that if ψ_i is an eigenvector of $\mathbf{X}^T\mathbf{X}$, then $\phi_i = \mathbf{X}\psi_i$ is an eigenvector of $\mathbf{S} = \mathbf{X}\mathbf{X}^T$.
- So, all we need is to compute the $N - 1$ eigenvectors of $\mathbf{X}^T\mathbf{X}$, which has size $N \times N$.
- Note that ϕ_i computed in this way is un-normalized. So, we need to normalize them by

$$\phi_i = \frac{\mathbf{X}\psi_i}{\|\mathbf{X}\psi_i\|}, \quad i = 1, \dots, N - 1$$

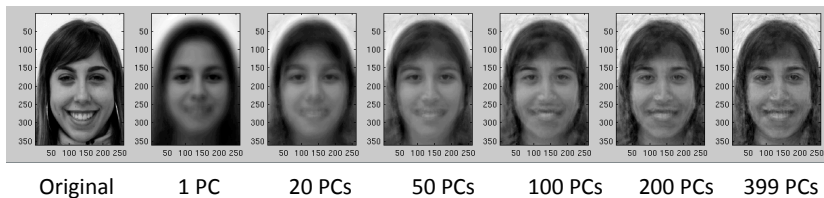
Example Application of PCA: Eigenface

- Eigenface is one of the most well-known applications of PCA.



Example Application of PCA: Eigenface

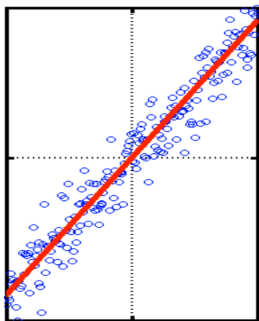
- Faces reconstructed using different numbers of principal components (eigenfaces):



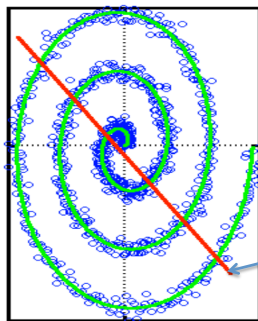
- See Lab2 of EIE4105 in <http://www.eie.polyu.edu.hk/~mwmak/myteaching.htm> for implementation.

Limitations of PCA

- PCA will fail if the subspace is non-linear



Linear subspace (PCA is fine)



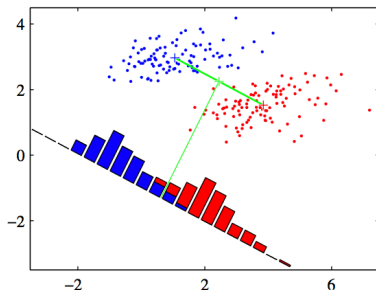
PCA can only
find this

Nonlinear subspace (PCA fails)

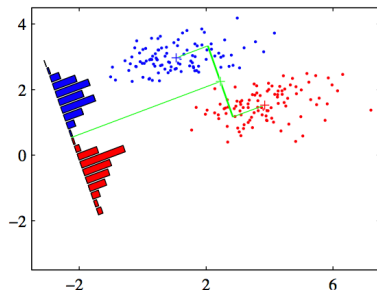
- Solution:* Use non-linear embedding such as ISOMAP or DNN

Fisher Discriminant Analysis

- FDA is a classification method to separate data into two classes.
- FDA could also be considered as a supervised dimension reduction method that reduces the dimension to 1.



Project data onto line joining the 2 means



Project data onto FDA subspace

Fisher Discriminant Analysis

- The idea of FDA is to find a 1-D line so that the projected data give a **large separation** between the means of two classes while also giving a **small variance** within each class, thereby minimizing the class overlap.
- Assume that training data are projected onto a 1-D space using

$$y_n = \mathbf{w}^T \mathbf{x}_n, \quad n = 1, \dots, N.$$

- Fisher criterion:

$$J(\mathbf{w}) = \frac{\text{Between-class scatter}}{\text{Within-class scatter}} = \frac{\mathbf{w}^T \mathbf{S}_B \mathbf{w}}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}}$$

where

$$\mathbf{S}_B = (\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)(\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)^T \quad \text{and} \quad \mathbf{S}_W = \sum_{k=1}^2 \frac{1}{N_k} \sum_{n \in \mathcal{C}_k} (\mathbf{x}_n - \boldsymbol{\mu}_k)(\mathbf{x}_n - \boldsymbol{\mu}_k)^T$$

are the **between-class** and **within-class** scatter matrices, respectively, and $\boldsymbol{\mu}_1$ and $\boldsymbol{\mu}_2$ are the class means.

Fisher Discriminant Analysis

- Note that only the direction of \mathbf{w} matters. Therefore, we can always find a \mathbf{w} that leads to $\mathbf{w}^T \mathbf{S}_W \mathbf{w} = 1$.
- The maximization of $J(\mathbf{w})$ can be rewritten as:

$$\begin{array}{ll} \max_{\mathbf{w}} & \mathbf{w}^T \mathbf{S}_B \mathbf{w} \\ \text{subject to} & \mathbf{w}^T \mathbf{S}_W \mathbf{w} = 1 \end{array}$$

- The Lagrangian function is

$$L(\mathbf{w}, \lambda) = \frac{1}{2} \mathbf{w}^T \mathbf{S}_B \mathbf{w} - \lambda (\mathbf{w}^T \mathbf{S}_W \mathbf{w} - 1)$$

- Setting $\frac{\partial L}{\partial \mathbf{w}} = 0$, we obtain

$$\begin{aligned} \mathbf{S}_B \mathbf{w} - \lambda \mathbf{S}_W \mathbf{w} &= 0 \\ \implies \mathbf{S}_B \mathbf{w} &= \lambda \mathbf{S}_W \mathbf{w} \\ \implies (\mathbf{S}_W^{-1} \mathbf{S}_B) \mathbf{w} &= \lambda \mathbf{w} \end{aligned} \tag{8}$$

- So, \mathbf{w} is the first eigenvector of $\mathbf{S}_W^{-1} \mathbf{S}_B$.

LDA on Multi-class Problems

- For multiple classes ($K > 2$ and $D > K$), we can use LDA to project D -dimensional vectors to M -dimensional vectors, where $1 < M < K$.
- \mathbf{w} is extended to a matrix $\mathbf{W} = [\mathbf{w}_1 \cdots \mathbf{w}_M]$ and the projected scalar y_i is extended to a vector \mathbf{y}_i :

$$\mathbf{y}_n = \mathbf{W}^T(\mathbf{x}_n - \boldsymbol{\mu}), \quad \text{where } y_{nj} = \mathbf{w}_j^T(\mathbf{x}_n - \boldsymbol{\mu}), \quad j = 1, \dots, M$$

where $\boldsymbol{\mu}$ is the global mean of training vectors.

- The between-class and within-class scatter matrices become

$$\mathbf{S}_B = \sum_{k=1}^K N_k (\boldsymbol{\mu}_k - \boldsymbol{\mu})(\boldsymbol{\mu}_k - \boldsymbol{\mu})^T$$
$$\mathbf{S}_W = \sum_{k=1}^K \sum_{n \in \mathcal{C}_k} (\mathbf{x}_n - \boldsymbol{\mu}_k)(\mathbf{x}_n - \boldsymbol{\mu}_k)^T$$

where N_k is the number of samples in the class k , i.e., $N_k = |\mathcal{C}_k|$.

LDA on Multi-class Problems

- The LDA criterion function:

$$J(\mathbf{W}) = \frac{\text{Between-class scatter}}{\text{Within-class scatter}} = \text{Tr} \left\{ \left(\mathbf{W}^T \mathbf{S}_B \mathbf{W} \right) \left(\mathbf{W}^T \mathbf{S}_W \mathbf{W} \right)^{-1} \right\}$$

- Constrained optimization:

$$\begin{array}{ll} \max_{\mathbf{W}} & \text{Tr}\{\mathbf{W}^T \mathbf{S}_B \mathbf{W}\} \\ \text{subject to} & \mathbf{W}^T \mathbf{S}_W \mathbf{W} = \mathbf{I} \end{array}$$

where \mathbf{I} is an $M \times M$ identity matrix.

- Note that unlike PCA in Eq. 5, because of the matrix \mathbf{S}_W in the constraint, we need to find one \mathbf{w}_j at a time.
- Note also that the constraint $\mathbf{W}^T \mathbf{S}_W \mathbf{W} = \mathbf{I}$ suggests that \mathbf{w}_j 's may not be orthogonal to each other [2].

LDA on Multi-class Problems

- To find \mathbf{w}_j , we write the Lagrangian function as:

$$L(\mathbf{w}_j, \lambda_j) = \mathbf{w}_j^T \mathbf{S}_B \mathbf{w}_j - \lambda_j (\mathbf{w}_j^T \mathbf{S}_W \mathbf{w}_j - 1)$$

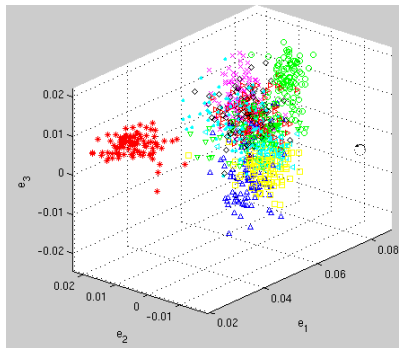
- Using Eq. 8, the optimal solution of \mathbf{w}_j satisfies

$$(\mathbf{S}_W^{-1} \mathbf{S}_B) \mathbf{w}_j = \lambda_j \mathbf{w}_j$$

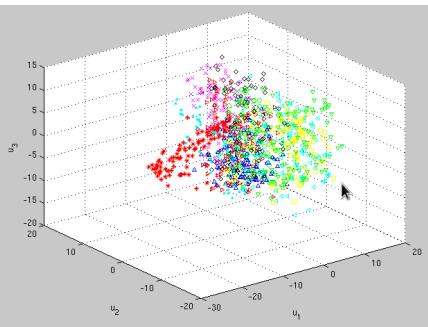
- Therefore, \mathbf{W} comprises the first M eigenvectors of $\mathbf{S}_W^{-1} \mathbf{S}_B$. A more formal proof can be found in [1].
- As the maximum rank of \mathbf{S}_B is $K - 1$, $\mathbf{S}_W^{-1} \mathbf{S}_B$ has at most $K - 1$ non-zero eigenvalues. As a result, M can be at most $K - 1$.
- After the projection, the vectors \mathbf{y}_n 's can be used to train a classifier (e.g., SVM) for classification.

PCA vs. LDA

- Project 784-dim vectors derived from 28×28 handwritten digits to 3-D space:

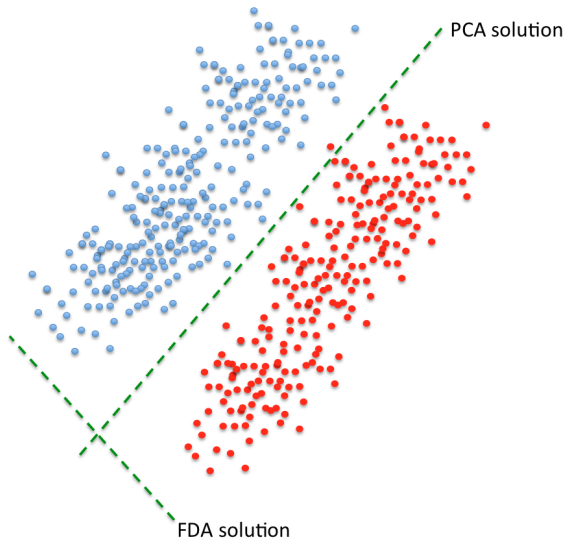


LDA



PCA

PCA vs. LDA



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- [2] Luo, Dijun Luo, Ding, Chris, and Huang, Heng (2011) “Linear Discriminant Analysis: New Formulations and Overfit Analysis”, *Proceedings of the Twenty-Fifth AAAI Conference on Artificial Intelligence*.