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CS549 – Computational Biology

LECTURE 16:
PCA AND SVD

Resource:

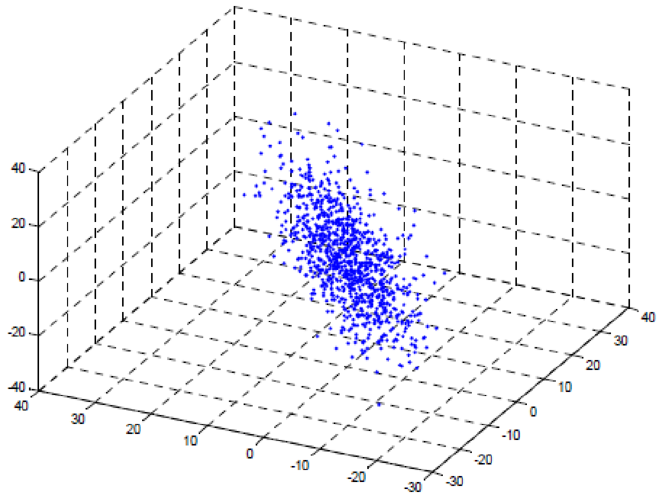
- PCA Slide by Iyad Batal
- Chapter 12 of PRML
- Shlens, J. (2003). A tutorial on principal component analysis.

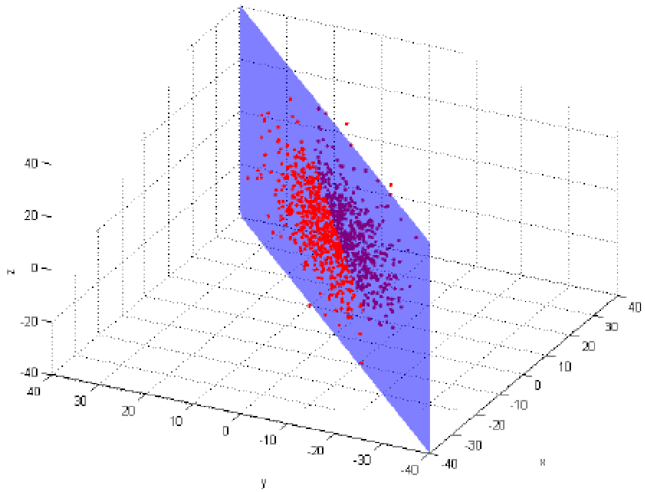
CONTENT

- Principal Component Analysis (PCA)
- Singular Value Decomposition (SVD)

PRINCIPLE COMPONENT ANALYSIS

- PCA finds a **linear** projection of high dimensional data into a lower dimensional subspace such as:
  - The variance retained is maximized.
  - The least square reconstruction error is minimized





PCA STEPS

Linearly transform an $N \times d$ matrix X into an $N \times m$ matrix Y

- Centralized the data (subtract the mean).
- Calculate the $d \times d$ covariance matrix: $C = \frac{1}{N-1} X^T X$
  - $C_{i,j} = \frac{1}{N-1} \sum_{q=1}^{N} X_{q,i} X_{q,i}$
  - $C_{i,i}$ (diagonal) is the variance of variable i.
  - $C_{i,j}$ (off-diagonal) is the covariance between variables i and j.
- Calculate the eigenvectors of the covariance matrix (orthonormal).
- Select *m* eigenvectors that correspond to the largest *m* eigenvalues to be the new basis.

EIGENVECTORS

- If A is a **square matrix**, a non-zero vector **v** is an eigenvector of A if there is a scalar λ (eigenvalue) such that

$$Av = \lambda v$$

- Example: $$\begin{pmatrix} 2 & 3 \\ 2 & 1 \end{pmatrix}\begin{pmatrix} 3 \\ 2 \end{pmatrix} = \begin{pmatrix} 12 \\ 8 \end{pmatrix} = 4\begin{pmatrix} 3 \\ 2 \end{pmatrix}$$
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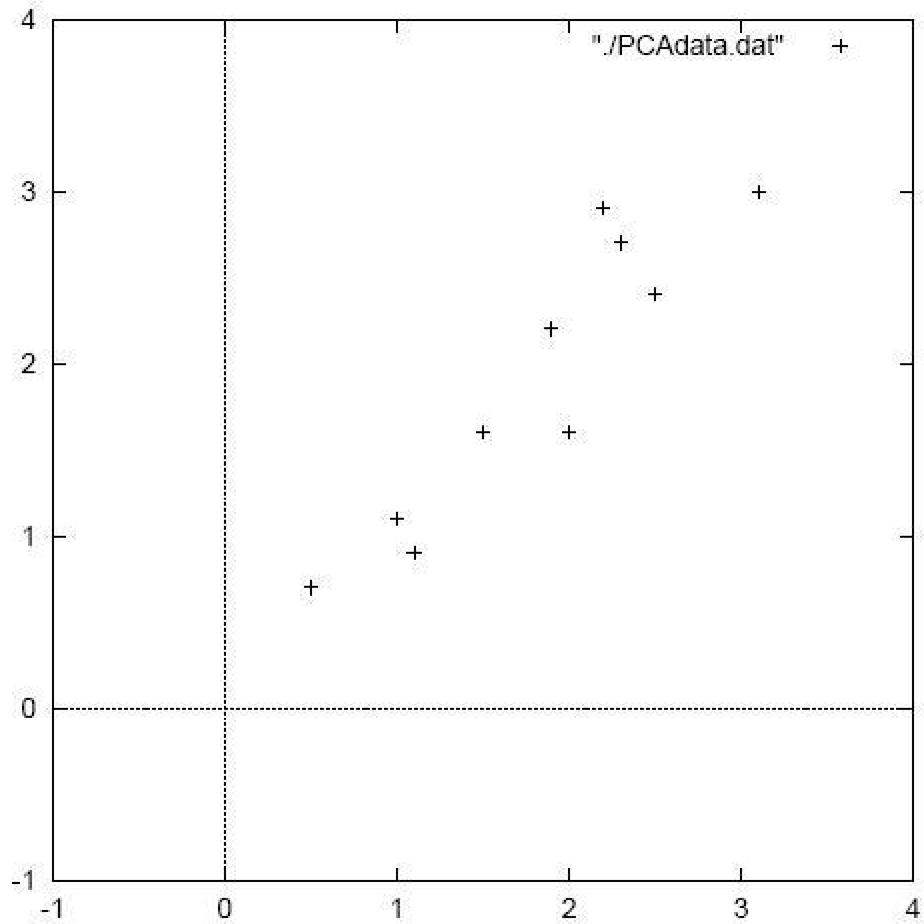
- If we think of the squared matrix A as a transformation matrix, then multiply it with the eigenvector do not change its direction.

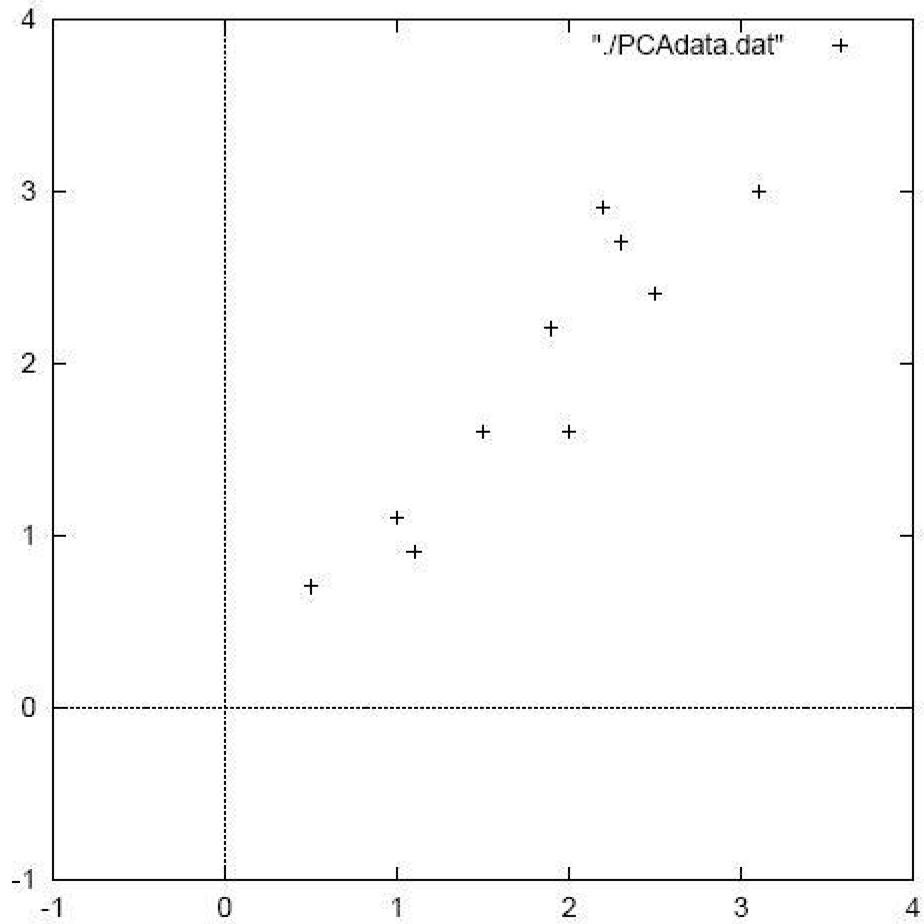
PCA EXAMPLE

X : the data matrix with $N=11$ objects and $d=2$ dimensions



* Step 1: subtract the mean and calculate the covariance matrix C.

$$C = \begin{pmatrix} 0.716 & 0.615 \\ 0.615 & 0.616 \end{pmatrix}$$

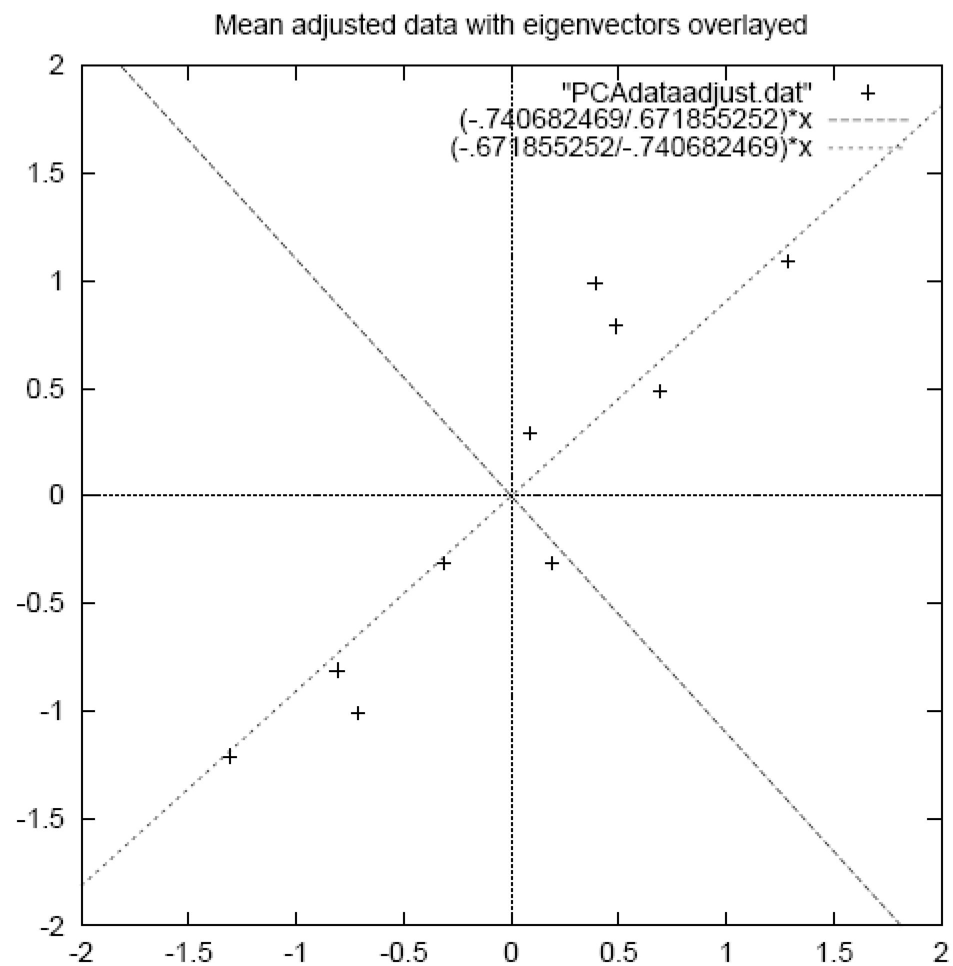


Step 2: Calculate the eigenvectors and eigenvalues of the covariance matrix:

$\lambda_1 \approx 1.28$, $v_1 \approx [-0.677 \;\; -0.735]^T$, $\lambda_2 \approx 0.49$, $v_2 \approx [-0.735 \;\; 0.677]^T$

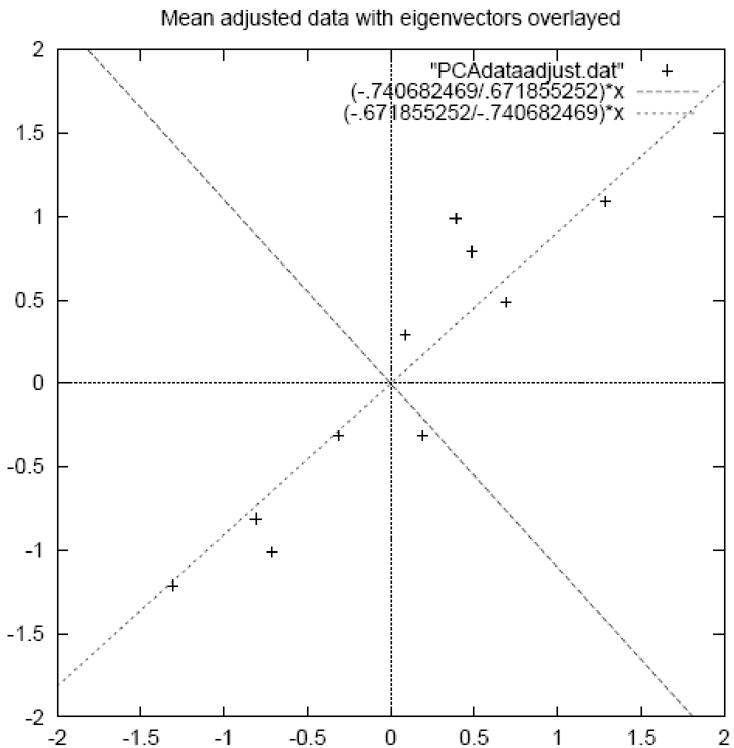
Notice that v1 and v2 are orthonormal:

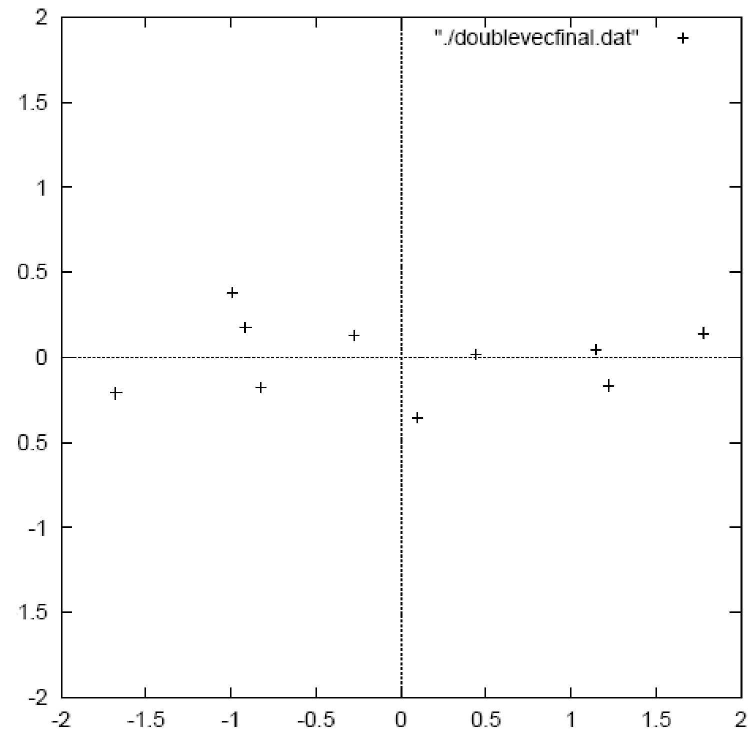
$$|v_1| = 1$$
$$|v_2| = 1$$
$$v_1 \,.\, v_2 = 0$$



Step 3: project the data

- Let $V = [v_1, \ldots v_m]$ is $d \times m$ matrix where the columns vi are the eigenvectors corresponding to the largest m eigenvalues
- The projected data: $Y = X\ V$ is $N \times m$ matrix.
- If m=d (more precisely rank(X)), then there is no loss of information!





- Step 3: project the data

$$\lambda_1 \approx 1.28,\ v_1 \approx [-0.677\ \ -0.735]^T,\ \lambda_2 \approx 0.49,\ v_2 \approx [-0.735\ \ 0.677]^T$$

- The eigenvector with the highest eigenvalue is the **principle component** of the data.
- *if we are allowed to pick only one dimension, the principle component is the best direction (retain the maximum variance).*
- Our PC is $v_1 \approx [-0.677\ \ -0.735]^T$

USEFUL PROPERTIES

- The covariance matrix is always symmetric

$$C^T = \left(\frac{1}{N-1} X^T X\right)^T = \frac{1}{N-1} X^T {X^T}^T = C$$

- The principal components of X are orthonormal

$$ {v_i}^T v_j = \begin{cases} 1 & if\ i = j \\ 0 & if\ i \neq j \end{cases} $$

- V=[v_1, … v_m], then $V^T = V^{-1}$, i.e $V^T V = I$

USEFUL PROPERTIES

Theorem 1: if square $d \times d$ matrix S is a real and symmetric matrix ($S = S^T$) then

$$\boldsymbol{S} = \boldsymbol{V} \boldsymbol{\Lambda} \boldsymbol{V}^{\boldsymbol{T}}$$

Where $V = [v_1, \ldots v_d]$ are the eigenvectors of S and $\Lambda = diag\,(\lambda_1, \ldots \lambda_d)$ are the eigenvalues.

Proof:

- $S\,V = V\,\Lambda$
- $[S\,v_1 \;\ldots\; S\,v_d] = [\lambda_1 . v_1 \;\ldots\; \lambda_d . v_d]$: the definition of eigenvectors.
- $S = V\,\Lambda\,V^{-1}$
- $S = V\,\Lambda\,V^T$ because V is orthonormal $V^{-1} = V^T$

USEFUL PROPERTIES

- The projected data: $Y = X\ V$
- The covariance matrix of Y is

$$C_Y = \frac{1}{N-1} Y^T Y = \frac{1}{N-1} V^T X^T X\ V = V^T C_X V$$

$$= \mathrm{V}^{\mathrm{T}} \mathrm{V}\ \Lambda\ \mathrm{V}^{\mathrm{T}} \mathrm{V}$$ because the covariance matrix C_X is symmetric

$$= \mathrm{V}^{-1} \mathrm{V}\ \Lambda\ \mathrm{V}^{-1} \mathrm{V}$$ because V is orthonormal

$$= \Lambda$$

After the transformation, the covariance matrix becomes diagonal.

DERIVATION OF PCA : 1. MAXIMIZING VARIANCE

- Assume the best transformation is one that maximize the variance of project data.
- Find the equation for variance of projected data.
- Introduce constraint
- Maximize the un-constraint equation. (find derivative w.r.t projection axis and set to zero)

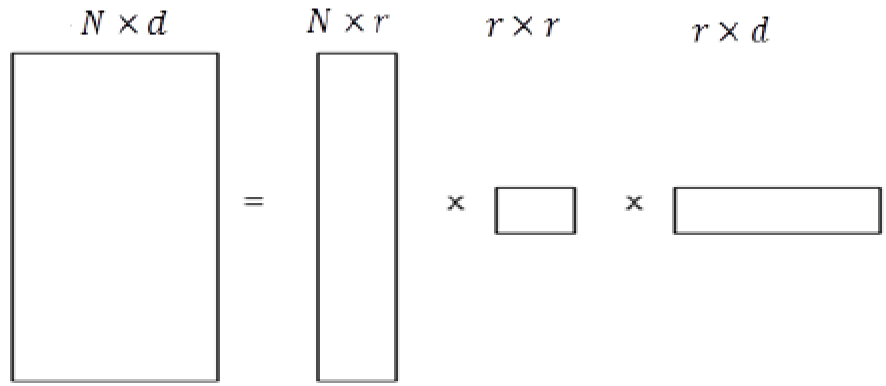
DERIVATION OF PCA :
2. MINIMIZING TRANSFORMATION ERROR

- Define error
- Identify variables that needs to be optimized in the error
- Minimize and solve for the variables.
- Interpret the information

SINGULAR VALUE DECOMPOSITION(SVD)

- Any $N \times d$ matrix X can be uniquely expressed as:

$$\mathbf{X = U \times \Sigma \times V^T}$$



- r is the rank of the matrix X (# of linearly independent columns/rows).
  - U is a column-orthonormal $N \times r$ matrix.
  - Σ is a **diagonal $r \times r$ matrix** where the singular values σi are sorted in descending order.
  - V is a column-orthonormal $d \times r$ matrix.

PCA AND SVD RELATION

Theorem:

Let $X = U \Sigma V^T$ be the SVD of an $N \times d$ matrix X and

$C = \frac{1}{N-1} X^T X$ be the $d \times d$ covariance matrix.

The eigenvectors of C are the same as the right singular vectors of X.

Proof:

$$X^T X = V \Sigma U^T U \Sigma V^T = V \Sigma \Sigma V^T = V \Sigma^2 V^T$$

$$C = V \frac{\Sigma^2}{N-1} V^T$$

But C is symmetric, hence $C = V \Lambda V^T$

Therefore, the eigenvectors of the covariance matrix C are the same as matrix V (right singular vectors) and

the eigenvalues of C can be computed from the singular values $\lambda_i = \frac{\sigma_i^2}{N-1}$

$$\mathbf{X} = \mathbf{U} \times \mathbf{\Sigma} \times \mathbf{V}^{\mathbf{T}}$$

The singular value decomposition and the eigendecomposition are closely related. Namely:

- The **left-singular vectors** of X are eigenvectors of XX^T
- The **right-singular vectors** of X are eigenvectors of X^TX.
- The **non-zero singular values** of X (found on the diagonal entries of Σ) are the square roots of the non-zero eigenvalues of both X^TX and XX^T.

ASSUMPTIONS OF PCA

- I. Linearity
- II. Mean and variance are sufficient statistics.
  - Gaussian distribution assumed
- III. Large variances have important dynamics.
- IV. The principal components are orthogonal

PCA WITH EIGENVALUE DECOMPOSITION

```
function [signals,PC,V] = pca1(data)

% PCA1: Perform PCA using covariance.
% data - MxN matrix of input data
% (M dimensions, N trials)
% signals - MxN matrix of projected data
% PC - each column is a PC
% V - Mx1 matrix of variances

[M,N] = size(data);

% subtract off the mean for each dimension
mn = mean(data,2);
data = data - repmat(mn,1,N);

% calculate the covariance matrix
covariance = 1 / (N-1) * data * data';

% find the eigenvectors and eigenvalues
[PC, V] = eig(covariance);

% extract diagonal of matrix as vector
V = diag(V);

% sort the variances in decreasing order
[junk, rindices] = sort(-1*V);
V = V(rindices);
PC = PC(:,rindices);

% project the original data set
signals = PC' * data;
```

Shlens, J. (2003). A tutorial on principal component analysis.

PCA WITH SVD

```
function [signals,PC,V] = pca2(data)

% PCA2: Perform PCA using SVD.
% data - MxN matrix of input data
% (M dimensions, N trials)
% signals - MxN matrix of projected data
% PC - each column is a PC
% V - Mx1 matrix of variances

[M,N] = size(data);

% subtract off the mean for each dimension
mn = mean(data,2);
data = data - repmat(mn,1,N);

% construct the matrix Y
Y = data' / sqrt(N-1);

% SVD does it all
[u,S,PC] = svd(Y);

% calculate the variances
S = diag(S);
V = S .* S;

% project the original data
signals = PC' * data;
```

Shlens, J. (2003). A tutorial on principal component analysis.