Principle Component Analysis (PCA)

Lecture 13

Rishabh Iyer

University of Texas at Dallas

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Eigenvalues

- λ is an eigenvalue of a matrix $A \in \mathbb{R}^{n \times n}$ if the linear system $Ax = \lambda x$ has at least one non-zero solution
  - If $Ax = \lambda x$ we say that λ is an eigenvalue of A with corresponding eigenvector x
  - Could be multiple eigenvectors for the same λ

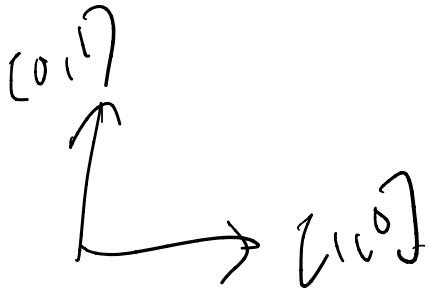
$$(A - I\lambda)x = 0$$

Eigenvalues of Symmetric Matrices

- If $A \in \mathbb{R}^{n \times n}$ is symmetric, then it has n linearly independent eigenvectors $v_1, \ldots, v_n$ corresponding to n real eigenvalues
  - Moreover, it has n linearly independent orthonormal eigenvectors
    - $v_i^T v_j = 0$ for all $i \neq j$
    - $v_i^T v_i = 1$ for all i

$A_{ij} = A_{ji}$

$\begin{bmatrix} 1 & 2 & 3 \\ 2 & 0 & 3 \\ 3 & 3 & 1 \end{bmatrix}$ ← Symmetric



Eigenvalues of Symmetric Matrices

- If $A \in \mathbb{R}^{n \times n}$ is symmetric, then it has n linearly independent eigenvectors $v_1, \ldots, v_n$ corresponding to n real eigenvalues

- A symmetric matrix is positive definite if and only if all of its eigenvalues are positive

  - The orthonormal eigenvectors form a basis of $\mathbb{R}^n$ (similar to the standard coordinate axes)

Examples

- The 2x2 identity matrix has all of its eigenvalues equal to 1 (it is positive definite) with orthonormal eigenvectors $\begin{bmatrix}1\\0\end{bmatrix}$ and $\begin{bmatrix}0\\1\end{bmatrix}$
- The matrix $\begin{bmatrix}1 & 1\\1 & 1\end{bmatrix}$ has eigenvalues 0 and 2 with orthonormal eigenvectors $\begin{bmatrix}\frac{-1}{\sqrt{2}}\\\frac{1}{\sqrt{2}}\end{bmatrix}$ and $\begin{bmatrix}\frac{1}{\sqrt{2}}\\\frac{1}{\sqrt{2}}\end{bmatrix}$
- The matrix $\begin{bmatrix}2 & 1\\1 & 2\end{bmatrix}$ has eigenvalues 1 and 3 with orthonormal eigenvectors $\begin{bmatrix}\frac{-1}{\sqrt{2}}\\\frac{1}{\sqrt{2}}\end{bmatrix}$ and $\begin{bmatrix}\frac{1}{\sqrt{2}}\\\frac{1}{\sqrt{2}}\end{bmatrix}$

Eigenvalues

- Suppose $A \in \mathbb{R}^{n \times n}$ is symmetric

- Any $x \in \mathbb{R}^n$ can be written as $x = \sum_{i=1}^{n} c_i v_i$ where $v_1, \ldots, v_n$ are the eigenvectors of A

  - $Ax = \sum_{i=1}^{n} \lambda_i c_i v_i$
  - $A^2 x = \sum_{i=1}^{n} \lambda_i^2 c_i v_i$
  - $\vdots$
  - $A^t x = \sum_{i=1}^{n} \lambda_i^t c_i v_i$

Eigenvalues

- Suppose $A \in \mathbb{R}^{n \times n}$ is symmetric

- Any $x \in \mathbb{R}^n$ can be written as $x = \sum_{i=1}^{n} c_i v_i$ where $v_1, \ldots, v_n$ are the eigenvectors of A

  - $c_i = \widetilde{v_i^T x}$, this is the projection of x along the line given by v_i (assuming that v_i is a unit vector)

Eigenvalues of Symmetric Matrices

- Let $Q \in \mathbb{R}^{n \times n}$ be the matrix whose i^{th} column is v_i and $D \in \mathbb{R}^{n \times n}$ be the diagonal matrix such that $D_{ii} = \lambda_i$
  - $Ax = QDQ^T x$
  - Can throw away some eigenvectors to approximate this quantity
    - For example, let Q_k be the matrix formed by keeping only the top k eigenvectors and D_k be the diagonal matrix whose diagonal consists of the top k eigenvalues

Frobenius Norm

- The Frobenius norm is a matrix norm given by

$$\|A\|_F = \sqrt{\sum_{i=1}^{n}\sum_{j=1}^{n}|A_{ij}|^2}$$

- $Q_k D_k Q_k^T$ is the best rank k approximation of the symmetric matrix A with respect to the Frobenius norm

$$Q_k D_k Q_k^T = \underset{B\in\mathbb{R}^{n\times n} s.t.\, rank(B)=k}{\operatorname{argmin}} \|A - B\|_F$$

Proof sketch:

Problem: $\min_{B \in \mathbb{R}^{m \times n} : \operatorname{rank}(B) = k} \|A - B\|_F$.

Know: $B' = Q_k D_k Q_k^T$ is rank k.

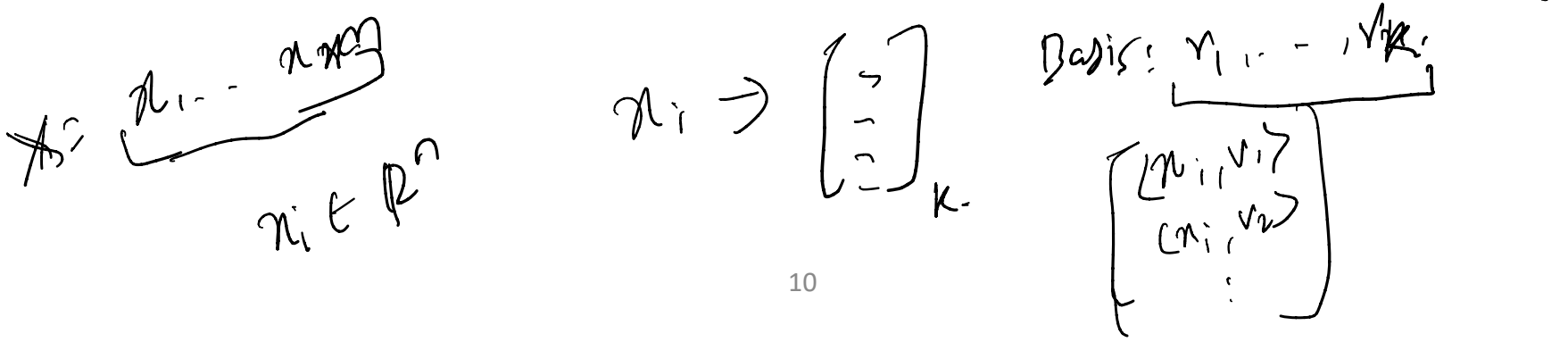
$\therefore B'$ is valid matrix.

$\|A - B\|_F^2 \geq \|QDQ^T - Q_k D_k Q_k^T\|^2$

$\forall B : \operatorname{rank}(B) = k$.

Principal Component Analysis

- Principle component analysis
  - Can be used to reduce the dimensionality of the data while still maintaining a good approximation of the sample mean and variance
  - Can also be used for selecting good features that are combinations of the input features
  - Unsupervised – just finds a good representation of the data in terms of combinations of the input features



Motivation of PCA

$x \in \mathbb{R}^n$ [Very large]

$1024 \times 1024 \rightarrow 10^6$

Reduce dim : 100

Eigen-vector space

$X^{n \times P}$ ↑ # examples, # feats

x_1 input images x_m → PCA → x_1' x_2' ⋮ $x_{n'}'$ → ML

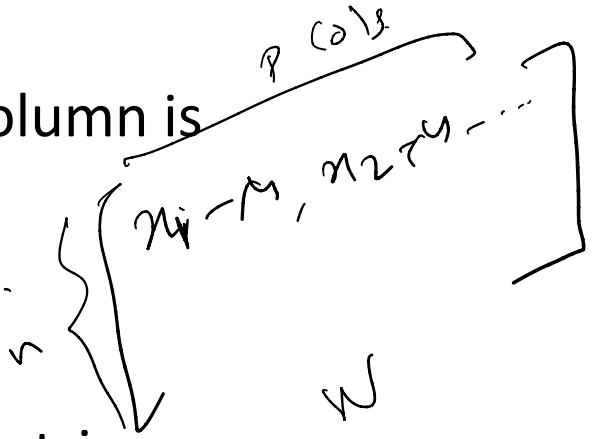
$$A = XX^T = QDQ^T$$

$$A_K = Q_K D_K Q_K^T$$

Principal Component Analysis

- Input a collection of data points sampled from some distribution $x_1, \ldots, x_p \in \mathbb{R}^n$
- Construct the matrix $W \in \mathbb{R}^{n \times p}$ whose i^{th} column is

$$x_i - \frac{\sum_j x_j}{p}$$



- The matrix WW^T is the sample covariance matrix
  - WW^T is symmetric and positive semidefinite

Principal Component Analysis

$eig(WW^T) \rightarrow sort \rightarrow \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_m$ (keep k) $\rightarrow v_1, v_2, \ldots v_k$

- PCA finds a set of orthogonal vectors that best explain the variance of the sample covariance matrix
  - From our previous discussion, these are exactly the eigenvectors of WW^T ← symmetric
  - We can discard the eigenvectors corresponding to small magnitude eigenvalues to yield an approximation
  - Simple algorithm to describe, MATLAB and other programming languages have built in support for eigenvector computation

PCA in Practice

1024 × 1024

$n \approx 1M$

- Forming the matrix WW^T can require a lot of memory (especially if $n \gg p$)
  - Need a faster way to compute this without forming the matrix explicitly
  - Typical approach: use the singular value decomposition (SVD)

Singular Value Decomposition (SVD)

- Every matrix $B \in \mathbb{R}^{n \times p}$ admits a decomposition of the form

$$B = U\Sigma V^T$$

$U, V \rightarrow$ Orthogonal matrices

  - where $U \in \mathbb{R}^{n \times n}$ is an orthogonal matrix, $\Sigma \in \mathbb{R}^{n \times p}$ is non-negative diagonal matrix, and $V \in \mathbb{R}^{p \times p}$ is an orthogonal matrix

  - A matrix $C \in \mathbb{R}^{m \times m}$ is orthogonal if $C^T = C^{-1}$. Equivalently, the rows and columns of C are orthonormal vectors

$$UU^T = U^TU = I$$

$$\Sigma = \begin{bmatrix} \sigma_1 & & 0 \\ & \sigma_2 & \\ & & \sigma_p \\ 0 & & \end{bmatrix} \quad (n \times p)$$

Singular Value Decomposition (SVD)

- Every matrix $B \in \mathbb{R}^{n \times p}$ admits a decomposition of the form

$$B = U \Sigma V^T$$

Diagonal elements of Σ called singular values

  - where $U \in \mathbb{R}^{n \times n}$ is an orthogonal matrix, $\Sigma \in \mathbb{R}^{n \times p}$ is non-negative diagonal matrix, and $V \in \mathbb{R}^{p \times p}$ is an orthogonal matrix

  - A matrix $C \in \mathbb{R}^{m \times m}$ is orthogonal if $C^T = C^{-1}$. Equivalently, the rows and columns of C are orthonormal vectors

$$U U^T = I = V V^T$$

SVD and PCA

$W = U\Sigma V^T$

$WW^T = U\Sigma \underbrace{V^T V}_{I} \Sigma^T U^T$

$= U\Sigma\Sigma^T U^T$

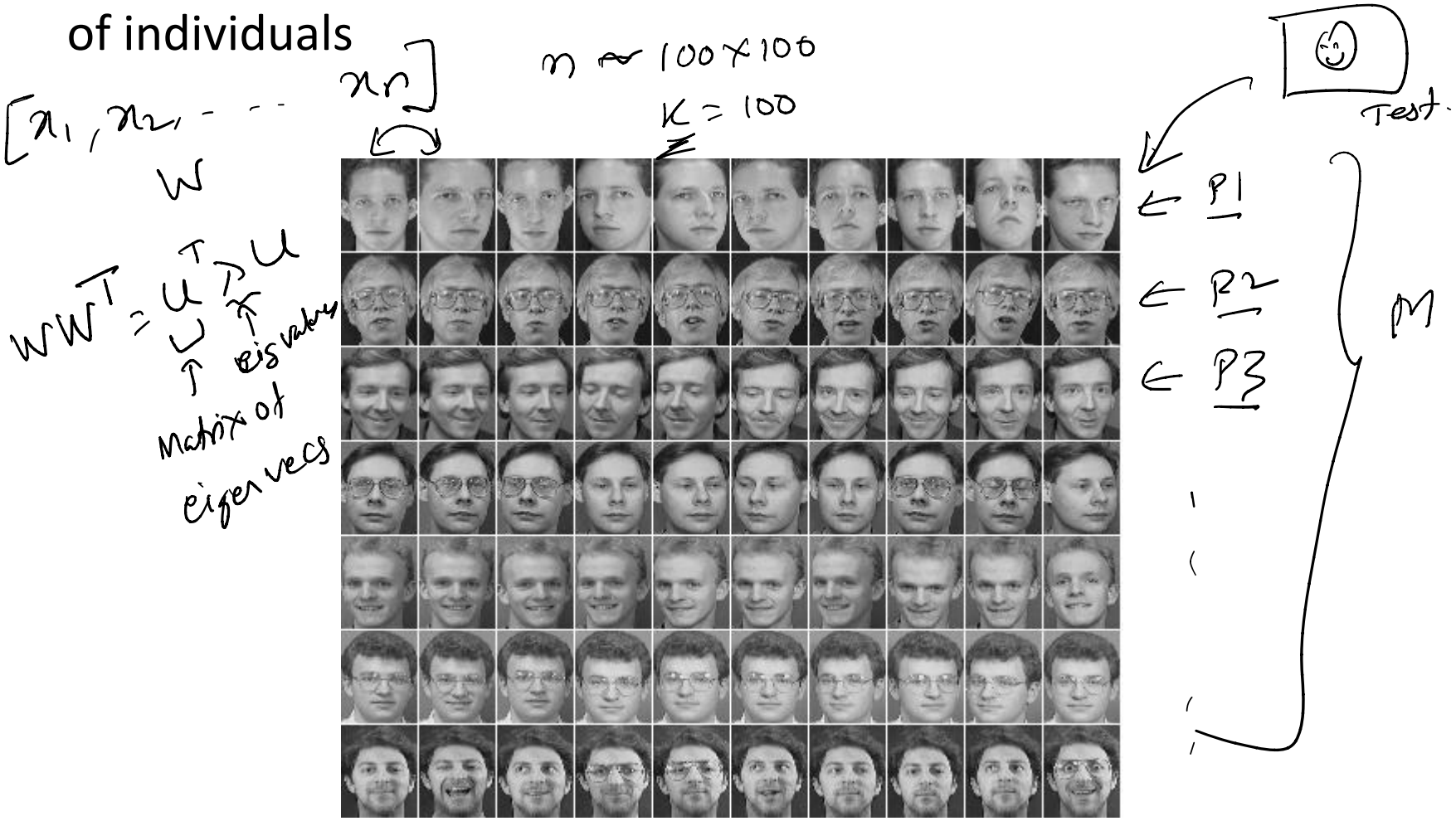
- Returning to PCA
  - Let $W = U\Sigma V^T$ be the SVD of W
  - $WW^T = U\Sigma V^T V\Sigma^T U^T = U\underbrace{\Sigma\Sigma^T}U^T$
  - If we can compute the SVD of W, then we don't need to form the matrix $\underbrace{WW^T}$

SVD and PCA

- For any matrix A, AA^T is symmetric and positive semidefinite
  - Let $A = U\Sigma V^T$ be the SVD of A
  - $AA^T = U\Sigma V^T V\Sigma^T U^T = U\Sigma\Sigma^T U^T$
  - U must be a matrix of eigenvectors of AA^T
  - The eigenvalues of AA^T are all non-negative because $\Sigma\Sigma^T = \Sigma^2$ which are the square of the singular values of A

An Example: "Eigenfaces"

- Let's suppose that our data is a collection of images of the faces of individuals



n = # feats

p = # examples

$$W = [x_1, x_2, \dots, x_p]$$

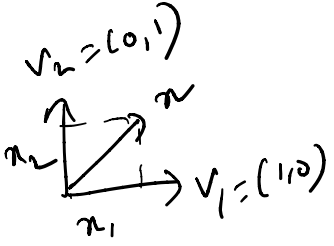
$$Cov(W) = WW^T$$

Eigen-Decomposition: $v_1, v_2, \dots v_k \in$ eig-vec(WW^T)

$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_k \in$ eig-val(WW^T)

$x_i \in \mathbb{R}^n$

$$PCA(x_i) = \begin{bmatrix} x_i^T v_1 \\ x_i^T v_2 \\ \vdots \\ x_i^T v_k \end{bmatrix} \in \mathbb{R}^k$$



$$\| Cov(W) - Cov_k(W) \|^2$$

v_i = orthogonal

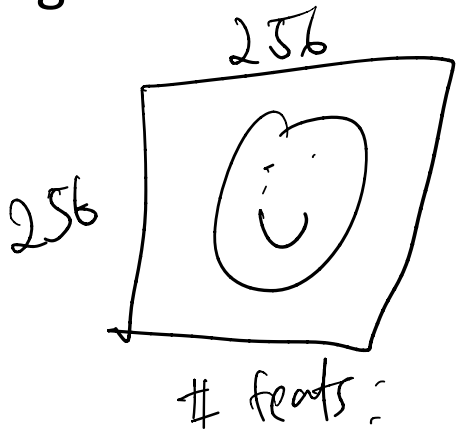
$DFE(x_i)$

An Example: "Eigenfaces"

- Let's suppose that our data is a collection of images of the faces of individuals
  - The goal is, given the "training data", to correctly match new images to the training data
  - Let's suppose that each image is an s × s array of pixels: $x_i \in R^n, n = s^2$
  - As before, construct the matrix $W \in \mathbb{R}^{n \times p}$ whose i^{th} column is $x_i - \sum_j \frac{x_j}{p}$

An Example: "Eigenfaces"

- Forming the matrix WW^T requires a lot of memory
  - $s = 256$ means WW^T is 65536×65536 = very large $\approx 36 \times 10^{10}$
  - Need a faster way to compute this without forming the matrix explicitly
  - Could use the singular value decomposition



An Example: "Eigenfaces"

- A different approach when $p \ll n$
  - Compute the eigenvectors of $A^T A$ (this is an $p \times p$ matrix)
  - Let v be an eigenvector of $A^T A$ with eigenvalue λ
  - $AA^T Av = \lambda Av$
  - This means that Av is an eigenvector of AA^T with eigenvalue λ (or 0)
  - Save the top k eigenvectors - called eigenfaces in this example

An Example: "Eigenfaces"

- The data in the matrix is "training data"
  - Given a new image, we'd like to determine which, if any, member of the data set that it is most similar to
- Step 1: Compute the projection of the recentered, new image onto each of the k eigenvectors
  - This gives us a vector of weights $c_1, \ldots, c_k$

An Example: "Eigenfaces"

- The data in the matrix is "training data"
  - Given a new image, we'd like to determine which, if any, member of the data set that it is most similar to
- Step 2: Determine if the input image is close to one of the faces in the data set
  - If the distance between the input and it's approximation is too large, then the input is likely not a face

$\underline{z_i} = PCA(x_i)$ $\quad z_i \in R^{k}$

An Example: "Eigenfaces"

- The data in the matrix is "training data"
  - Given a new image, we'd like to determine which, if any, member of the data set that it is most similar to
- Step 3: Find the person in the training data that is closest to the new input
  - Replace each group of training images by its average
  - Compute the distance to the i^{th} average $\|c - a^i\|$ where a^i are the coefficients of the average face for person i

An Example: "Eigenfaces"

$E[XX^T] \neq$ cov.

$E((X-\mu)(X-\mu)^T)$

- The data in the matrix is "training data"
  - Given a new image, we'd like to determine which, if any, member of the data set that it is most similar to
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Eigen Faces Example.

(1) Create mean-normalized Dataset: $(x_1, x_2, \ldots x_p)$

each $x_i \in \mathbb{R}^n$

(2) Do SVD (W), Compute Eig Dec (WW^T)

Get top k eig vec: $v_1, v_2, \ldots, v_k$.

(3) For each x_i, $z_i = PCA(x_i) = \begin{bmatrix} v_1^T x_i \\ v_2^T x_i \\ \vdots \\ v_k^T x_i \end{bmatrix}$

$D = (z_1, \ldots, z_p)$

(4) For test x_t, $z_t = PCA(x_t)$

Use NN classifier to get Id of person!!

$Cov(WW^T)$

1, 5, 100, 500, ...

$Cov_K((X-M)(X-M)^T)$

M + Delta(

$X_i \sim M_i + Noise$

Cov

$X_i = M_i + Z_i$

$\hat{X}_i = M_i + Approx(Z_i)$

better than $Approx(X_i)$