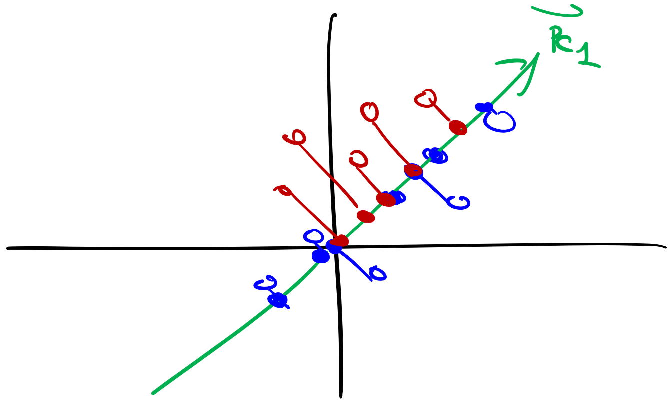
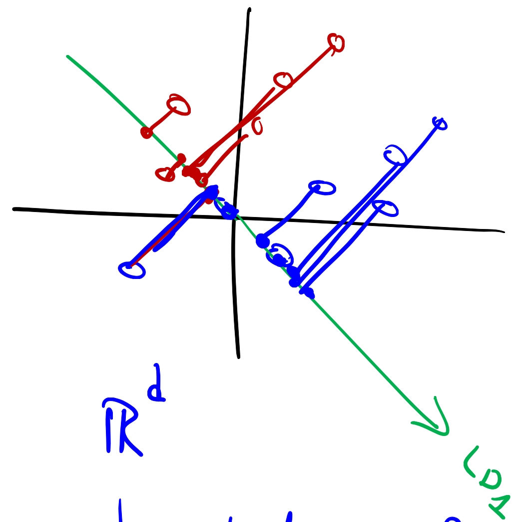
Linear Discriminant Analysis (LDA)





$\mathbb{R}^d$

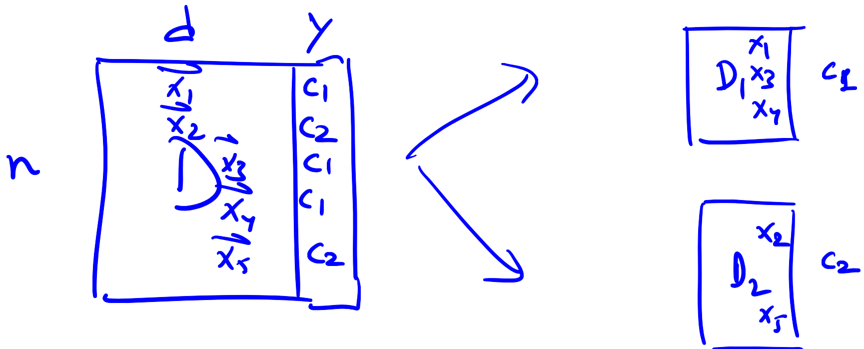
Fischer Objective

$$J = \max_{\vec{w}} \frac{(m_1 - m_2)^2}{s_1^2 + s_2^2}$$

how to find LD_1 ?

$$\vec{w} = \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_d \end{pmatrix}$$

assume 2 classes c_1 and c_2



$|D_1| = n_1$ $\quad \vec{\mu}_1$

$|D_2| = n_2$ $\quad \vec{\mu}_2$

$D_1 \xrightarrow[\text{scalar project onto } \vec{w}]{} \underbrace{a_1,\ a_3,\ a_4}_{\text{scalars}}$

$$a_1 = \left(\frac{\vec{x}_1^T \vec{w}}{\vec{w}^T \vec{w}} \right) = \mathrm{Proj}_{\vec{w}}\left(\vec{x}_1\right)$$

If $\vec{w}$ is unit vector

$$a_1 = \vec{x}_1^T \vec{w}$$

Proj D_1 $\quad$ Proj D_2

$\boxed{a_1, a_3, a_4}$ $\quad$ $\boxed{a_2, a_5}$

$$\Downarrow$$

m_1

$$m_2 = \frac{1}{n_2} \sum_{i=1}^{n_2} \vec{x}_i^T \vec{\omega} = \vec{\omega}^T \vec{\mu}_2$$

$$m_1 = \frac{1}{n_1} \sum_{i=1}^{n_1} a_i = \frac{1}{n_1} \sum_{i=1}^{n_1} \vec{x}_i^T \vec{\omega}$$

$$= \frac{1}{n_1} \sum_{i=1}^{n_1} \vec{\omega}^T \vec{x}_i$$

$$= \vec{\omega}^T \underbrace{\left(\frac{1}{n_1} \sum_{i=1}^{n_1} \vec{x}_i \right)}$$

$$= \vec{\omega}^T \vec{\mu}_1$$

$\vec{\mu}_1$ = mean of D_1 $\in \mathbb{R}^d$

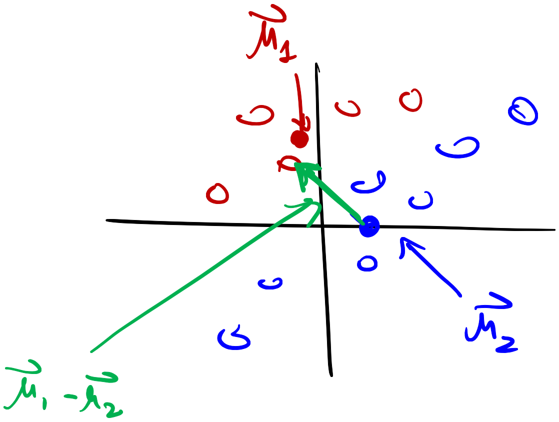
Numerator : $(m_1 - m_2)^2$

$$= \left(\vec{\omega}^T \vec{\mu}_1 - \vec{\omega}^T \vec{\mu}_2 \right)^2$$

$$= \left[\underbrace{\vec{\omega}^T (\vec{\mu}_1 - \vec{\mu}_2)} \right]^2$$

$$= \left[\vec{\omega}^T (\vec{\mu}_1 - \vec{\mu}_2) \right] \left[(\vec{\mu}_1 - \vec{\mu}_2)^T \vec{\omega} \right]$$

$$= \underset{1 \times d}{\vec{\omega}^T} \underbrace{\left((\vec{\mu}_1 - \vec{\mu}_2)(\vec{\mu}_1 - \vec{\mu}_2)^T \right)}_{\substack{\text{Outer product} \\ d \times d}} \underset{d \times 1}{\vec{\omega}}$$



$\vec{w} \in \mathbb{R}^d$

$\vec{\mu}_i \in \mathbb{R}^d$

$$B = (\vec{\mu}_1 - \vec{\mu}_2)(\vec{\mu}_1 - \vec{\mu}_2)^T$$

between class scatter

$d \times d$ matrix

numerator: $\vec{w}^T B \vec{w}$

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denominator : $s_1^2 + s_2^2$

$s_1 \equiv$ projected scatter for c_1

$$D_1 \downarrow \boxed{a_1 \; a_3 \; a_4} \qquad D_2 \downarrow \boxed{a_2, \; a_5}$$

Un-normalized Variance

$$s_1^2 = \boxed{n_1 \sigma_1^2}$$

$$= \sum_{i=1}^{n_1} (a_i - m_1)^2$$

proj point

proj mean

$$= \sum (\vec{w}^T \vec{x}_i - \vec{w}^T \vec{\mu}_1)^2$$

$$= \sum [\vec{w}^T (\vec{x}_i - \vec{\mu}_1)]^2$$

$$= \vec{\omega}^T \Big(\underbrace{\sum (x_i - \mu_1)(x_i - \mu_1)^T}_{\vec{\omega}^T \left(\underbrace{n_1 \cdot \Sigma_1}_{S_1} \right) \vec{\omega}} \Big) \vec{\omega}$$

$$S_2 = \vec{\omega} \left(n_2 \Sigma_2 \right) \vec{\omega}$$

$$\underline{s_1}^2 = \vec{\omega}^T S_1 \vec{\omega} \qquad s_2^2 = \vec{\omega}^T S_2 \vec{\omega}$$

$$D \to D_1 \longrightarrow \mu_1, \Sigma_1, \underline{S_1 = n_1 \cdot \Sigma_1}$$

$$D \to D_2 \longrightarrow \mu_2, \Sigma_2, \underline{S_2 = n_2 \Sigma_2}$$

$$J = \max_{\vec{\omega}} \frac{\vec{\omega}^T B \vec{\omega}}{\vec{\omega}^T (S_1 + S_2) \vec{\omega}} = \boxed{\max_{\vec{\omega}} \frac{\vec{\omega}^T B \vec{\omega}}{\vec{\omega}^T S \vec{\omega}}}$$

$$\underbrace{S_2, S_1, S}_{\text{PSD}}, \; B : \mathbb{R}^{d \times d}$$

rank one

$$\underline{\underline{\vec{\omega} \in \mathbb{R}^d}}$$

$$S = S_1 + S_2$$

within class scatter

Q: how to find $\vec{\omega}$?

$$\boxed{\frac{\partial J}{\partial \vec{\omega}} = 0} \implies \frac{2 B \vec{\omega} \left(\vec{\omega}^T S \vec{\omega} \right) - 2 S \vec{\omega} \left(\vec{\omega}^T B \vec{\omega} \right)}{\left(\vec{\omega}^T S \vec{\omega} \right)^2} = 0$$

$$\underbrace{B\vec{w}\left(\vec{w}^T S\vec{w}\right)} = S\vec{w}\left(\underline{\vec{w}^T B\vec{w}}\right)$$

$$B\vec{w} = \left(\frac{\vec{w}^T B w}{\vec{w}^T S w}\right) S\vec{w}$$

$\lambda \equiv$ objective value

$$\Rightarrow \boxed{\boxed{B\vec{w} = \lambda S\vec{w}}}$$

generalized eigendecomp

$B\vec{w} = \lambda\vec{w}$

eigen decomp

If S^{-1} exists

replace $S^{-1} = S^{+}$

pseudo-inverse

Compute from non-zero singular values of S

$$S^{-1}\left(B\vec{w}\right) = S^{-1}\left(\lambda S\vec{w}\right)$$

$$\boxed{\boxed{\left(S^{-1}B\right)\vec{w} = \lambda\vec{w}}}$$

$\vec{w}$ is dominant eigenvector of $S^{-1}B$

λ is largest eigenvalue of $S^{-1}B$

$$\nabla_{\vec{w}} = \frac{\partial J}{\partial \vec{w}}$$

$$\vec{w}_t = \vec{w}_{t-1} + \eta \cdot \nabla_{\vec{w}}$$

generalized eigen decomp

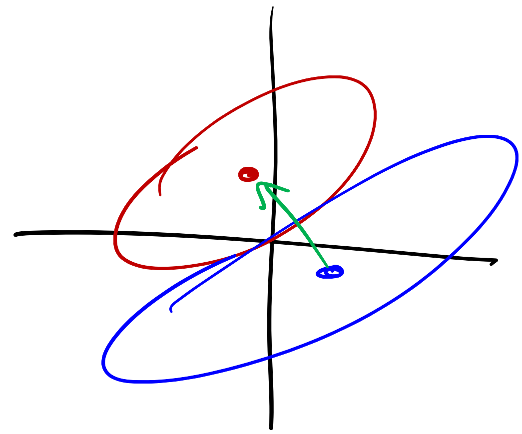
$$B\vec{w} = \lambda S\vec{w}$$

$$(S^{-1}B)\vec{w} = \lambda\vec{w}$$

$$(\vec{\mu}_1-\vec{\mu}_2)\underbrace{(\mu_1-\mu_2)^T\vec{w}}_{b} = \lambda S\vec{w}$$

$$\lambda S\vec{w} = b.(\vec{\mu}_1-\vec{\mu}_2)$$

$$\vec{w} = S^{-1}\left(\frac{b}{\lambda}(\vec{\mu}_1-\vec{\mu}_2)\right)$$



$$\vec{w} = \cancel{\frac{b}{\lambda}}\, S^{-1}(\vec{\mu}_1-\vec{\mu}_2)$$

geometrically, the LDA is a linear transformation of $\vec{\mu}_1-\vec{\mu}_2$ vector

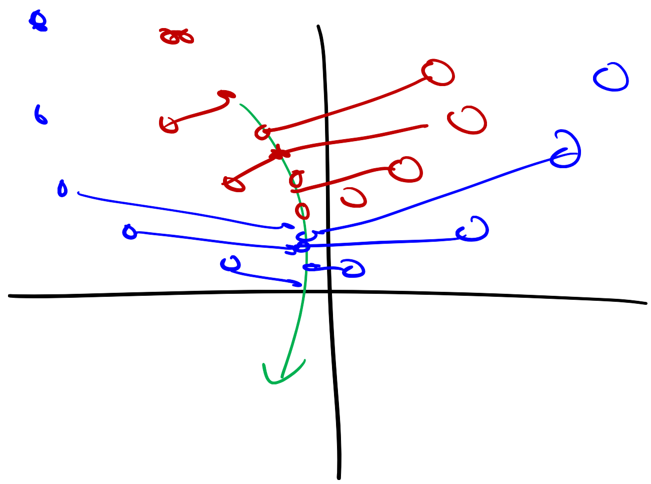
make $\vec{w}$ a unit vector

$$\boxed{\vec{w} = S^{-1}(\vec{\mu}_1-\vec{\mu}_2)}$$

exam!

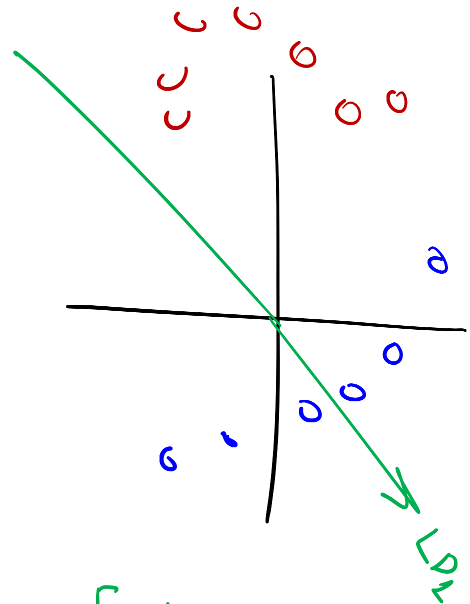
$$\vec{w} = \frac{\vec{w}}{\|\vec{w}\|}$$

Kernel LDA



Input space

$\xrightarrow{\phi}$ quadratic



Feature space

$\Downarrow$

$K \Leftarrow$ pairs of dot-products in conceptual feature space

$\vec{w}$ will not be materialized

$$\boxed{\vec{w} = \sum_{i=1}^{n} a_i \phi(\vec{x}_i)}$$

Representer Theorem

$\vec{w}$ is a linear combination of feature points

$\phi(\vec{x}_i) = \vec{x}_i$

leads to linear kernel

$$\vec{x}_i^T x_j = \phi(\vec{x}_i)^T \phi(\vec{x}_j)$$

$$\vec{a} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}$$

$$\boxed{\vec{\omega} = \sum_{i=1}^{n} a_i \, \underline{\phi(\vec{x_i})}} \quad X$$

we can project any point onto $\vec{\omega}$

$$\boxed{p_j = \phi(x_j)^T \vec{\omega} = \sum_{i=1}^{n} a_i \, k(x_j, x_i)}$$

$$\boxed{J = \max_{\vec{a}} \frac{\vec{a}^T M \vec{a}}{\vec{a}^T N \vec{a}}}$$

$$\frac{\vec{\omega}^T B \vec{\omega}}{\vec{\omega}^T S \vec{\omega}}$$

$$\vec{\omega}\left(\underline{\underline{S^{-1} B}}\right)\vec{\omega}$$

M: between class

N: within class

} from $\underline{K}$

$$\vec{a}^T \left(\frac{M}{N}\right) \vec{a}$$

$$\vec{a}\left(N^{-1} M\right) \vec{a}$$

$\vec{a}$ is the dominant eigenvector of $N^{-1} M$

λ is largest eigenvalue

$$\lambda = \frac{\vec{a}^T M \vec{a}}{\vec{a} \, N \vec{a}}$$

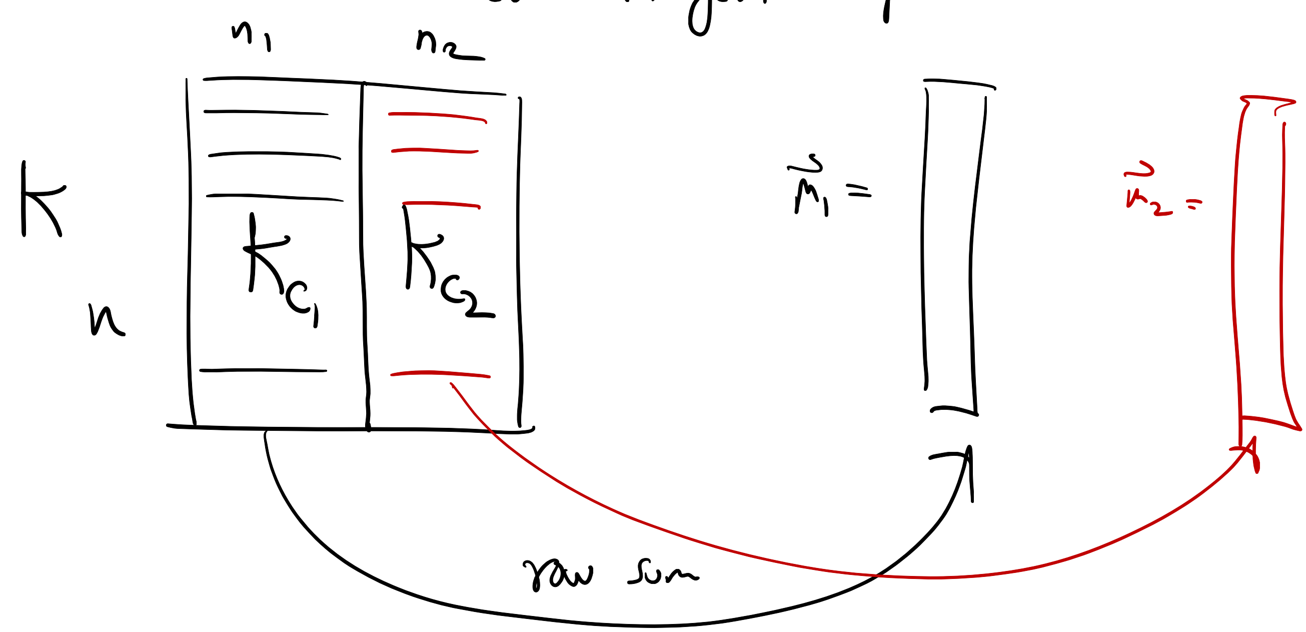
$$M\vec{a} = \lambda N \vec{a}$$

generalized eigendecomp

$$\underline{\underline{N^{-1} M}} \vec{a} = \lambda \vec{a}$$

$$\vec{a} = N^{-1}\left(\vec{\mu}_1 - \vec{\mu}_2\right)$$

means in feature space



$$\underset{n \times n}{M} = (\vec{\mu}_1 - \vec{\mu}_2)(\vec{\mu}_1 - \vec{\mu}_2)^T$$

| B

$$N = N_1 + N_2$$

$$N_1 = (K_{c_1})\left[I_{n_1} - 0\right](K_{c_1})^T$$

$$I_n = \begin{bmatrix} 1 & & & 0 \\ & 1 & & \\ & & 1 & \\ 0 & & & 1 \end{bmatrix}$$

$$O_n = \frac{1}{n} \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ & & \vdots & & \end{bmatrix}$$

$n \times n$