## Singular Value Decomposition (SVD)



U and V are orthogonal matrices, and S is a diagonal matrix consisting of singular values.

#### Singular Value Decomposition (SVD)

**SVD of a Matrix: observations**

 $M = U S V<sup>T</sup>$ 

Multiply both sides by M<sup>T</sup>

 $\mathsf{M}^\mathsf{T}\mathsf{M} = (\mathsf{U}\ \mathsf{S}\ \mathsf{V}^\mathsf{T})^\mathsf{T}\ \mathsf{U}\ \mathsf{S}\ \mathsf{V}^\mathsf{T}$  $M<sup>T</sup>M = (V S U<sup>T</sup>) U S V<sup>T</sup>$  $U^TU = I$  $M<sup>T</sup>M = V S<sup>2</sup> V<sup>T</sup>$ Multiplying on the left Multiplying on the right

 $MM^{\mathsf{T}} = U S V^{\mathsf{T}} (U S V^{\mathsf{T}})^{\mathsf{T}}$  $MM<sup>T</sup> = U S V<sup>T</sup> (V S U<sup>T</sup>)$  $V<sup>T</sup>V = I$  $MM<sup>T</sup> = U S<sup>2</sup> U<sup>T</sup>$ 

### Singular Value Decomposition (SVD)

#### **SVD of a Matrix: observations**

 $M<sup>T</sup>M = V S<sup>2</sup> V<sup>T</sup>$   $\longleftarrow$  diagonalizations  $\longrightarrow$   $MM<sup>T</sup> = U S<sup>2</sup> U<sup>T</sup>$ 

Diagonalization of a Matrix: (finding eigenvalues)

#### $A = W \wedge W^{T}$

where:

- A is a square, symmetric matrix
- Columns of W are eigenvectors of A
- $\wedge$  is a diagonal matrix containing the eigenvalues

Therefore, if we know U (or V) and S, we basically have found out the eigenvectors and eigenvalues of MM<sup>T</sup> (or M<sup>T</sup>M) !

What is PCA?

- Analysis of n-dimensional data
- Observes correspondence between different dimensions

• Determines principal dimensions along which the variance of the data is high

#### Why PCA?

- Determines a (lower dimensional) basis to represent the data
- Useful compression mechanism
- Useful for decreasing dimensionality of high dimensional data

Steps in PCA: #1 Calculate Adjusted Data Set



Steps in PCA: #2 Calculate Co-variance matrix, C, from Adjusted Data Set, A

#### Co-variance Matrix: C



$$
cov(X,Y) = \frac{\sum_{i=1}^{\infty} (X_i - X)(Y_i - Y)}{(n-1)}
$$

 $\mathbf{\nabla}$ n

 $\sqrt{V}$ 

 $\bar{\mathbf{V}}$   $\vee$ 

 $\bar{V}$ 

Note: Since the means of the dimensions in the adjusted data set, A, are 0, the covariance matrix can simply be written as:

$$
C = (A AT) / (n-1)
$$

 $C_{ii} = cov(i,j)$ 

Steps in PCA: #3 Calculate eigenvectors and eigenvalues of C



If some eigenvalues are 0 or very small, we can essentially discard those eigenvalues and the corresponding eigenvectors, hence reducing the dimensionality of the new basis.

Steps in PCA: #4 Transforming data set to the new basis

 $F = F<sup>T</sup>A$ 

where:

• F is the transformed data set

 $\cdot$  E<sup>T</sup> is the transpose of the E matrix containing the eigenvectors

• A is the adjusted data set

Note that the dimensions of the new dataset, F, are less than the data set A

To recover A from F:

 $(E<sup>T</sup>)<sup>-1</sup>F = (E<sup>T</sup>)<sup>-1</sup>E<sup>T</sup>A$  $(E<sup>T</sup>)<sup>T</sup>F = A$  $EF = A$ 

\* E is orthogonal, therefore  $E^{-1} = E^{T}$ 

# PCA using SVD

Recall: In PCA we basically try to find eigenvalues and eigenvectors of the covariance matrix, C. We showed that  $C = (AA^{T}) / (n-1)$ , and thus finding the eigenvalues and eigenvectors of C is the same as finding the eigenvalues and eigenvectors of AA<sup>T</sup>

Recall: In SVD, we decomposed a matrix A as follows:  $A = U S V<sup>T</sup>$ 

and we showed that:

 $AA<sup>T</sup> = U S<sup>2</sup> U<sup>T</sup>$ 

where the columns of U contain the eigenvectors of AAT and the eigenvalues of AA<sup>T</sup> are the squares of the singular values in S

Thus SVD gives us the eigenvectors and eigenvalues that we need for PCA