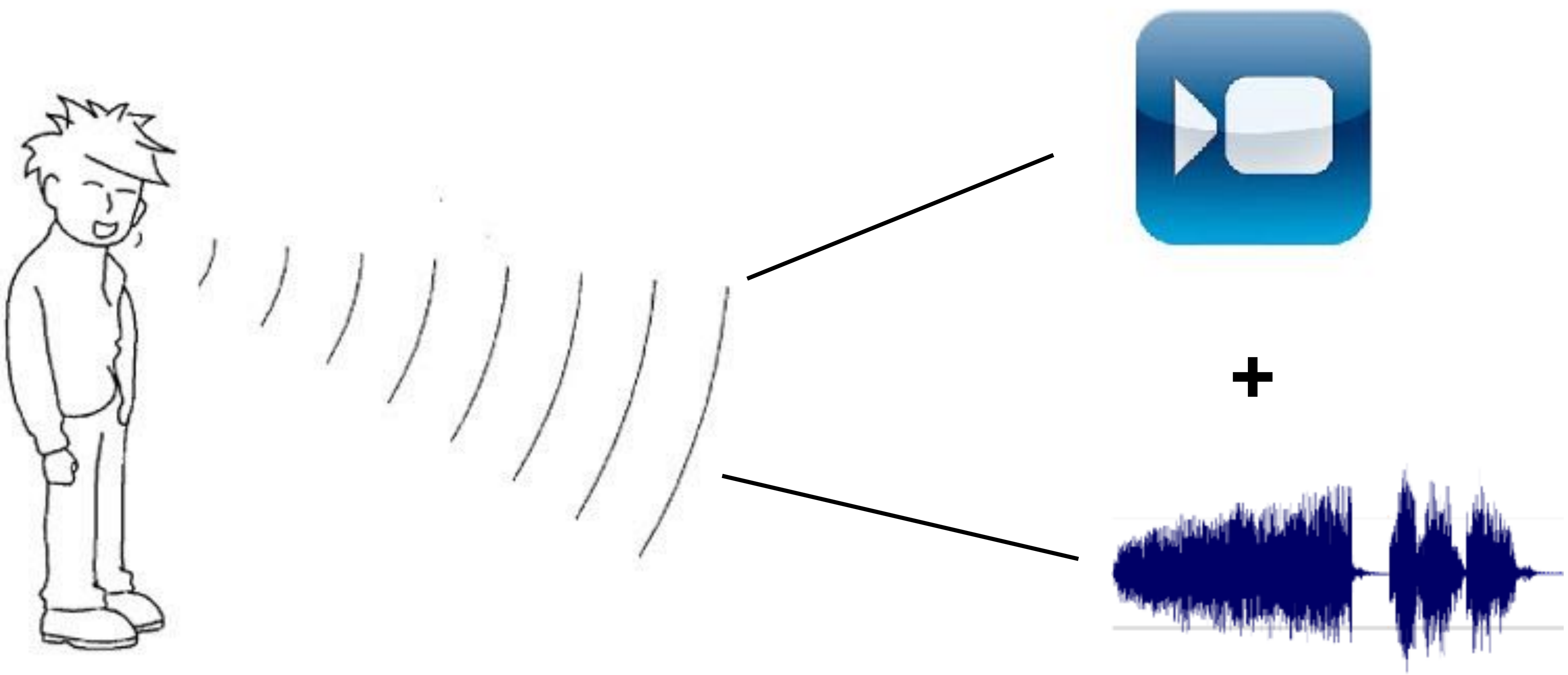
Machine Learning for Data Science (CS4786)
Lecture 6

Canonical Correlation Analysis
+
Kernel PCA

Example I: Speech Recognition



- Audio might have background sounds uncorrelated with video
- Video might have lighting changes uncorrelated with audio
- Redundant information between two views: the speech

Example II: Combining Feature Extractions

- Method A and Method B are both equally good feature extraction techniques
- Concatenating the two features blindly yields large dimensional feature vector with redundancy
- Applying techniques like CCA extracts the key information between the two methods
- Removes extra unwanted information

Canonical Correlation Analysis

Age

+ Gender

Candies per week

Favorite Cartoon

Two View Dimensionality Reduction

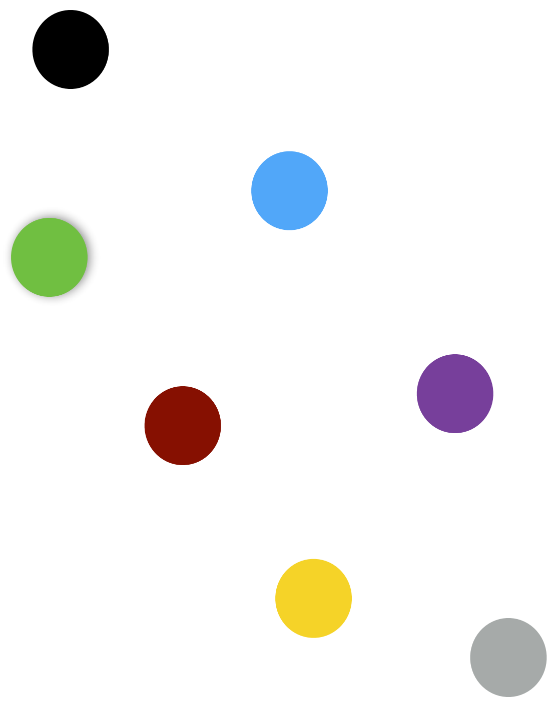
- Data comes in pairs $(\mathbf{x}_1, \mathbf{x}'_1), \ldots, (\mathbf{x}_n, \mathbf{x}'_n)$ where $\mathbf{x}_t$'s are d dimensional and $\mathbf{x}'_t$'s are d' dimensional

- Goal: Compress say view one into $\mathbf{y}_1, \ldots, \mathbf{y}_n$, that are K dimensional vectors

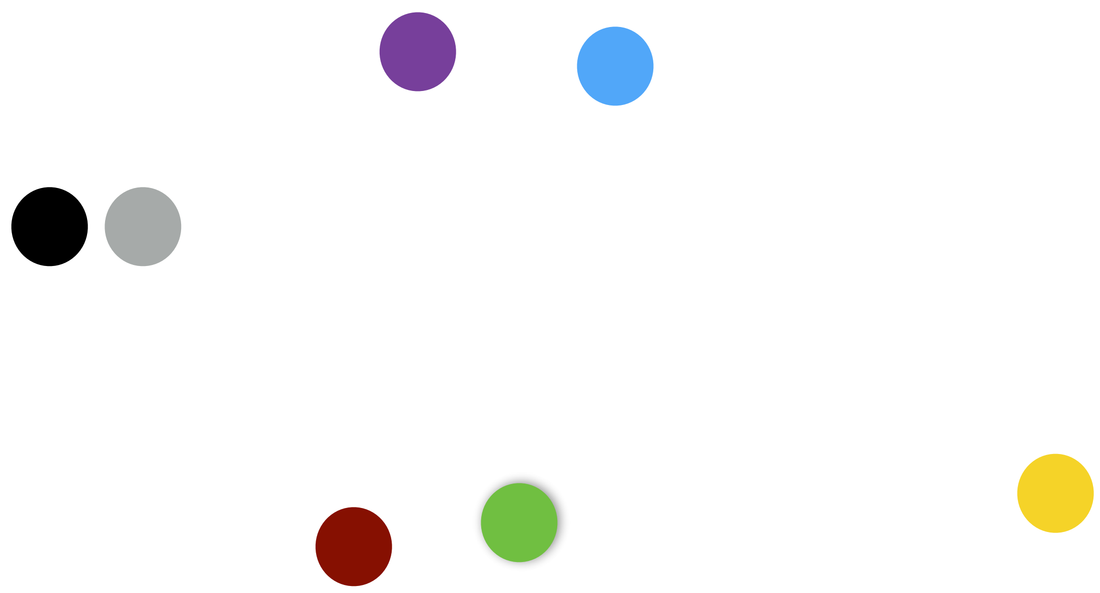
    - Retain information redundant between the two views

    - Eliminate "noise" specific to only one of the views

Which Direction to Pick?



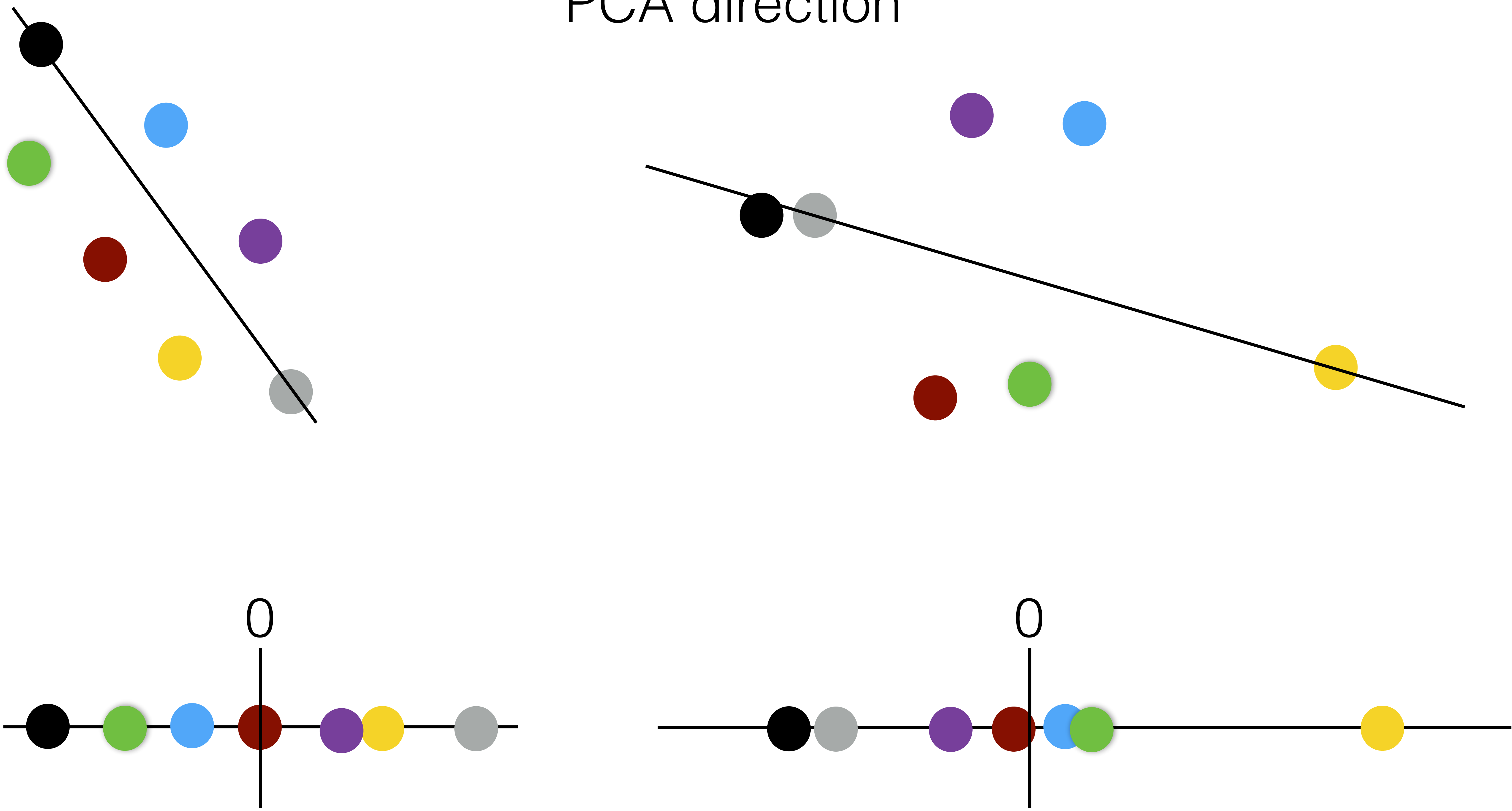
View I



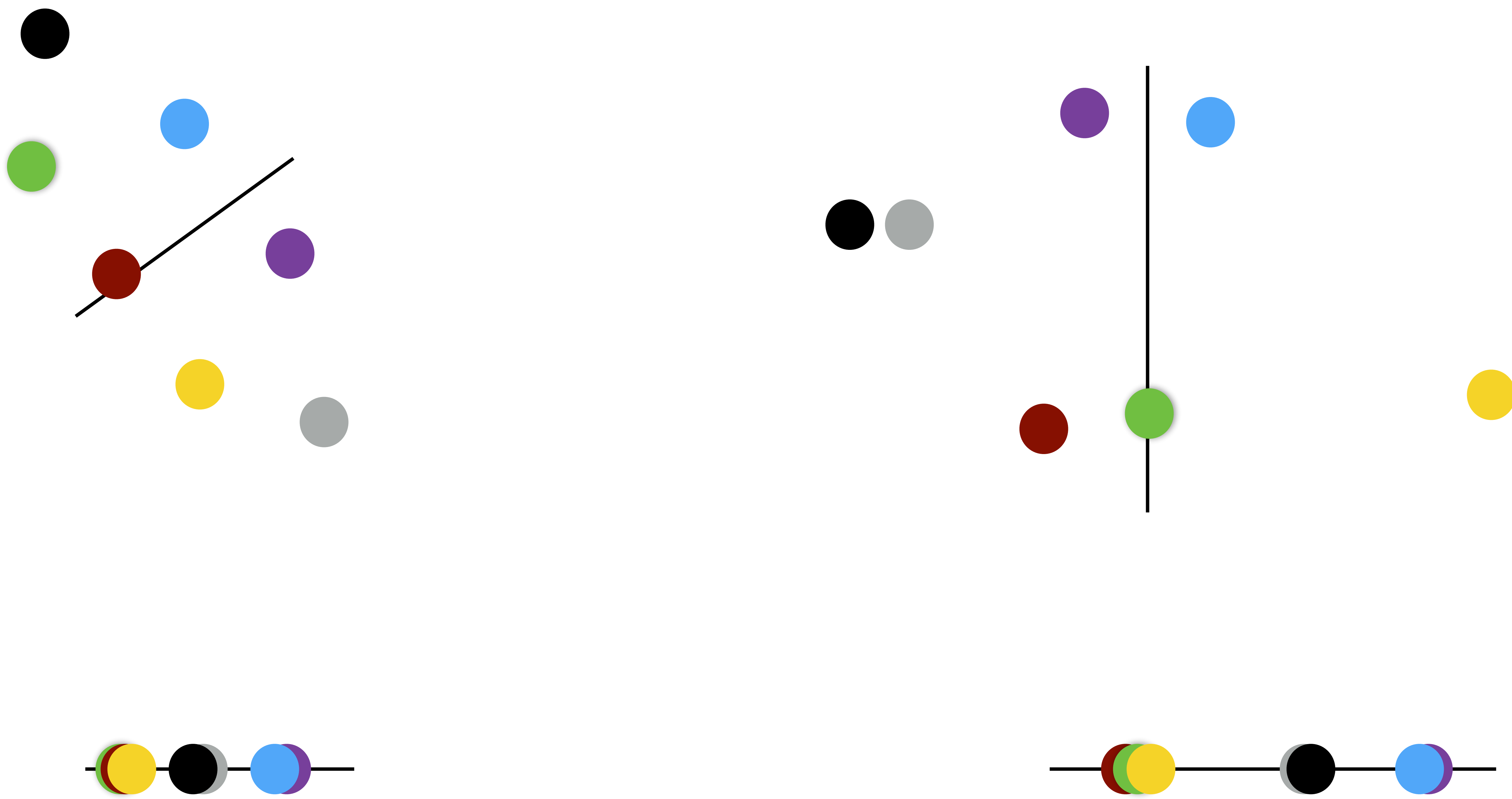
View II

WHICH DIRECTION TO PICK?

PCA direction



Which Direction to Pick?



Direction has large covariance

Maximizing Correlation Coefficient

- Say $\mathbf{w}_1$ and $\mathbf{v}_1$ are the directions we choose to project in views 1 and 2 respectively we want these directions to maximize,

$$\frac{\frac{1}{n}\sum_{t=1}^{n}\left(\mathbf{y}_t[1]-\frac{1}{n}\sum_{t=1}^{n}\mathbf{y}_t[1]\right)\cdot\left(\mathbf{y}'_t[1]-\frac{1}{n}\sum_{t=1}^{n}\mathbf{y}'_t[1]\right)}{\sqrt{\frac{1}{n}\sum_{t=1}^{n}\left(\mathbf{y}_t[1]-\frac{1}{n}\sum_{t=1}^{n}\mathbf{y}_t[1]\right)^2}\sqrt{\frac{1}{n}\sum_{t=1}^{n}\left(\mathbf{y}'_t[1]-\frac{1}{n}\sum_{t=1}^{n}\mathbf{y}'_t[1]\right)}}$$

Maximizing Correlation Coefficient

- Say $\mathbf{w}_1$ and $\mathbf{v}_1$ are the directions we choose to project in views 1 and 2 respectively we want these directions to maximize,

$$\frac{1}{n}\sum_{t=1}^{n}\left(\mathbf{y}_t[1] - \frac{1}{n}\sum_{t=1}^{n}\mathbf{y}_t[1]\right)\cdot\left(\mathbf{y}'_t[1] - \frac{1}{n}\sum_{t=1}^{n}\mathbf{y}'_t[1]\right)$$

s.t. $\frac{1}{n}\sum_{t=1}^{n}\left(\mathbf{y}_t[1] - \frac{1}{n}\sum_{t=1}^{n}\mathbf{y}_t[1]\right)^2 = \frac{1}{n}\sum_{t=1}^{n}\left(\mathbf{y}'_t[1] - \frac{1}{n}\sum_{t=1}^{n}\mathbf{y}'_t[1]\right) = 1$

where $\mathbf{y}_t[1] = \mathbf{w}_1^\top \mathbf{x}_t$ and $\mathbf{y}'_t[1] = \mathbf{v}_1^\top \mathbf{x}'_t$

- Hence we want to solve for projection vectors $\mathbf{w}_1$ and $\mathbf{v}_1$ that

$$\begin{aligned}\text{maximize } &\frac{1}{n}\sum_{t=1}^{n}\mathbf{w}_1^\top(\mathbf{x}_t-\mu)\cdot\mathbf{v}_1^\top(\mathbf{x}'_t-\mu') \\ \text{subject to } &\frac{1}{n}\sum_{t=1}^{n}(\mathbf{w}_1^\top(\mathbf{x}_t-\mu))^2=\frac{1}{n}\sum_{t=1}^{n}(\mathbf{v}_1^\top(\mathbf{x}'_t-\mu'))^2=1\end{aligned}$$

where $\mu=\frac{1}{n}\sum_{t=1}^{n}\mathbf{x}_t$ and $\mu'=\frac{1}{n}\sum_{t=1}^{n}\mathbf{x}'_t$

Canonical Correlation Analysis

- Hence we want to solve for projection vectors $\mathbf{w}_1$ and $\mathbf{v}_1$ that

$$\begin{aligned}&\text{maximize } \mathbf{w}_1^\top \Sigma_{1,2} \mathbf{v}_1 \\ &\text{subject to } \mathbf{w}_1^\top \Sigma_{1,1} \mathbf{w}_1 = \mathbf{v}_1^\top \Sigma_{2,2} \mathbf{v}_1 = 1\end{aligned}$$

$$\Sigma = \begin{matrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{matrix} = \mathrm{cov}\left(X \; X' \right)$$

CCA Algorithm

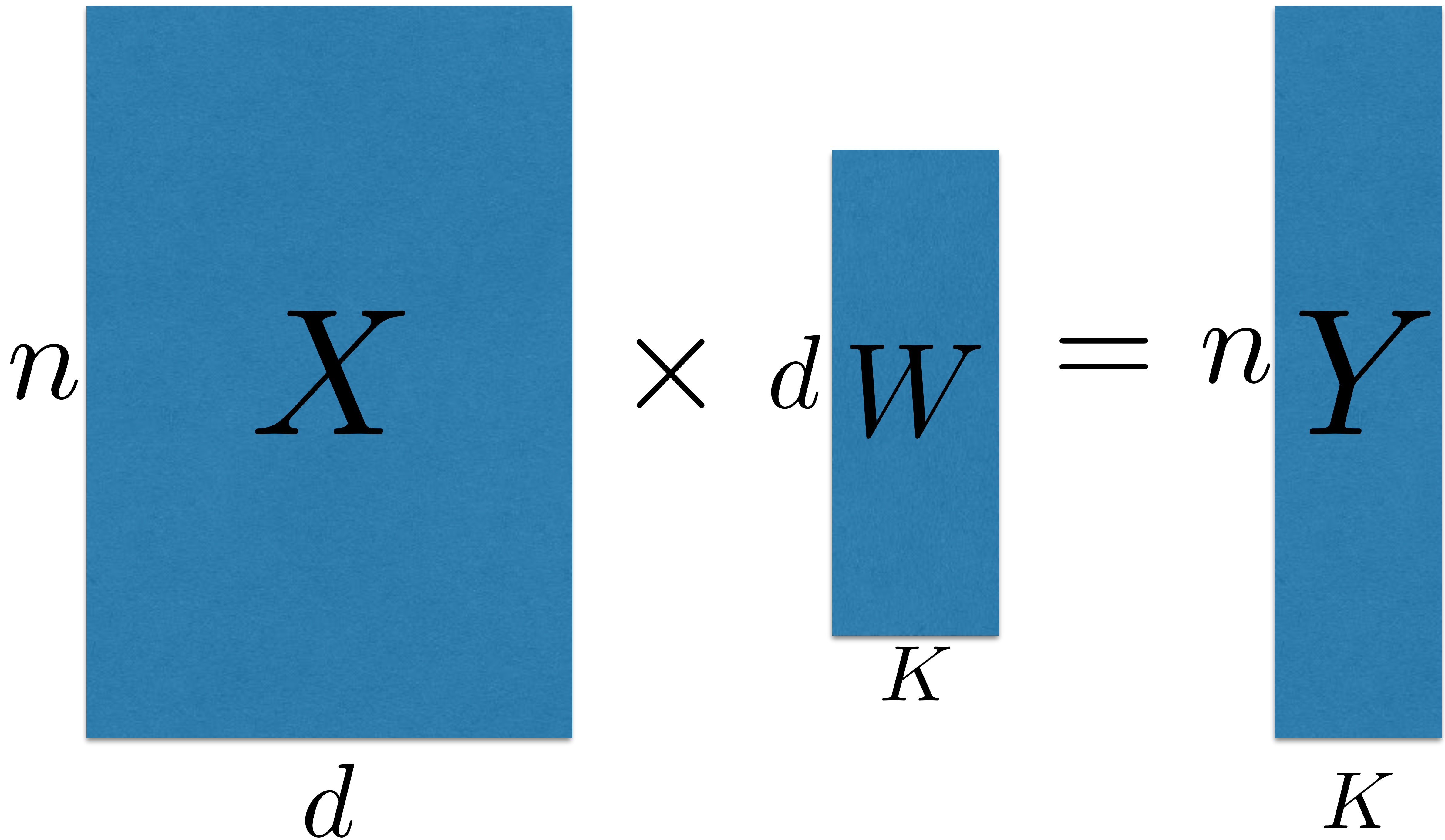
1. $$X = \left({}^{n}\underset{d_1}{X_1}, \underset{d_2}{X_2} \right)$$

2. $$\Sigma = \begin{matrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{matrix} = \mathrm{cov}\left(X \right)$$

3. $$W = \mathrm{eigs}\left(\Sigma_{11}^{-1}\Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}, K \right)$$

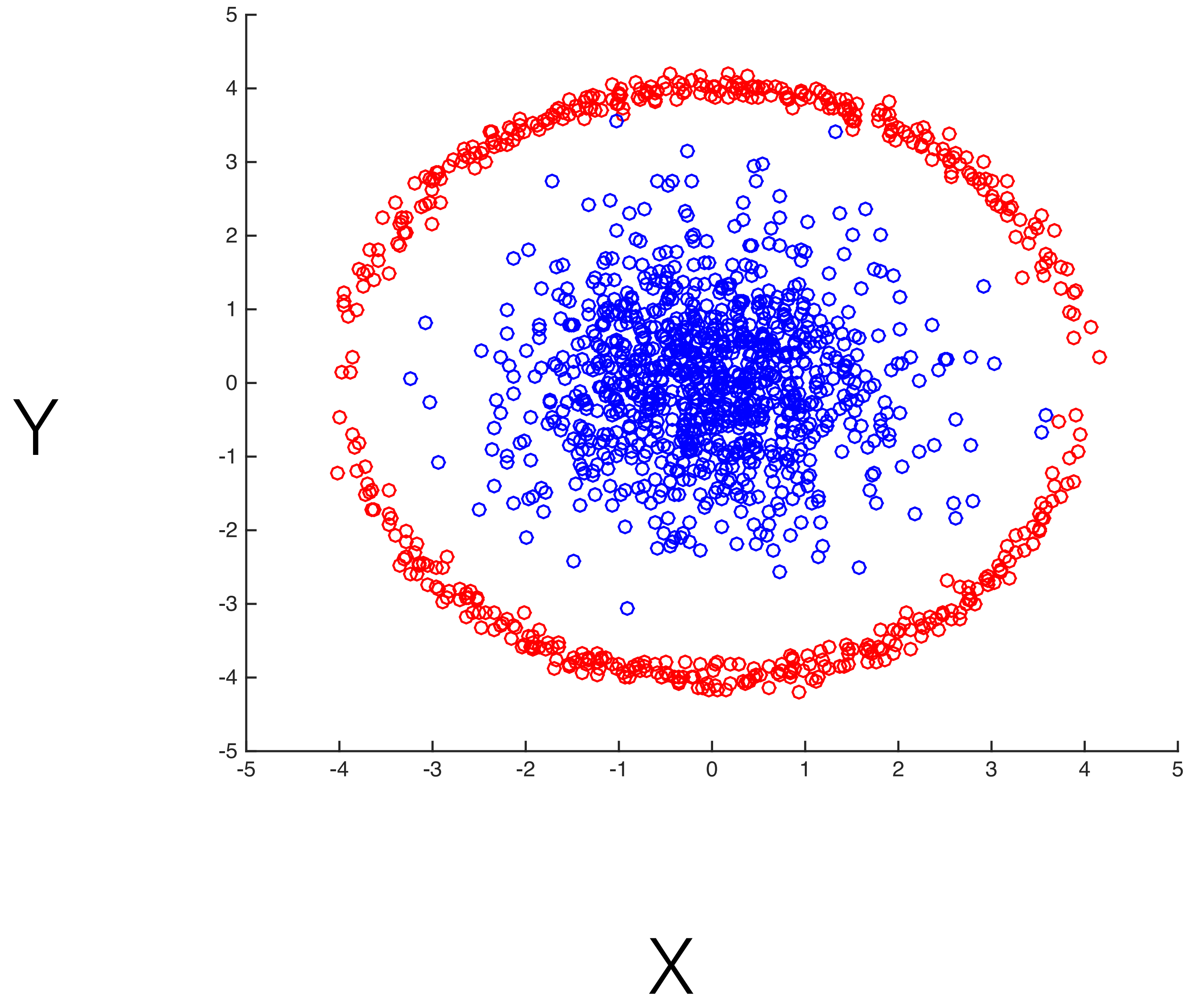
4. $$Y_1 = X_1 - \mu_1 \times W$$

Linear Projections



Works when data lies in a low dimensional linear sub-space

Example



Kernel Trick

- Lift to higher dimensions to introduce non-linearity
  - Linear in high dim = non-linear in lower dim
- Project to lower dimension using PCA

A First Cut

- Given $\mathbf{x}_t \in \mathbb{R}^d$, the feature space vector is given by mapping

$$\Phi(\mathbf{x}_t) = (\mathbf{x}_t[1], \ldots, \mathbf{x}_t[d], \mathbf{x}_t[1] \cdot \mathbf{x}_t[1], \mathbf{x}_t[1] \cdot \mathbf{x}_t[2], \ldots, \mathbf{x}_t[d] \cdot \mathbf{x}_t[d], \ldots)^\top$$

- Enumerating products up to order K (ie. products of at most K coordinates) we can get degree K polynomials.

- However dimension blows up as d^K

- Is there a way to do this without enumerating Φ?

Kernel Trick

- Essence of Kernel trick:
  - **If** we can write down an algorithm only in terms of $\Phi(\mathbf{x}_t)^\top \Phi(\mathbf{x}_s)$ for data points $\mathbf{x}_t$ and $\mathbf{x}_s$
  - **Then** we don't need to explicitly enumerate $\Phi(\mathbf{x}_t)$'s but instead, compute $k(\mathbf{x}_t, \mathbf{x}_s) = \Phi(\mathbf{x}_t)^\top \Phi(\mathbf{x}_s)$ (even if Φ maps to infinite dimensional space)
- Example: RBF kernel $k(\mathbf{x}_t, \mathbf{x}_s) = \exp(-\sigma \|\mathbf{x}_t - \mathbf{x}_s\|_2^2)$, polynomial kernel $k(\mathbf{x}_t, \mathbf{x}_s) = \left(\mathbf{x}_t^\top \mathbf{y}_t\right)^p$
- Kernel function measures similarity between points.

Kernel Trick

$$
\begin{aligned}
(\mathbf{x}_t^\top \mathbf{y}_t)^p &= \sum_{k_1+k_2+\ldots+k_d=p} \binom{c}{k_1,k_2,\ldots,k_d} \prod_{j=1}^{d} (x_t[j] y_t[j])^{k_j} \\
&= \sum_{k_1+k_2+\ldots+k_d=p} \left(\sqrt{\binom{c}{k_1,k_2,\ldots,k_d}} \prod_{j=1}^{d} x_t[j]^{k_t} \right) \cdot \left(\sqrt{\binom{c}{k_1,k_2,\ldots,k_d}} \prod_{j=1}^{d} y_t[j]^{k_j} \right)
\end{aligned}
$$

$$
\Phi(\mathbf{x})^\top = \left(\ldots, \sqrt{\binom{c}{k_1,k_2,\ldots,k_d}} \prod_{j=1}^{d} x_t[j]^{k_t}, \ldots \right)_{k_1+k_2+\ldots+k_d=p}
$$

Lets Rewrite PCA

Lets start with the assumption that Data is centered! (i.e. Sum of x_t's is 0)

- k^{th} column of W is eigenvector of covariance matrix
  That is, $\lambda_k W_k = \Sigma W_k$. Rewriting, for centered X

$$\lambda_k W_k = \frac{1}{n}\left(\sum_{t=1}^{n} \mathbf{x}_t \mathbf{x}_t^\top\right) W_k = \frac{1}{n}\sum_{t=1}^{n}\left(\mathbf{x}_t^\top W_k\right)\mathbf{x}_t$$

But $\mathbf{x}_t^\top W_k = \mathbf{y}_t[k]$

$$\lambda_k W_k = \frac{1}{n}\sum_{t=1}^{n} \mathbf{y}_t[k]\mathbf{x}_t$$

Lets Rewrite PCA

$$\begin{aligned}
\mathbf{y}_s[k] &= W_k^\top \mathbf{x}_s \\
&= \frac{1}{\lambda_k} \left(\frac{1}{n} \sum_{t=1}^{n} \mathbf{y}_t[k] \mathbf{x}_t \right)^\top \mathbf{x}_s \\
&= \frac{1}{n\lambda_k} \sum_{t=1}^{n} \mathbf{y}_t[k] \mathbf{x}_t^\top \mathbf{x}_s \\
&= \frac{1}{n\lambda_k} \sum_{t=1}^{n} \mathbf{y}_t[k] \tilde{K}_{s,t}
\end{aligned}$$

Where $\tilde{K}_{s,t} = \mathbf{x}_t^\top \mathbf{x}_s$ is the kernel matrix for centered data

Lets Rewrite PCA

- Hence, the k'th column on Y matrix is such that

$$\mathbf{y}[k] = \frac{1}{n\lambda_k}\mathbf{y}[k]\tilde{K}$$

$$\text{Also we have, } 1 = \|W_k\|^2 = \frac{1}{\lambda_k^2 n^2}\left(\sum_{t=1}^{n}\mathbf{y}_t[k]\mathbf{x}_t\right)^\top\left(\sum_{s=1}^{n}\mathbf{y}_s[k]\mathbf{x}_s\right)$$

$$= \frac{1}{\lambda_k^2 n^2}\sum_{t=1}^{n}\sum_{s=1}^{n}\mathbf{y}_s[k]\mathbf{x}_s^\top\mathbf{x}_t\ \mathbf{y}_t[k]$$

$$= \frac{1}{\lambda_k^2 n^2}\mathbf{y}[k]\tilde{K}\mathbf{y}[k]^\top = \frac{1}{n\lambda_k}\|\mathbf{y}[k]\|^2$$

Hence $P_k = \mathbf{y}[k]/\sqrt{n\lambda_k}$ is an eigenvector of $\tilde{K}$ with eigen value $\gamma_k = n\lambda_k$

Rewritting PCA

- We assumed centered data, what if its not,

$$
\begin{aligned}
\tilde{K}_{s,t} &= \left(\mathbf{x}_t - \frac{1}{n}\sum_{u=1}^{n}\mathbf{x}_u)\right)^\top \left(\mathbf{x}_s - \frac{1}{n}\sum_{u=1}^{n}\mathbf{x}_u\right) \\
&= \mathbf{x}_t^\top \mathbf{x}_s - \left(\frac{1}{n}\sum_{u=1}^{n}\mathbf{x}_u\right)^\top \mathbf{x}_s - \left(\frac{1}{n}\sum_{u=1}^{n}\mathbf{x}_u\right)^\top \mathbf{x}_t \\
&\quad + \frac{1}{n^2}\left(\sum_{u=1}^{n}\mathbf{x}_u\right)^\top \left(\sum_{v=1}^{n}\mathbf{x}_v\right) \\
&= \mathbf{x}_t^\top \mathbf{x}_s - \frac{1}{n}\sum_{u=1}^{n}\mathbf{x}_u^\top \mathbf{x}_s - \frac{1}{n}\sum_{u=1}^{n}\mathbf{x}_u^\top \mathbf{x}_t + \frac{1}{n^2}\sum_{u=1}^{n}\sum_{v=1}^{n}\mathbf{x}_u^\top \mathbf{x}_v
\end{aligned}
$$

Rewriting PCA

- Equivalently, if Kern is the matrix ($\text{Kern}_{t,s} = x_t^\top x_s$),

$$\tilde{K} = \text{Kern} - \frac{(\mathbf{1}_{n\times n} \times \text{Kern})}{n} - \frac{(\text{Kern} \times \mathbf{1}_{n\times n})}{n} + \frac{(\mathbf{1}_{n\times n} \times \text{Kern} \times \mathbf{1}_{n\times n})}{n^2}$$

Kernel PCA

All we need to be able to compute, to perform PCA are $\mathbf{x}_t^\top \mathbf{x}_s$

Replace $\mathbf{x}_t^\top \mathbf{x}_s$ with $\Phi(\mathbf{x}_t)^\top \Phi(\mathbf{x}_s) = k(x_t, x_s)$ to perform PCA in feature space

Kernel PCA

1.

$$\underbrace{\text{Kern}}_{n \times n} = \begin{bmatrix} k(x_1,x_1) & k(x_1,x_2) & \dots & k(x_1,x_n) \\ k(x_2,x_1) & k(x_2,x_2) & \dots & k(x_2,x_n) \\ \vdots & \vdots & \vdots & \vdots \\ k(x_{n-1},x_1) & k(x_{n-1},x_2) & \dots & k(x_{n-1},x_n) \\ k(x_n,x_1) & k(x_n,x_2) & \dots & k(x_n,x_n) \end{bmatrix}$$

2.

$$\underbrace{\tilde{K}}_{n \times n} = \text{Kern} - \frac{1}{n}\left(\mathbf{1}\ \text{Kern} + \text{Kern}\ \mathbf{1}\right) + \frac{1}{n^2}\mathbf{1}\ \text{Kern}\ \mathbf{1}$$

Kernel PCA

3. $$\left[\,{}^{n}\underset{K}{P},\ \gamma\,\right] = \text{eigs}\left(\tilde{K},\ K\right)$$

4. $${}^{n}\underset{K}{Y} = \underset{K}{\left[\,P_1\sqrt{\gamma_1}\ \cdots\ P_K\sqrt{\gamma_K}\,\right]}$$