Scientific Computing for Biologists

Singular Value Decomposition and Biplots

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Overview of Lecture

- Singular Value Decomposition
  - Algebra of SVD
  - Geometry of SVD
  - Relationship to Eigendecomposition
  - Applications of SVD
- Biplots
  - Simultaneous representation of rows and columns of a matrix

Hands-on Session

- SVD and Biplots in R
- SVD in Python
- Applications of SVD in R and Python
  - ‘Seriation’ using SVD
  - Matrix approximation and image compression using SVD

Eigendecomposition

$$A = UDU^{-1}$$

where:

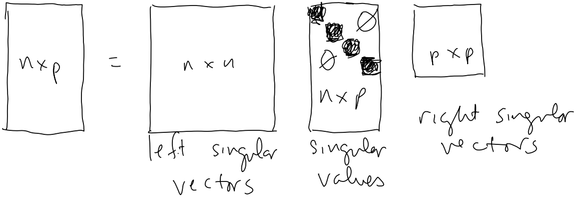
- U is a matrix of eigenvectors (in columns)
- D is a diagonal matrix with eigenvalues along diagonal.

when A is real-valued and symmetric than U is orthgonal.

Singular Value Decomposition

$$\underset{(n \times p)}{A} = \underset{(n \times n)}{U} \quad \underset{(n \times p)}{S} \quad \underset{(p \times p)}{V^T}$$

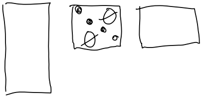
assume $n \geq p$



when written like this U & V are orthonormal

sometimes written as

$$\underset{}{A} = \underset{(n \times p)}{U} \quad \underset{(p \times p)}{S} \quad \underset{(p \times p)}{V^T} =$$



Facts about SVD

- Singular Value Decomposition is often referred to as giving the "basic structure" of a matrix
- The rank of A is equivalent to the number of non-zero singular values in $A = USV^T$

$$\mathrm{rank}(A) \leq \min(n, p)$$

- The Euclidean norm (L_2) norm of a matrix is the relative amount it stretches a vector:

$$|A|_E = \frac{|Ax|}{|x|}$$

The L_2 norm of A is given by S_{11}.

Geometric Interpretation of SVD

Any matrix, $A_{n \times p}$, represents a linear transformation from $\mathbb{R}^p \mapsto \mathbb{R}^n$.

SVD can be thought of decomposing the transformation specified by A into a simple form:

$$A = (\text{rotation})(\text{scaling})(\text{rotation})$$

- U and V are orthonormal matrices $\rightsquigarrow$ Orthonormal matrices represent rigid rotations (or rotation plus reflection)
- Diagonal matrices represent “stretching”

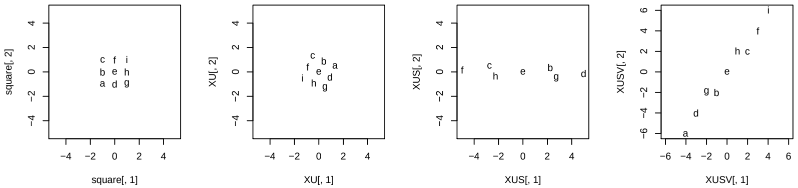
SVD Example

$$A = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} = USV^T$$

where $U = \begin{bmatrix} -0.41 & -0.91 \\ -0.91 & 0.41 \end{bmatrix}$ $S = \begin{bmatrix} 5.47 & 0 \\ 0 & 0.37 \end{bmatrix}$

$$V^T = \begin{bmatrix} -0.58 & -0.82 \\ 0.82 & -0.58 \end{bmatrix}$$

Geometry



Relationship of SVD to Eigendecomposition

$A = U S V^T$, let $D = SS$

$$A^T A = (V S U^T)(U S V^T) = V S \underbrace{U^T U}_{= I \text{ (since orthonormal)}} S V^T$$

$$= V D V^T$$

so the singular values S_{ii} are $\sqrt{D_{ii}}$ where D_{ii} are the eigenvalues of $A^T A$

columns of V are the eigenvectors of $A^T A$

Using SVD to do PCA

let X be a mean-centered data matrix

covariance matrix of X

$$C = \frac{1}{n} X^T X$$

By SVD we can write $X = USV^T$

$$C = \frac{1}{n} VSU^T USV^T$$
$$= \frac{1}{n} VS^2V^T$$

Principal Components given by columns of V

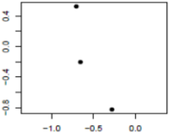
PC Scores given by UD

Another Way of Thinking about SVD

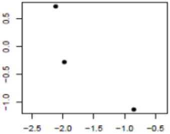
Observations in measurement space = (Observations in PC space) $\xleftarrow{\text{rotation}}$ Inverse of Eigenvectors

$$A = U\,S\;V^T$$

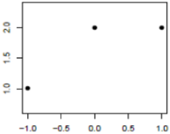
e.g. $A = \begin{bmatrix} 1 & 2 \\ 0 & 2 \\ -1 & 1 \end{bmatrix} =$



U



US (note change of scale)



USV^T

Applications of SVD

- Pseudoinverse of an arbirary matrix
- Matrix approximation
- Motivates the Biplot and Correspondence Analysis

Pseudoinverse via SVD

The pseudoinverse of a matrix is a generalization of the concept of a matrix inverse. Only square matrices have a matrix inverse; the pseudoinverse applies to an arbitrary $n \times p$ matrix.

Given an $n \times p$ matrix A find matrix A^+ such that:

$$
\begin{aligned}
AA^+A &= A \\
A^+AA^+ &= A^+ \\
(AA^+)^T &= AA^+ \\
(A^+A)^T &= A^+A
\end{aligned}
$$

Moore-Penrose Inverse via SVD:

$$
\begin{aligned}
\text{if } A &= USV^T \\
A^+ &= VS^+U^T
\end{aligned}
$$

where S^+ has the reciprocal of non-zero elements of S.

SVD for Matrix Approximation

If $A = USV^T$ then the optimal (least-squares) k-dimensional approximation of A (where $k < \text{rank}(A)$) is given by:

$$\tilde{A} = US^{\star}V^T$$

where:

$$\begin{aligned} S^{\star}_{ii} &= S_{ii} \text{ for } i \leq k \\ S^{\star}_{ii} &= 0 \text{ for } i > k \end{aligned}$$

Biplots

- Technique for simultaneously displaying row and column data
- Invented by K. Gabriel (see also papers by Gower)

Given data matrix X, write

$$\underset{(n \times p)}{X} = \underset{(n \times p)}{U} \; \underset{(p \times p)}{S} \; \underset{(p \times p)}{V^T}$$

$$\tilde{X}_k = U \, S^* \, T \qquad \text{(}k\text{-dimensional approximation to } X\text{)}$$

reduce $\tilde{X}$ to a product

$$\tilde{X} = G H^T$$

where $\underset{\text{(row effects)}}{G = U (S^*)^{\alpha}}$ $\quad \underset{\text{(column effects)}}{H^T = (S^*)^{1-\alpha} V^T}$

if $\alpha = 1$, PCs are "sphered"

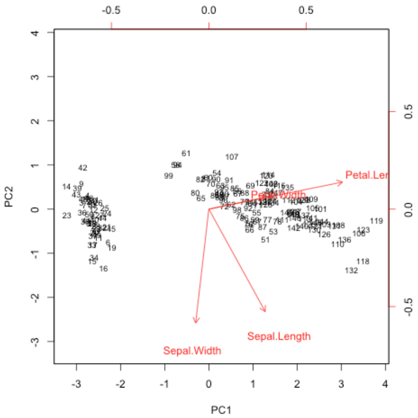
Biplots

$$
\begin{aligned}
G &= U(S^\star)^\alpha \text{ (row effects)} \\
H^T &= (S^\star)^{1-\alpha} V^T \text{ (columns effects)}
\end{aligned}
$$

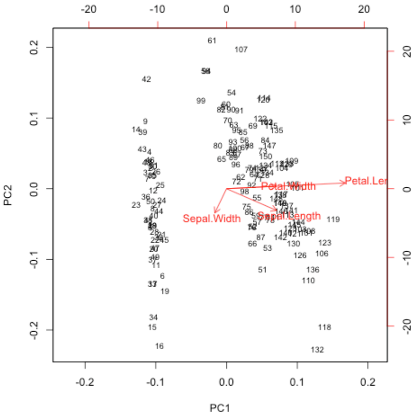
Different choices of α emphasize different relationships in the data.

- $\alpha = 0$, column-metric preserving biplot; optimally approximates variance-covariance structure. Cosine of angles between vectors approximate correlations; distances between points approximate Mahalanobis distance (“correlation biplot”)
- $\alpha = 1$, row-metric preserving biplot; optimally approximates Euclidean distances among observations. Coordinates of observations correspond to PC scores; coordinates of variables correspond to eigenvector coefficients (“distance biplot”)
- $\alpha = 0.5$, optimally approximates observational values (“symmetric biplot”)

Biplots, Example



alpha = 0

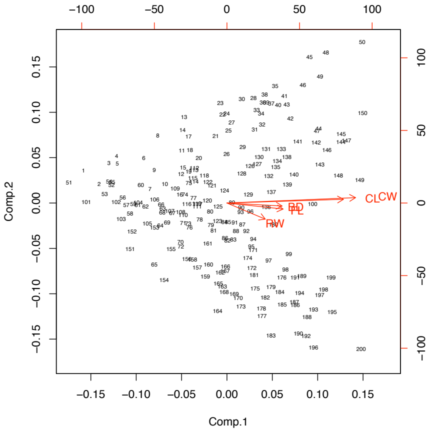


alpha = 1

Anderson's famous iris data set.

Biplots, Example II

- Observations drawn as points in space of PCs
- Variables drawn as vectors in PC space



Biplot ($\alpha = 1$) for dataset of five morphological measurements on crabs.