Data Modelling Methods-V

CS771: Introduction to Machine Learning
Purushottam Kar



Outline of today's discussion

- Recap of PCA, PPCA
- Details of PCA and applications



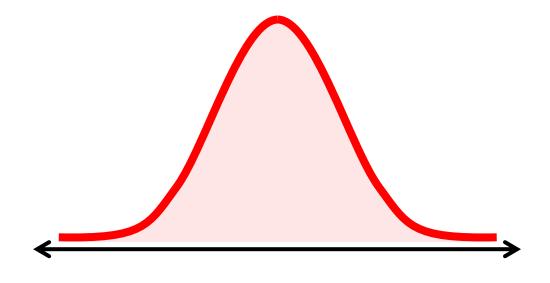
Recap

Modelling Low-dimensional structure in data

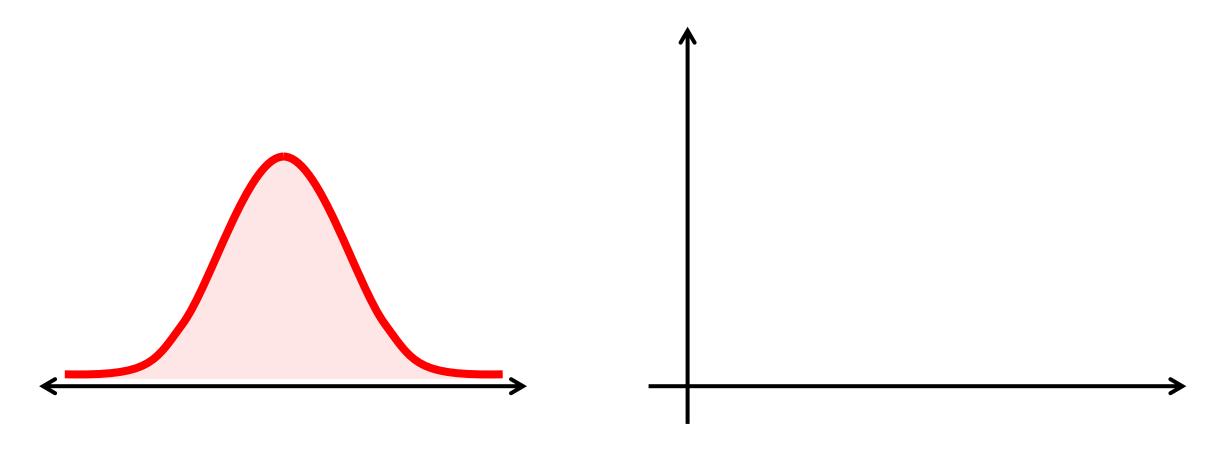




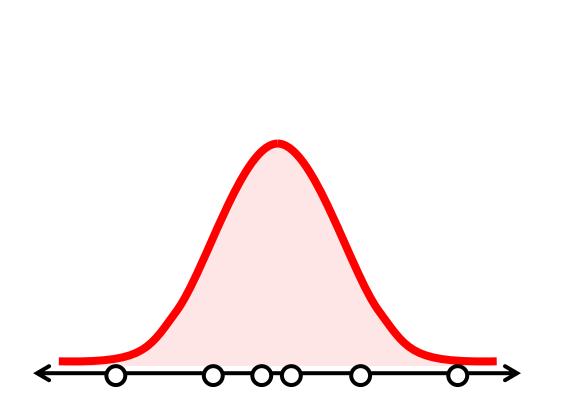








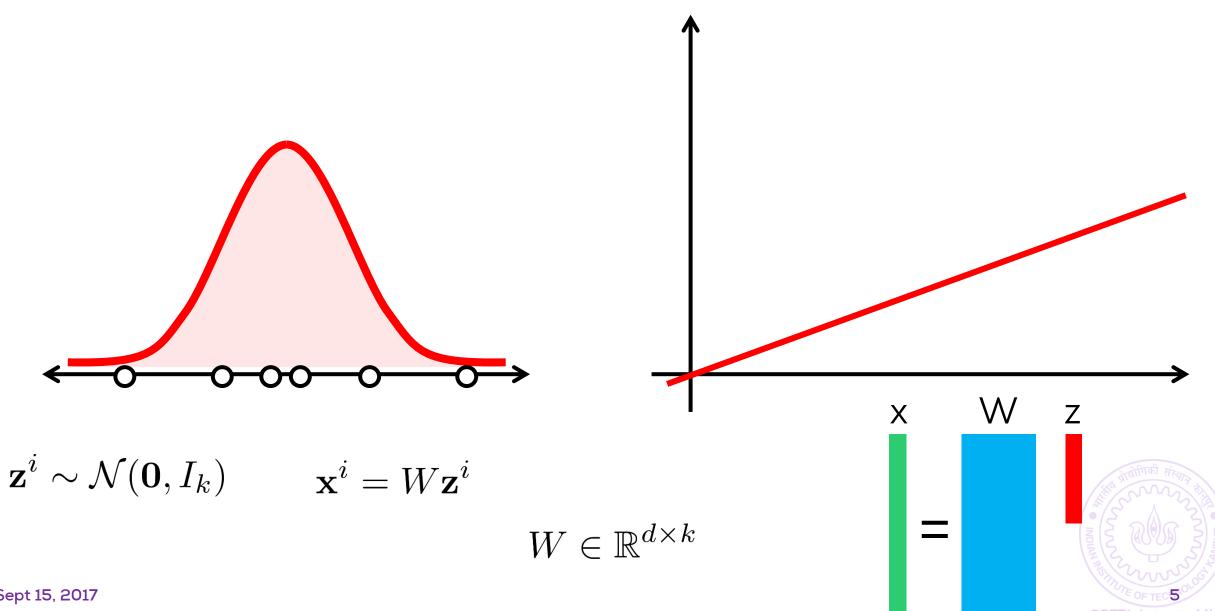


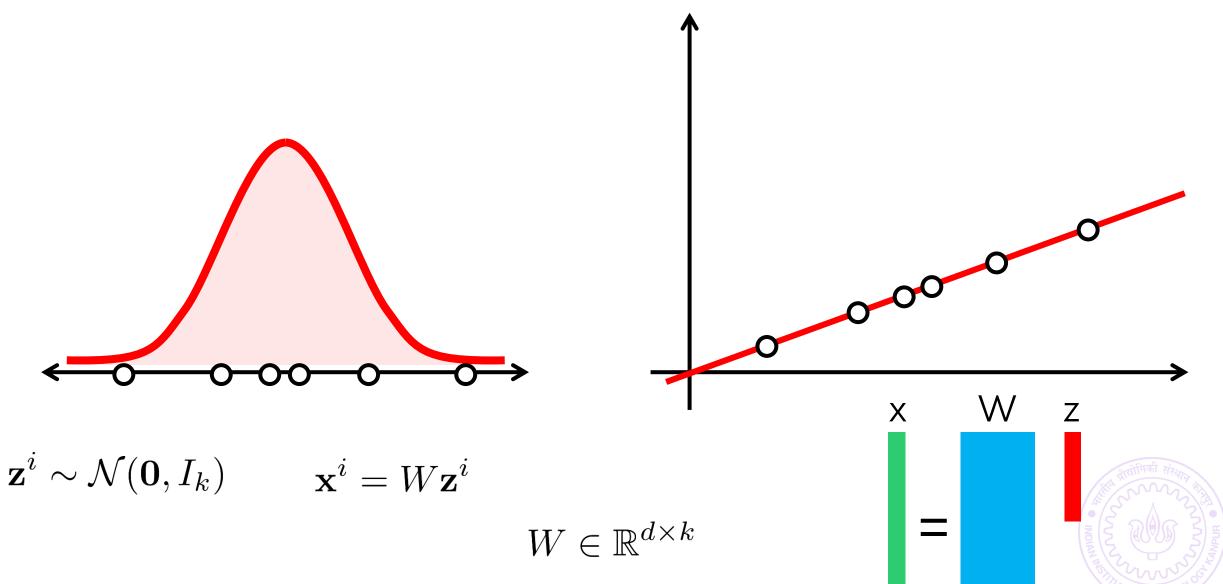


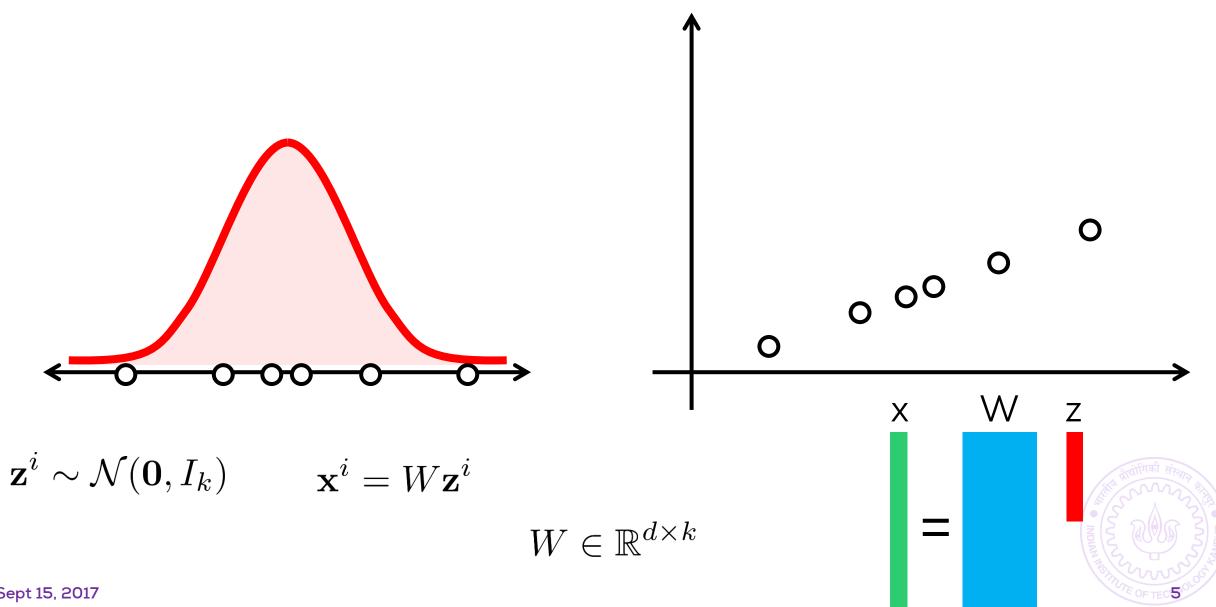


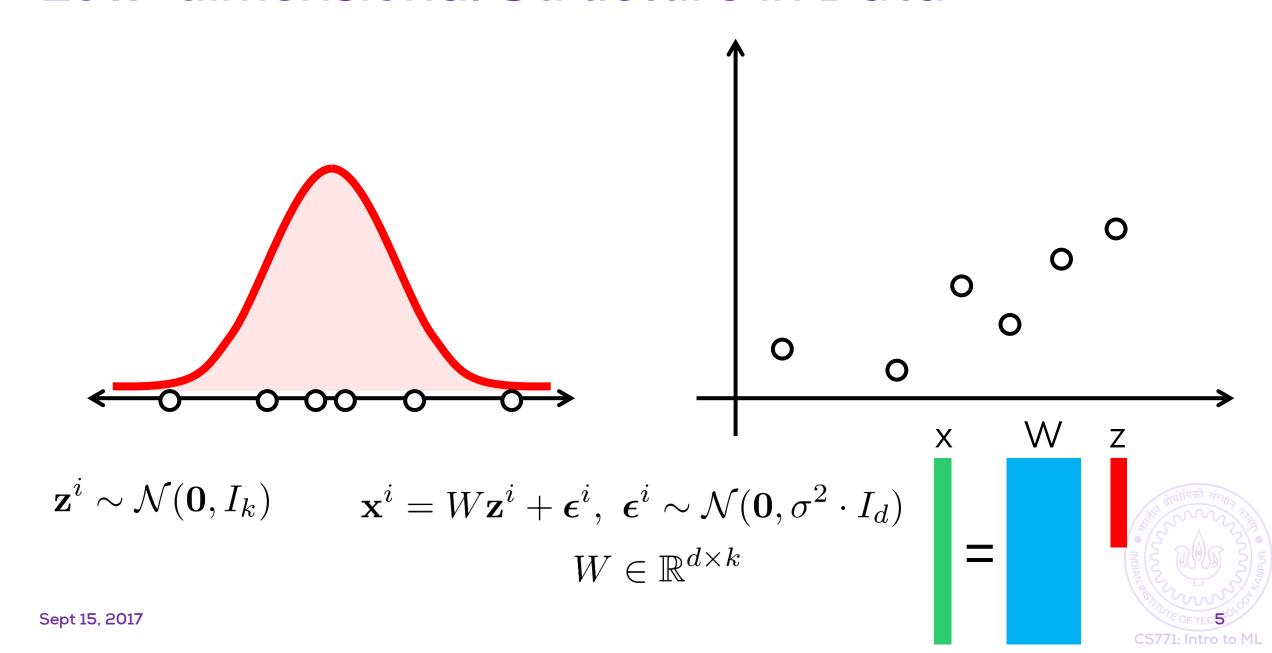
$$\mathbf{z}^i \sim \mathcal{N}(\mathbf{0}, I_k)$$

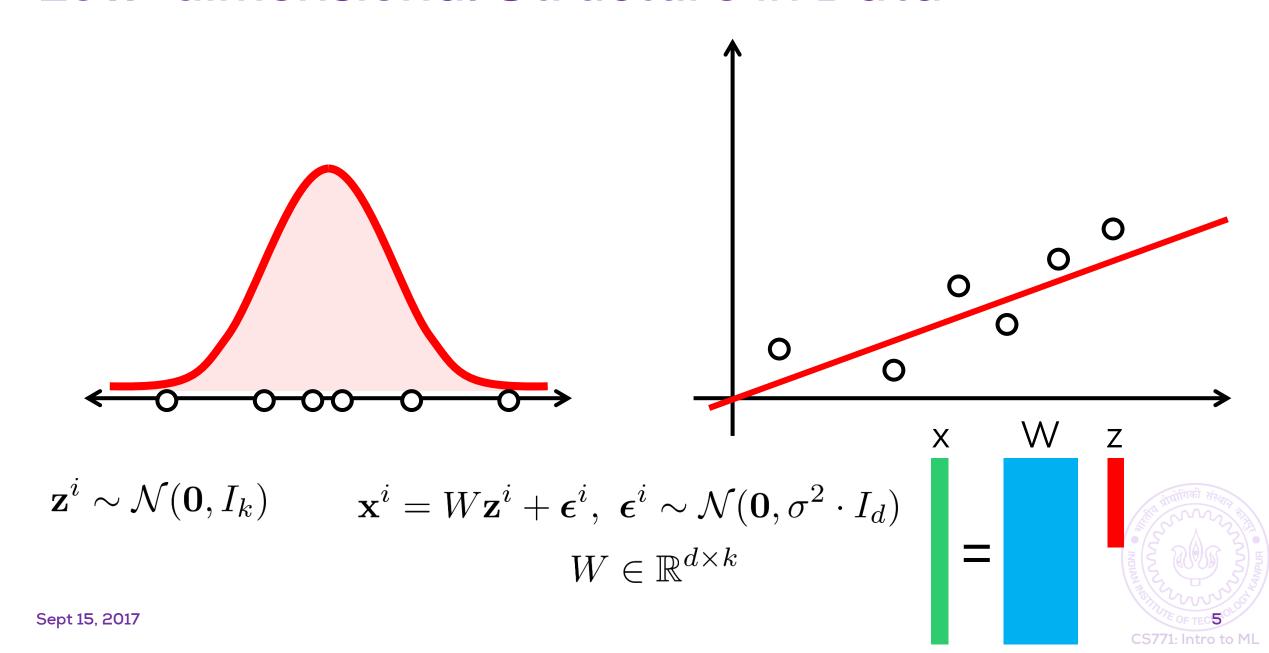


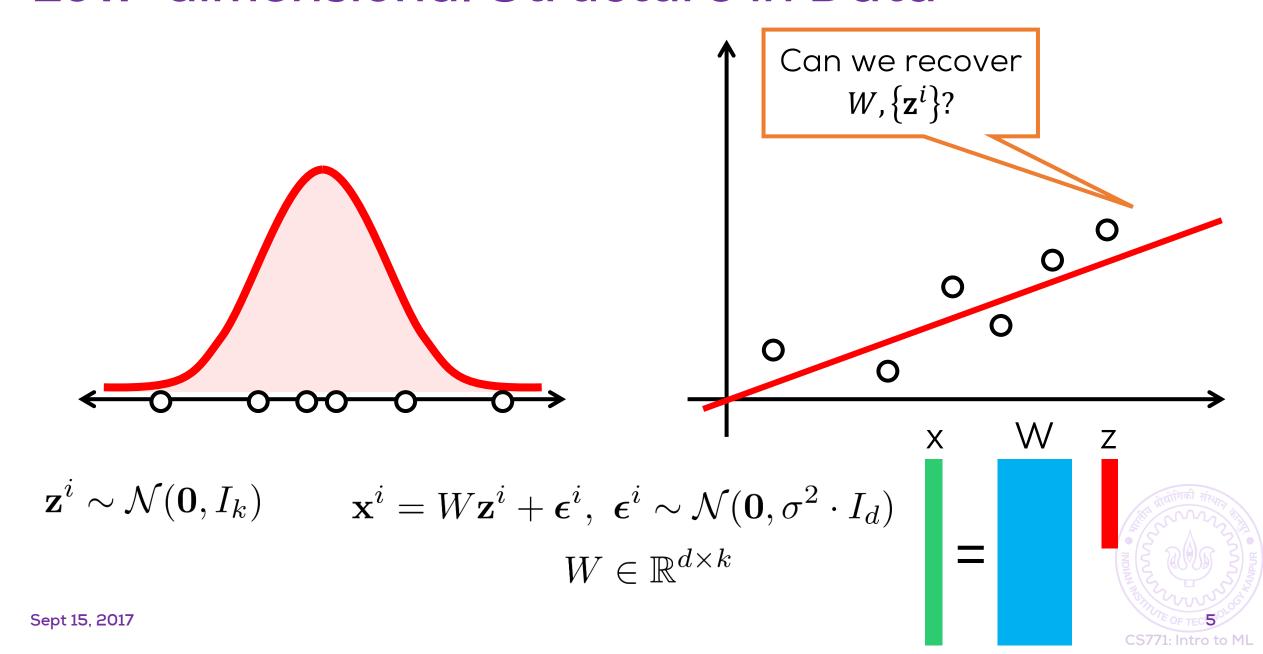


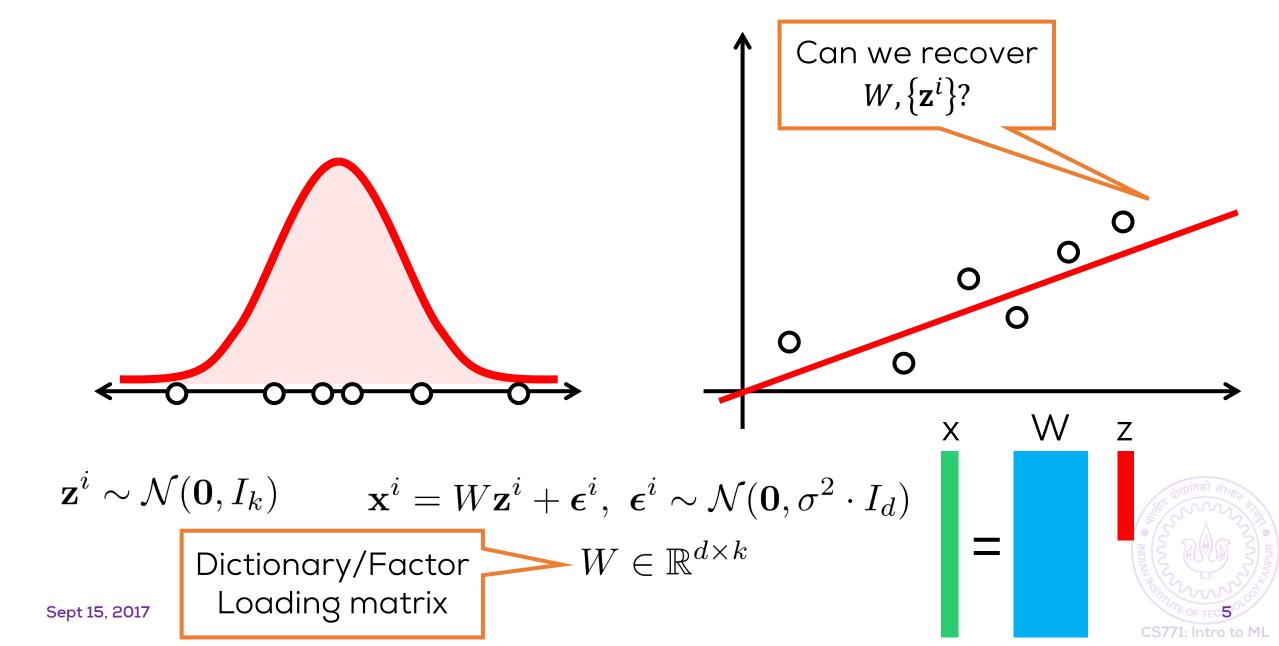








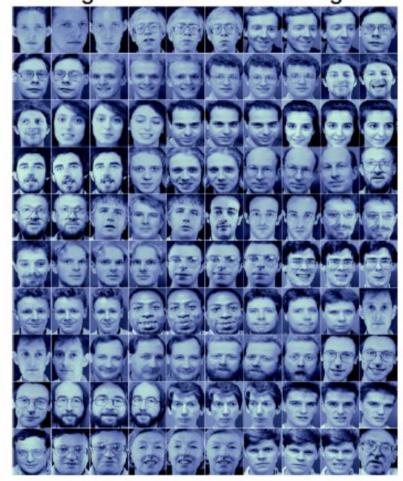




- Space savings: store k-dim \mathbf{z}^i instead of d-dim \mathbf{x}^i , $k \ll d$
- ullet Discover meaningful structure in data captured by W



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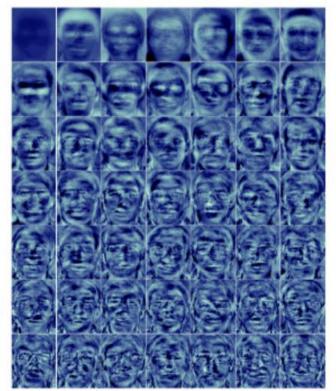
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Discover meaningful structure in data captured by W

Original Collection of Images



K=49 Eigenvectors ("eigenfaces") learned by PCA on this data

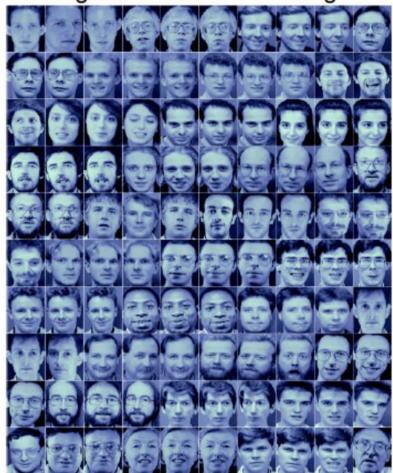




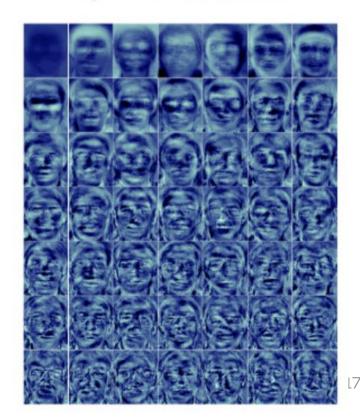
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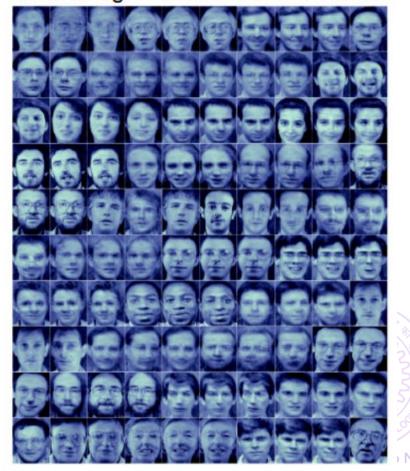
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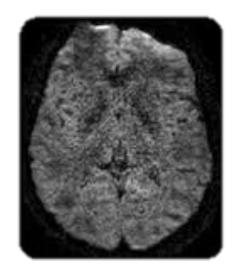
K=49 Eigenvectors ("eigenfaces") learned by PCA on this data

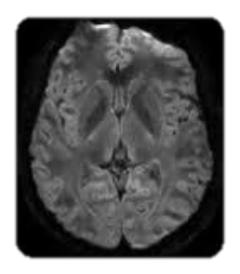


Each image's reconstructed version



ullet Noise removal: low-dim \mathbf{z}^i contains all useful info, rest is noise





• Or ... the "noise" could be the useful stuff (fore/background sep)



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http://personales.upv.es/jmanjon/ Netrapalli et al, Non-convex Robust PCA, NIPS 2014



CS771: Intro to ML

What we have and what we want

- In secret, someone generates a low-dim data $\mathbf{z}^i \sim \mathcal{N}(\mathbf{0}, I_k) \in \mathbb{R}^k$
- The point is projected into a high-dim space $W\mathbf{z}^i \in \mathbb{R}^d$ ($W \in \mathbb{R}^{d \times k}$)
- Noise is added to the point $\mathbf{x}^i | \mathbf{z}^i \sim \mathcal{N}(W\mathbf{z}^i, \sigma^2 \cdot I_d)$
- We get to see \mathbf{x}^i , $i=1\dots n$ but only for say $n\approx dk$ points
- Want to recover W,σ and \mathbf{z}^i
- It turns out that likelihood $\mathbb{P}[\mathbf{x}^i \mid \sigma, W] = \mathcal{N}(0, \Sigma)$ where $\Sigma = \sigma^2 \cdot I_d + WW^{\top} \in \mathbb{R}^{d \times d}$
- ullet However, estimating Σ directly is bad
 - Too many samples $n \approx d^2$ required
 - Not clear how to extract W, σ from Σ



An MLE Estimate for W, σ



MLE Estimation

- Given samples $\mathbf{x}^1, \mathbf{x}^2, ..., \mathbf{x}^n$ from $\mathcal{N}(0, \sigma^2 \cdot I_d + WW^\top)$, log-likelihood is $\log \mathbb{P}[X \mid W, \sigma] = \frac{n}{2} \left(d \log 2\pi + \log |\mathcal{C}| + \mathrm{tr}(\mathcal{C}^{-1}S) \right)$ where $\mathcal{C} = WW^\top + \sigma^2 \cdot I_d$, and $S = \frac{1}{n} \sum_{i=1}^n \mathbf{x}^i \left(\mathbf{x}^i \right)^\top$
- Let $S = U\Lambda U^{\mathsf{T}}$ be the eigen-decomposition of S
 - $U = [\mathbf{u}^1, ..., \mathbf{u}^d] \in \mathbb{R}^{d \times d}$, $\Lambda = \operatorname{diag}(\lambda_1, ..., \lambda_d) \in \mathbb{R}^{d \times d}$, $\lambda_1 \ge \lambda_2 \ge \cdots$
- $\widehat{W}_{\text{MLE}} = U_k \sqrt{\Lambda_k \widehat{\sigma}^2_{\text{MLE}} \cdot I}$
- where $U_k = [\mathbf{u}^1, ..., \mathbf{u}^k]$ and $\Lambda_k = [\lambda_1, ..., \lambda_k]$
- ullet Top k eigenvalues and eigenvectors
- $\hat{\sigma}_{\text{MLE}} = \frac{1}{d-k} \sum_{j=k+1}^{d} \lambda_j$

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Need to find and all some eigenvalues eigenvalues

Probabilistic Principal Component Analysis (Tipping and Bishop, 1999)

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• Let $\sigma=0$, then the MLE looks like (no need to estimate σ) $\widehat{W}_{\rm MLE}={\rm U_k}\sqrt{\Lambda_k}$



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PRINCIPAL COMPONENT ANALYSIS

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- 2. Initialize $S^0 \leftarrow S$
- 3. For j = 1, ..., k
 - 1. Let $(\hat{\lambda}_j, \hat{\mathbf{u}}_j) \leftarrow \mathsf{POWER-METHOD}(S^{j-1})$
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- 4. Return $\widehat{W}_{\text{MLE}} = \left[\sqrt{\widehat{\lambda}_j} \cdot \widehat{\mathbf{u}}_j \right]_{j=1,\dots,k}$



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The peeling technique

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The peeling technique

How to recover \mathbf{z}^i ?
Wait a bit.

The Power Method

THE POWER METHOD

- 1. Matrix $S \in \mathbb{R}^{d \times d}$
- 2. Initialize \mathbf{x}^0 randomly $\sim \mathcal{N}(\mathbf{0}, I)$
- 3. For t = 1, 2, ..., T

$$\mathbf{y}^t = S\mathbf{x}^{t-1}$$

$$\mathbf{x}^t = \frac{\mathbf{y}^t}{\|\mathbf{y}^t\|_2}$$

- 4. Repeat until convergence
- !5. Return eigenvector estimate as \mathbf{x}^T
- 6. Return eigenvalue estimate as $||S\mathbf{x}^T||_2$



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Overall $O(d^2)$ time

PROBABILISTIC PCA

- !1. Matrix $S \in \mathbb{R}^{d \times d}$
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- 3. For j = 1, ..., d
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PROBABILISTIC PCA

Recall that

 $\widehat{W}_{\text{MLE}} = U_{k} \sqrt{\Lambda_{k} - \widehat{\sigma}^{2}_{\text{MLE}} \cdot I}$

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How to recover z^i ? Wait a bit.

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Takes $O(d^3)$ time \otimes

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Probabilistic PCA (not assuming $\sigma = 0$)

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time 😊

Can we do better?

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Need to find and all Need to find and all eigenvectors and all eigenvalues

Probabilistic Principal Component Analysis (Tipping and Bishop, 1999)

- Given samples $\mathbf{x}^1, \mathbf{x}^2, ..., \mathbf{x}^n$ from $\mathcal{N}(0, \sigma^2 \cdot I_d + WW^\top)$, log-likelihood is $\log \mathbb{P}[X \mid W, \sigma] = \frac{n}{2} \left(d \log 2\pi + \log |\mathcal{C}| + \mathrm{tr}(\mathcal{C}^{-1}S) \right)$ where $\mathcal{C} = WW^\top + \sigma^2 \cdot I_d$, and $S = \frac{1}{n} \sum_{i=1}^n \mathbf{x}^i \left(\mathbf{x}^i \right)^\top$
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Need to find and an eigenvalues

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Need to find not ten eigenvectors and ten eigenvalues

Probabilistic Principal Component Analysis (Tipping and Bishop, 1999)

- Given samples $\mathbf{x}^1, \mathbf{x}^2, \dots, \mathbf{x}^n$ from \mathcal{N} Power method takes og-likelihood is $\log \mathbb{P}[X \mid W, \sigma] = \frac{n}{2} \left(d \log \frac{\text{only } O(d^2k) \text{ time and } 1S)}{\text{not } O(d^3) \text{ time to}} \right)$ where $C = WW^{T} + \sigma^{2} \cdot I_{d}$, and $S = \text{solve this problem} \odot$

- Let $S = U\Lambda U^{\mathsf{T}}$ be the eigen-decomposition of S
 - $U = [\mathbf{u}^1, ..., \mathbf{u}^d] \in \mathbb{R}^{d \times \bar{d}}, \Lambda = \operatorname{diag}(\lambda_1, ..., \lambda_d) \in \mathbb{R}^{d \times d}, \lambda_1 \geq \lambda_2$
- $\widehat{W}_{\text{MLE}} = U_{k} \sqrt{\Lambda_{k} \widehat{\sigma}^{2}_{\text{MLE}} \cdot I}$
- where $U_k = [u^1, ..., u^k]$ and $\Lambda_k = [\lambda_1, ..., \lambda_k]$
- ullet Top k eigenvalues and eigenvectors
- $\hat{\sigma}_{\text{MLE}} = \frac{1}{d-k} \sum_{j=k+1}^{d} \lambda_j = \frac{1}{d-k} \left(\text{tr}(S) \sum_{j=1}^{k} \lambda_i \right)$

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$$C = WW^{T} + \sigma^{2} \cdot I_{d}$$
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 $\log \mathbb{P}[X \mid W, \sigma] = \frac{n}{2} \left(d \log \frac{\text{only } O(d^2k) \text{ time and } 1S)}{\text{not } O(d^3) \text{ time to}} \right)$

Improvement over last lecture's claim

- Let $S = U\Lambda U^{\mathsf{T}}$ be the eigen-decomposition of S
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FA Interpretations for PCA



- Dates back more than a century [Pearson, 1901; Hotelling, 1930]
- Seeks to find the "closest" low-dim representation of data
- Also seeks to capture the maximum "variance" in the data

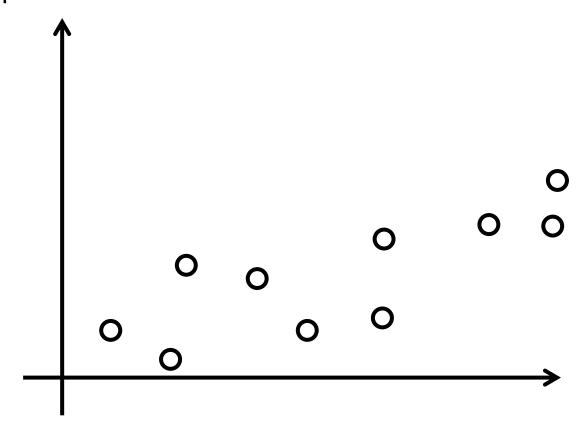


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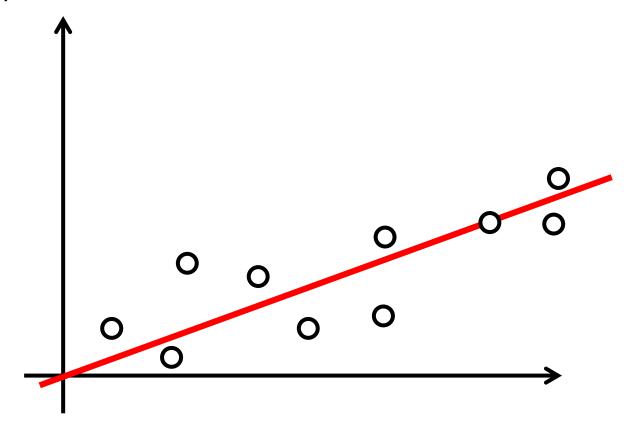


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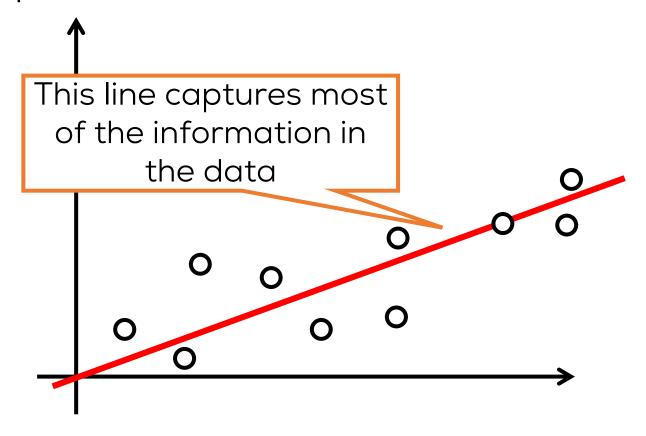


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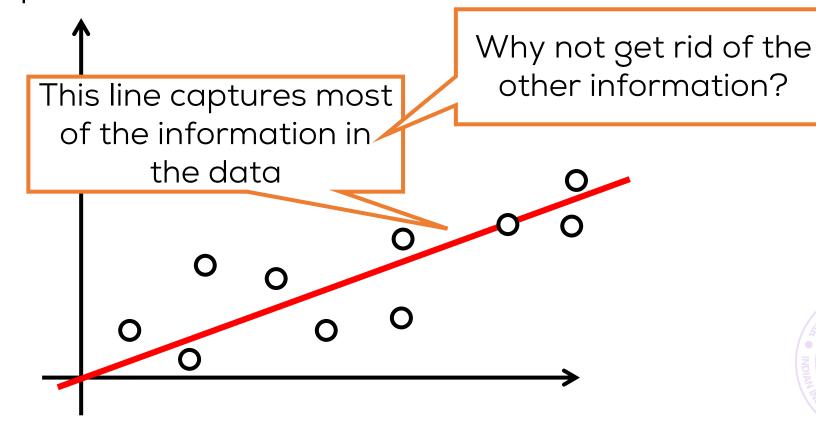


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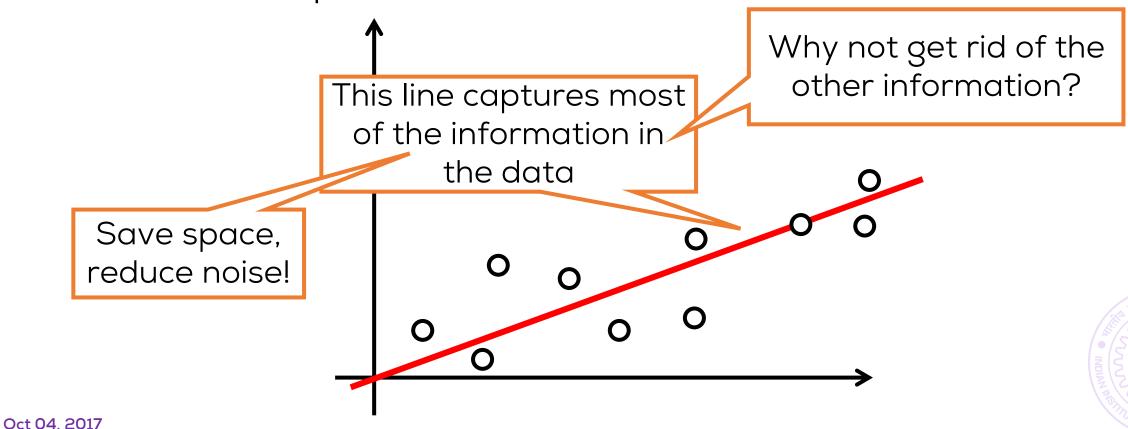




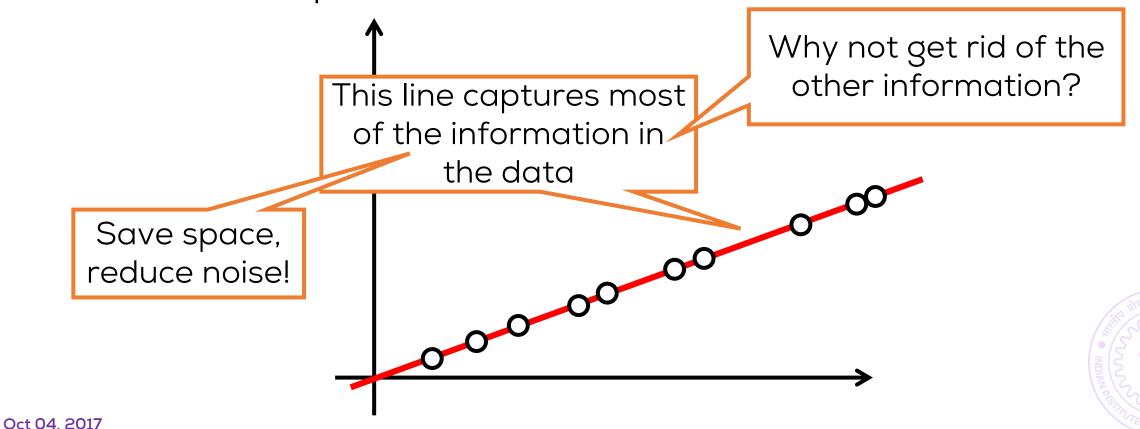
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- Given: n data points $\mathbf{x}^1, \dots, \mathbf{x}^n \in \mathbb{R}^d$
- \bullet Goal: find a line in \mathbb{R}^d such that all points lie "close" to the line (actually finding the best 1-d representation for the points)
- Every line in d-dimensions is indexed by a unit vector $\mathbf{w} \in \mathbb{R}^d$ (assume the line passes through the origin for simplicity)
- Every point on this line is of the form $z \cdot \mathbf{w}$ for some $z \in \mathbb{R}$
- Closest point on the line (Euclidean dist.) to a point x is $\langle w, x \rangle \cdot w$
- Given data points $\mathbf{x}^1, ..., \mathbf{x}^n \in \mathbb{R}^d$ and line corresponding to $\mathbf{w} \in \mathbb{R}^d$, can find out how well the line "fits" the points

$$\sum_{i=1}^{n} \left\| \mathbf{x}^{i} - \left\langle \mathbf{w}, \mathbf{x}^{i} \right\rangle \cdot \mathbf{w} \right\|_{2}^{2}$$

- Given: n data points $\mathbf{x}^1, \dots, \mathbf{x}^n \in \mathbb{R}^d$
- ullet Goal: find a line in \mathbb{R}^d such that all points lie "close" to the line (actually finding the best 1-d representation for the points)
- \bullet So our problem reduces to the following optimization problem

$$\underset{\|\mathbf{W}\|_{2}=1}{\arg\min} \sum_{i=1}^{\infty} \|\mathbf{x}^{i} - \langle \mathbf{w}, \mathbf{x}^{i} \rangle \cdot \mathbf{w}\|_{2}^{2} = \sum_{i=1}^{\infty} \|\mathbf{x}^{i} - \mathbf{w}\mathbf{w}^{\mathsf{T}}\mathbf{x}^{i}\|_{2}^{2}$$

• Simple calculations show that the above is equivalent to $\underset{\text{arg max } \mathbf{w}^{\mathsf{T}} \mathcal{S} \mathbf{w}}{\text{arg max } \mathbf{w}^{\mathsf{T}} \mathcal{S} \mathbf{w}}$

where
$$S = \frac{1}{n} \sum_{i=1}^{n} \mathbf{x}^{i} (\mathbf{x}^{i})^{\mathsf{T}} \in \mathbb{R}^{d \times d}$$



- Given: n data points $\mathbf{x}^1, ..., \mathbf{x}^n \in \mathbb{R}^d$
- ullet Goal: find a line in \mathbb{R}^d such that all points lie "close" to the line (actually finding the best 1-d representation for the points)
- So our problem further reduces to arg max $\mathbf{w}^T S \mathbf{w}$ $\|\mathbf{w}\|_{2}=1$

- Power method can find this in $O(d^2)$ time \odot
- The solution to (2) is the leading eigenvector of S (the one corresponding to the largest eigenvalue λ_1) i.e. ${m w}={m u}^1$
- Proof: write $S = U\Lambda U^{\top}$, $U = [\mathbf{u}^1, ..., \mathbf{u}^d]$, $\Lambda = \operatorname{diag}(\lambda_1, ..., \lambda_d)$, $\lambda_1 \ge \lambda_2 \ge \cdots$
- Then $\mathbf{w}^{\mathsf{T}} S \mathbf{w} = \sum_{j=1}^{d} \lambda_j \left(\langle \mathbf{u}^j, \mathbf{w} \rangle \right)^2$. Makes sense to align \mathbf{w} with \mathbf{u}^1 fully.
- Exercise: complete the above proof (Hint: U is a basis for \mathbb{R}^d)
- Alternate proof: find and solve the dual problem!

- Given: n data points $\mathbf{x}^1, \dots, \mathbf{x}^n \in \mathbb{R}^d$
- Goal: find the k-dimensional hyperplane in \mathbb{R}^d such that all points lie "closest" to that hyperplane
- Every k-dimensional hyperplane in d-dimensions is indexed by k orthonormal unit vectors $\mathbf{w}^1, \mathbf{w}^2, ..., \mathbf{w}^k \in \mathbb{R}^d$ (assume the plane passes through the origin for simplicity)
- Let us represent this using a matrix $W \in \mathbb{R}^{d \times k}$ with $W^\top W = I_k \in \mathbb{R}^{k \times k}$
- Be careful ... we may not have $WW^{\mathsf{T}} = I_d \in \mathbb{R}^{d \times d}$
- Every point on the plane is of the form $W\mathbf{z}$ for some $\mathbf{z} \in \mathbb{R}^k$
- Is this z that same latent variable z we had earlier?
- Yeah ... we will now see how to recover \mathbf{z}^i as well \odot



- Given: n data points $\mathbf{x}^1, \dots, \mathbf{x}^n \in \mathbb{R}^d$
- Goal: find the k-dimensional hyperplane in \mathbb{R}^d such that all points lie "closest" to that hyperplane
- The closest point (in Euclidean dist.) to \mathbf{x} on the plane given by W is $WW^{\mathsf{T}}\mathbf{x}$. (Hint: use the fact that U has orthonormal columns)
- \bullet We can thus, setup an opt. problem to find the best W

$$\underset{W^{\mathsf{T}}W=I_k}{\operatorname{arg min}} \sum_{i=1}^{\infty} \left\| \mathbf{x}^i - WW^{\mathsf{T}}\mathbf{x}^i \right\|_2^2 \equiv \underset{W^{\mathsf{T}}W=I_k}{\operatorname{arg max}} \operatorname{tr}(W^{\mathsf{T}}SW)$$

• One can show that the optimal solution are the top k eigenvectors of S i.e. $W=U_k=[\mathbf{u}^1,\dots,\mathbf{u}^k]\in\mathbb{R}^{d\times k}$

Exercise! Exercise!

- Proof: by induction. Base case k=1 already done
- Do a bit of rewriting

• Now apply induction to get $\widetilde{W} = [\mathbf{u}^2, \mathbf{u}^3, ..., \mathbf{u}^k]$

- Given: n data points $\mathbf{x}^1, \dots, \mathbf{x}^n \in \mathbb{R}^d$
- Goal: find the k-dimensional hyperplane in \mathbb{R}^d such that all points lie "closest" to that hyperplane
- The closest point (in Euclidean dist.) to \mathbf{x} on the plane given by W is $WW^{\mathsf{T}}\mathbf{x}$. (Hint: use the fact that U has orthonormal columns)
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- ullet Goal: find the k-dimensional hyperplane in \mathbb{R}^d such that all points lie "closest" to that hyperplane
- The closest point (in Euclidean dist.) to ${\bf x}$ on the plane given by Wis $WW^{\mathsf{T}}\mathbf{x}$. (Hint: use the fact that U has orthonormal columns)
- We can thus, setup an opt. problem to find the best W

$$\underset{W^{\mathsf{T}}W=I_{k}}{\operatorname{arg\,min}} \sum_{i=1}^{n} \left\| \mathbf{x}^{i} - WW^{\mathsf{T}}\mathbf{x}^{i} \right\|_{2}^{2} \equiv \underset{W^{\mathsf{T}}W=I_{k}}{\operatorname{arg\,max}} \operatorname{tr}(W^{\mathsf{T}}SW) \text{ can find these in } O(d^{2}k) \text{ time}$$

• One can show that the optimal solution are the top k eigenvectors of S i.e. $W=U_k=[\mathbf{u}^1,\dots,\mathbf{u}^k]\in\mathbb{R}^{d\times k}$

Power method

- Given: n data points $\mathbf{x}^1, \dots, \mathbf{x}^n \in \mathbb{R}^d$
- Goal: find the k-dimensional hyperplane in \mathbb{R}^d such that all points lie "closest" to that hyperplane
- ullet Having recovered the optimal W we can now recover \mathbf{z}^i
- Recall that the closest point on the plane to \mathbf{x}^i is $WW^\mathsf{T}\mathbf{x}^i$
- However, recall that every point in the plane is expressed as $W\mathbf{z}$
- This means that $WW^{\mathsf{T}}\mathbf{x}^i = W\mathbf{z}^i$
- Multiply both sides by W^{\top} and use the fact that $W^{\top}W = I_k$ $W^{\top}WW^{\top}\mathbf{x}^i = W^{\top}W\mathbf{z}^i$ $\mathbf{z}^i = W^{\top}\mathbf{x}^i$



Wait a second!

- Didn't the PML discussion tell us that $W_{\mathrm{MLE}} = U_k \sqrt{\Lambda_k}$
- Now the FA discussion is telling us $W=U_k$. What gives??
- Note that the FA forced W to have orthonormal columns $W^TW = I_k$
- This is why we got $W=U_k$ since we also have $U_k^{\mathsf{T}}U_k=I_k$
- Both FA/PML are valid. They just shift normalization constants
- FA view: $W_{\text{FA}} = U_k$ and $\mathbf{z}_{\text{FA}}^i = W_{\text{FA}}^\mathsf{T} \mathbf{x}^i$
- PML view: $W_{\mathrm{PML}} = U_k \sqrt{\Lambda_k}$ and $\mathbf{z}_{\mathrm{PML}}^i = \Lambda_k^{-1} W_{\mathrm{PML}}^\mathsf{T} \mathbf{x}^i$
- The PML \mathbf{z}^i are "normalized" since PML models $\mathbf{z}^i \sim N(\mathbf{0}, I_k)$
- ullet The FA W is "normalized" as they are constrained to be so
- Note that $W_{\text{FA}}\mathbf{z}_{\text{FA}}^{\text{i}} = W_{\text{PML}}\,\mathbf{z}_{\text{PML}}^{\text{i}} = U_k U_k^{\mathsf{T}}\mathbf{x}^i$



Some practical issues

- We kept assuming that "lines" and "planes" (that approximate the data points) pass through the origin
- This may not be true in general. To make this true, we need to mean-centre the data.
- Let $\mu = \frac{1}{n} \sum_{i=1}^n \mathbf{x}^i$. Convert data to $\tilde{\mathbf{x}}^i = \mathbf{x}^i \mu$ and work with $\tilde{\mathbf{x}}^i$
- Use $S = \frac{1}{n} \sum_{i=1}^{n} \tilde{\mathbf{x}}^{i} (\tilde{\mathbf{x}}^{i})^{\mathsf{T}}$ to perform PCA, PPCA
- How to decide *k*?
 - \bullet Choose k that is small but gives reasonable reconstruction
 - Some tuning required on training data itself
 - Other criterion also used (model selection later lectures)

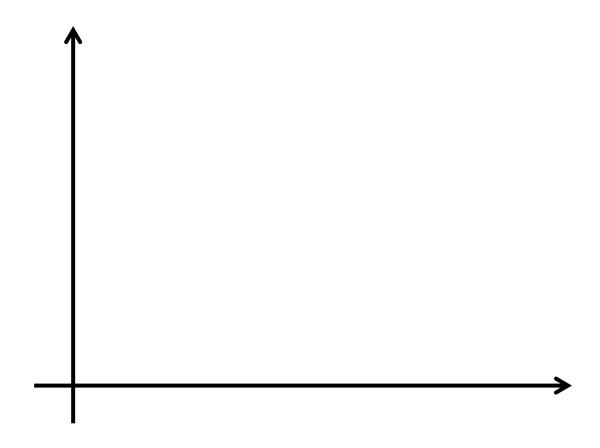
Data may vary differently along different directions



- Data may vary differently along different directions
- Directions with more spread useful and informative

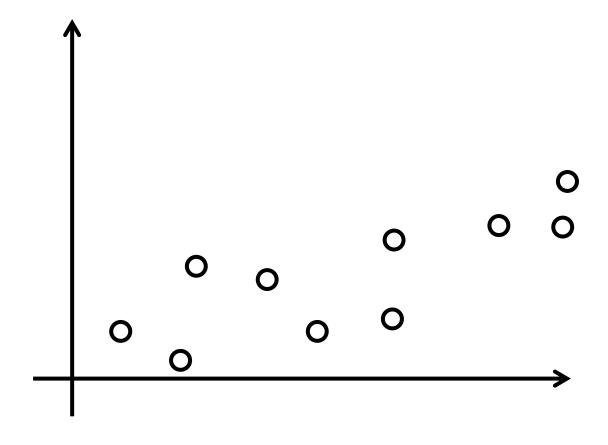


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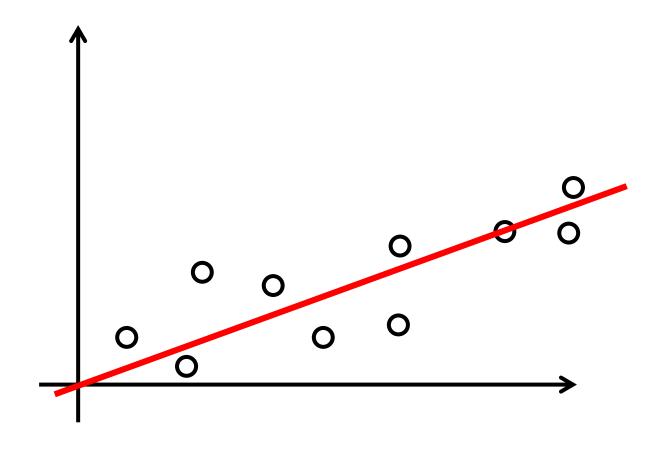


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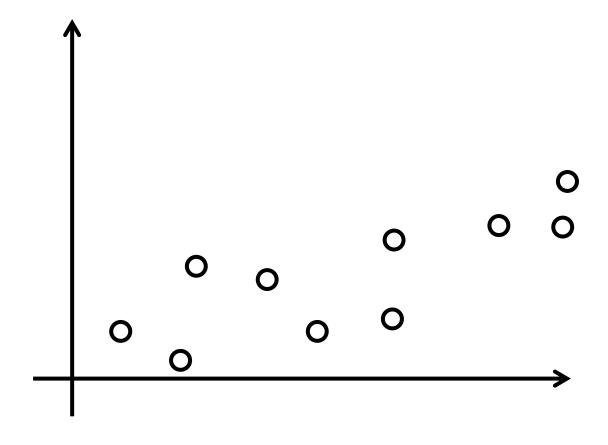


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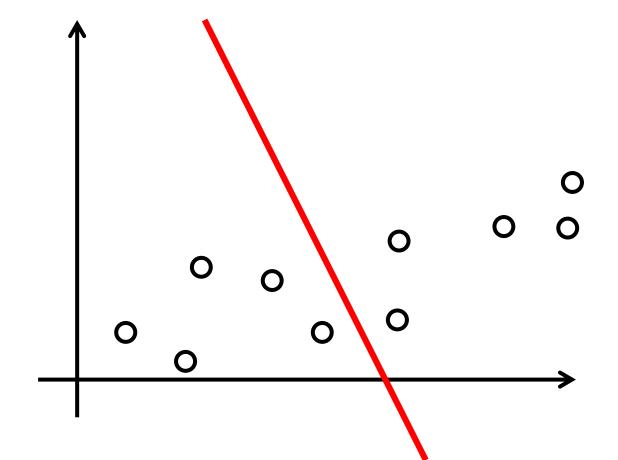


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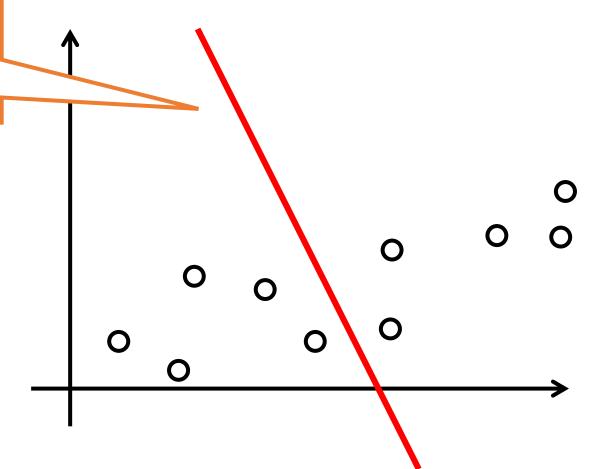
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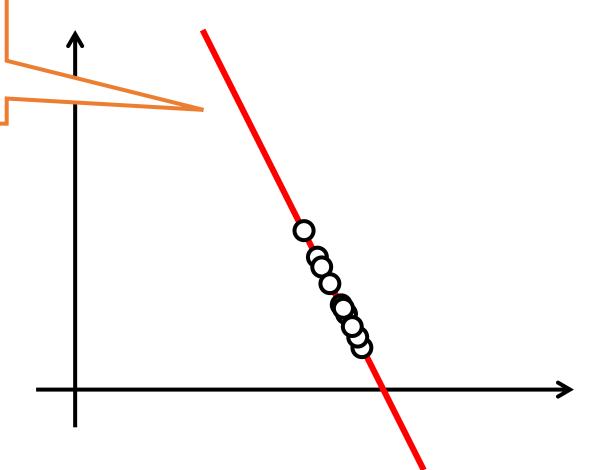
Projecting onto this line throws away a lot of information about the data





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Projecting onto this line throws away a lot of information about the data

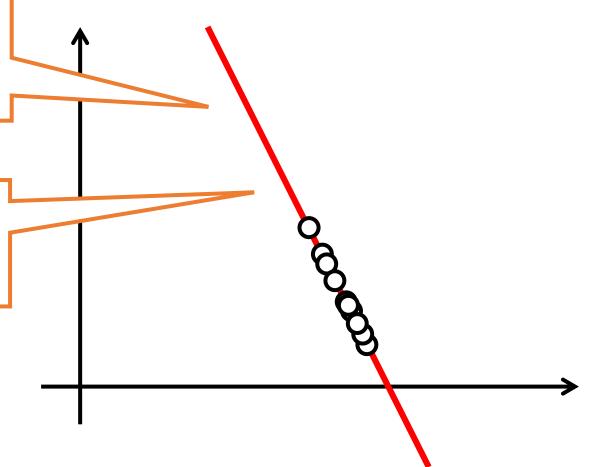




- Data may vary differently along different directions
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Projecting onto this line throws away a lot of information about the data

Save space, but introduces large amount of noise!





- Given: n data points $\mathbf{x}^1, \dots, \mathbf{x}^n \in \mathbb{R}^d$ (assume mean centered)
- Suppose we approximate each of these points by the closest point on a line given by \mathbf{u}
- The approximations will be $\langle \mathbf{u}, \mathbf{x}^i \rangle \cdot \mathbf{u}$
- Means of these approximations will be $\mathbf{0}$ (data is mean centered)
- "Variance" of these approximations will be

• Variance of these approximations will be
$$\frac{1}{n}\sum_{i=1}^{n}\left\|\left\langle \mathbf{u},\mathbf{x}^{i}\right\rangle \cdot \mathbf{u} - \mathbf{0}\right\|_{2}^{2} = \frac{1}{n}\sum_{i=1}^{n}\left\|\mathbf{u}\mathbf{u}^{\mathsf{T}}\mathbf{x}^{i}\right\|_{2}^{2} = \mathbf{u}^{\mathsf{T}}S\mathbf{u}$$
 where $S = \frac{1}{n}\sum_{i=1}^{n}\mathbf{x}^{i}\left(\mathbf{x}^{i}\right)^{\mathsf{T}}$

- But PCA maximizes this!
- PCA discovers directions of maximum spread in data!



Some practical issues

- We saw how to recover a low-dim. representation of data
- PCA gave us a way to express $\mathbf{x}^i \approx U\mathbf{z}^i$
- For the entire data matrix $X = [\mathbf{x}^1, \mathbf{x}^2, ..., \mathbf{x}^n] \in \mathbb{R}^{d \times n}$, this means X = UZ, where $Z = [\mathbf{z}^1, \mathbf{z}^2, ..., \mathbf{z}^n] \in \mathbb{R}^{k \times n}$
- This gives a low-rank factorization of the matrix X

• Note: Eigen-decomposition on $S = \frac{1}{n}XX^T \equiv PCA$ on XHigh rank (upto min(n, d)) dOct 04, 2017

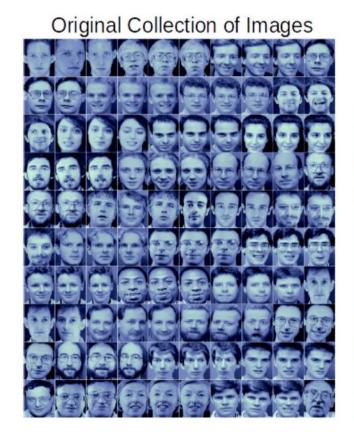
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Oct 04, 2017

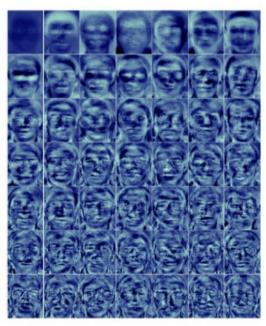
- The k vectors in U give us a useful basis for representing new data points!
- Time savings, space savings and noise removal
- Such bases (not necessarily orthonormal) often called dictionaries
- Dictionary Learning, Topic Modelling, other advanced methods for learning "simple" but latent structure in the data
- Excellent applications in image and signal processing, large-scale learning



- Eigen-faces [Sirovich and Kirby, Turk and Pentland]
- Each face represented as just a 49-dim vector!



K=49 Eigenvectors ("eigenfaces") learned by PCA on this data



Each image's reconstructed version







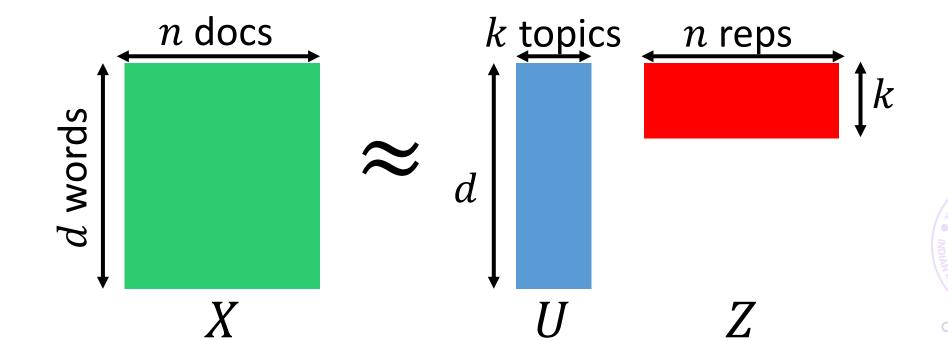
 \boldsymbol{X}

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Latent Semantic Analysis

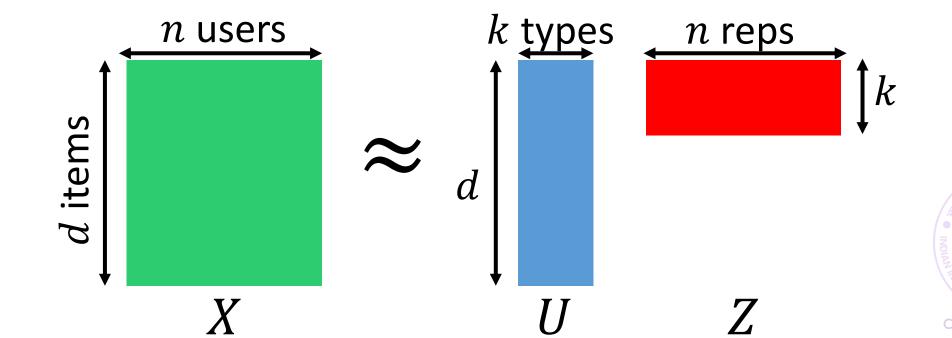
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- Given a collection of n documents/articles (e.g. Wikipedia)
- Discover of k topics and a representation of each article in terms of these topics. E.g. topics can be sports, education, science etc.
- Each document represented as a bag of d words ($d \approx 10^6$)

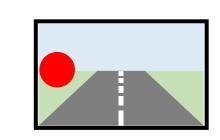


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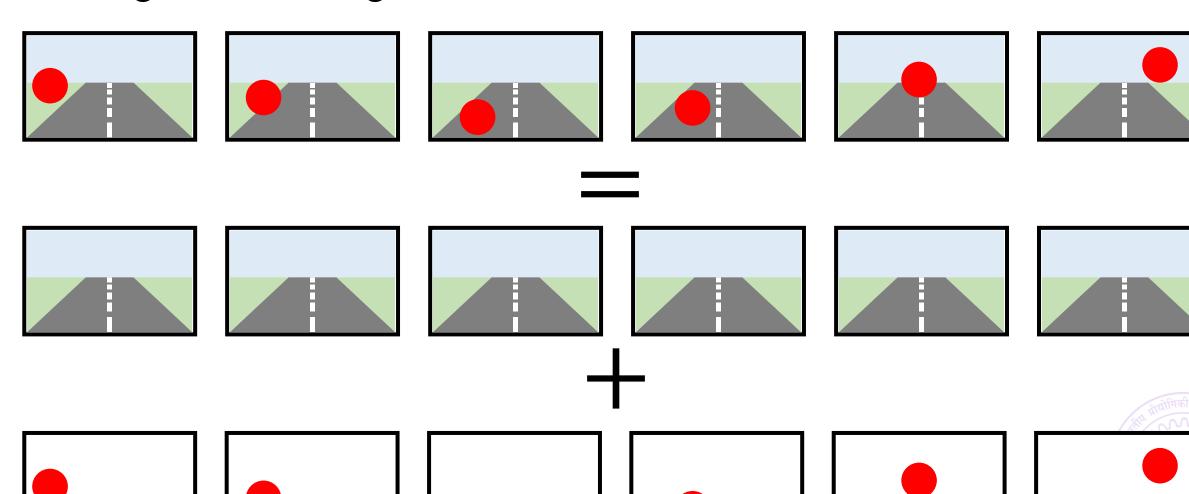
- Recommendation systems (collaborative filtering)
- ullet Given a collection of n users who have rated d movies each
- Discover of k user-types and a representation of each user in terms of these types.



Foreground/background separation



CS771: Intro to ML



- Make every frame a vector $\mathbf{x}^i \in \mathbb{R}^d$. n frames $\mathbf{X} = [\mathbf{x}^1, \mathbf{x}^2, ..., \mathbf{x}^n] \in \mathbb{R}^{d \times n}$
- Background is a constant vector $\mathbf{b} \in \mathbb{R}^d$. Let $\mathbf{1} = [1,1,1,...1]^{\mathsf{T}} \in \mathbb{R}^n$
- Foreground treated as noise $\mathbf{f}^i \in \mathbb{R}^d$. Let $F = [\mathbf{f}^1, \mathbf{f}^2, ..., \mathbf{f}^n] \in \mathbb{R}^{d \times n}$
- We have $X = \mathbf{b} \cdot \mathbf{1}^{\mathsf{T}} + F$
- Decompose X into low-rank components and recover F as noise







Please give your Feedback

http://tinyurl.com/ml17-18afb

