SVD and PCA

Dimensionality Reduction

The curse of dimensionality

- Real data usually have thousands, or millions of dimensions
  - E.g., web documents, where the dimensionality is the vocabulary of words
  - Facebook graph, where the dimensionality is the number of users
- Huge number of dimensions causes problems
  - Data becomes very sparse, some algorithms become meaningless (e.g. density based clustering)
  - The complexity of several algorithms depends on the dimensionality and they become infeasible.

Dimensionality Reduction

- Usually the data can be described with fewer dimensions, without losing much of the meaning of the data.
  - The data reside in a space of lower dimensionality
- Essentially, we assume that some of the data is noise, and we can approximate the useful part with a lower dimensionality space.
  - Dimensionality reduction does not just reduce the amount of data, it often brings out the useful part of the data

Dimensionality Reduction

- We have already seen a form of dimensionality reduction
- LSH, and random projections reduce the dimension while preserving the distances

SVD is "**the Rolls-Royce and the Swiss Army Knife of Numerical Linear Algebra.**"*

*Dianne O'Leary, MMDS '06

Data in the form of a matrix

- We are given n objects and d attributes describing the objects. Each object has d numeric values describing it.
- We will represent the data as a $n \times d$ real matrix A.
  - We can now use tools from linear algebra to process the data matrix
- Our goal is to produce a new $n \times k$ matrix B such that
  - It preserves as much of the information in the original matrix A as possible
  - It reveals something about the structure of the data in A

[redacted]

d terms
(e.g., theorem, proof, etc.)

n documents

$$\left(\begin{array}{c} A \\ \\ A_{ij} = \text{frequency of the } j\text{-th} \\ \text{term in the } i\text{-th document} \end{array}\right)$$

Find subsets of terms that bring documents together

d movies

n customers

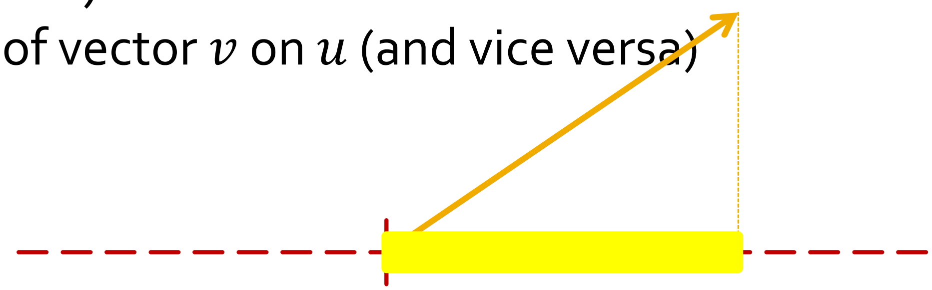
$$A$$

A_{ij} = rating of **j**-th product by the **i**-th customer

Find subsets of movies that capture the behavior or the customers

Linear algebra

- We assume that vectors are column vectors.
- We use v^T for the transpose of vector v (row vector)
- Dot product: $u^T v$ $(1\times n, n\times 1 \ \rightarrow \ 1\times 1)$
  - The dot product is the projection of vector v on u (and vice versa)
- $[1, 2, 3]\begin{bmatrix}4\\1\\2\end{bmatrix} = 12$
- $u^T v = \|v\|\|u\|\cos(u, v)$
  - If $||u|| \ = \ 1$ (unit vector) then $u^T v$ is the projection length of v on u
- $[-1, 2, 3]\begin{bmatrix}4\\-1\\2\end{bmatrix} = 0$ orthogonal vectors
  - Orthonormal vectors: two unit vectors that are orthogonal



Matrices

- An n×m matrix A is a collection of n row vectors and m column vectors

$$A = \begin{bmatrix} | & | & | \\ a_1 & a_2 & a_3 \\ | & | & | \end{bmatrix} \qquad A = \begin{bmatrix} - & \alpha_1^T & - \\ - & \alpha_2^T & - \\ - & \alpha_3^T & - \end{bmatrix}$$

- Matrix-vector multiplication
  - Right multiplication Au: projection of u onto the row vectors of A, or projection of row vectors of A onto u.
  - Left-multiplication $u^T A$: projection of u onto the column vectors of A, or projection of column vectors of A onto u
- Example:

$$[1,2,3]\begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix} = [1,2]$$

Rank

- Row space of A: The set of vectors that can be written as a linear combination of the rows of A
  - All vectors of the form $v = u^T A$

- Column space of A: The set of vectors that can be written as a linear combination of the columns of A
  - All vectors of the form $v = Au$.

- Rank of A: the number of linearly independent row (or column) vectors
  - These vectors define a basis for the row (or column) space of A

Rank-1 matrices

- In a rank-1 matrix, all columns (or rows) are multiples of the same column (or row) vector

$$A = \begin{bmatrix} 1 & 2 & -1 \\ 2 & 4 & -2 \\ 3 & 6 & -3 \end{bmatrix}$$

- All rows are multiples of $r = [1,2,-1]$
- All columns are multiples of $c = [1,2,3]^T$
- External product: uv^T $(n\times 1\,,1\times m \;\rightarrow\; n\times m)$
  - The resulting $n\times m$ has rank 1: all rows (or columns) are linearly dependent
  - $A = rc^T$

Eigenvectors

- (Right) Eigenvector of matrix A: a vector v such that $Av = \lambda v$
- λ: eigenvalue of eigenvector v

- A square matrix A of rank r, has r orthonormal eigenvectors $u_1, u_2, \ldots, u_r$ with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_r$.
- Eigenvectors define an orthonormal basis for the column space of A

Singular Value Decomposition

$$A = U \;\; \Sigma \;\; V^T = [u_1, u_2, \cdots, u_r] \begin{bmatrix} \sigma_1 & & & 0 \\ & \sigma_2 & & \\ & & \ddots & \\ 0 & & & \sigma_r \end{bmatrix} \begin{bmatrix} v_1^T \\ v_2^T \\ \vdots \\ v_r^T \end{bmatrix}$$

$[n \times m] = [n \times r] \;\; [r \times r] \;\; [r \times m]$

r: rank of matrix A

- $\sigma_1, \geq \sigma_2 \geq \cdots \geq \sigma_r$: singular values of matrix A (also, the square roots of eigenvalues of AA^T and $A^T A$)
- $u_1, u_2, \ldots, u_r$: left singular vectors of A (also eigenvectors of AA^T)
- $v_1, v_2, \ldots, v_r$: right singular vectors of A (also, eigenvectors of $A^T A$)

$$A = \sigma_1 u_1 v_1^T + \sigma_2 u_2 v_2^T + \cdots + \sigma_r u_r v_r^T$$

Symmetric matrices

- Special case: A is symmetric positive definite matrix

$$A = \lambda_1 u_1 u_1^T + \lambda_2 u_2 u_2^T + \cdots + \lambda_r u_r u_r^T$$

- $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_r \geq 0$: Eigenvalues of A
- $u_1, u_2, \ldots, u_r$: Eigenvectors of A

Singular Value Decomposition

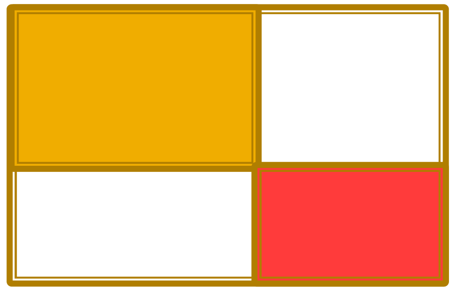
- The left singular vectors are an orthonormal basis for the row space of A.
- The right singular vectors are an orthonormal basis for the column space of A.

- If A has rank r, then A can be written as the sum of r rank-1 matrices

- There are r "linear components" (trends) in A.
  - Linear trend: the tendency of the row vectors of A to align with vector **v**
  - Strength of the i-th linear trend: $||Av_i|| = \boldsymbol{\sigma_i}$

An (extreme) example

- Document-term matrix
  - Blue and Red rows (colums) are linearly dependent

A =


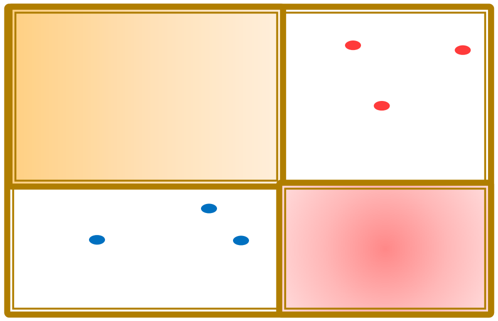
- There are two prototype documents (vectors of words): blue and red
  - To describe the data is enough to describe the two prototypes, and the projection weights for each row

- A is a rank-2 matrix

$$A = [w_1, w_2] \begin{bmatrix} d_1^T \\ d_2^T \end{bmatrix}$$

An (more realistic) example

- Document-term matrix

A = 

- There are two prototype documents and words but they are noisy
  - We now have more than two singular vectors, but the strongest ones are still about the two types.
  - By keeping the two strongest singular vectors we obtain most of the information in the data.
    - This is a rank-2 approximation of the matrix A

k

$$
\begin{array}{ccccccc}
\begin{pmatrix} \\ \quad A_k \quad \\ \\ \end{pmatrix} & = & \begin{pmatrix} \\ \quad U_k \quad \\ \\ \end{pmatrix} & \cdot & \begin{pmatrix} \quad \Sigma_k \quad \end{pmatrix} & \cdot & \begin{pmatrix} \quad V_k^T \quad \end{pmatrix} \\
\mathbf{n \times d} & & \mathbf{n \times k} & & \mathbf{k \times k} & & \mathbf{k \times d}
\end{array}
$$

U_k (V_k): orthogonal matrix containing the top *k* left (right) singular vectors of A.

Σ_k: diagonal matrix containing the top *k* singular values of A

A_k is an approximation of A

A_k is the **best** approximation of A

SVD as an optimization

- The rank-k approximation matrix A_k produced by the top-k singular vectors of A minimizes the Frobenious norm of the difference with the matrix A

$$A_k = \arg \max_{B:rank(B)=k} \|A - B\|_F^2$$

$$\|A - B\|_F^2 = \sum_{i,j} \left(A_{ij} - B_{ij}\right)^2$$

What does this mean?

- We can project the row (and column) vectors of the matrix A into a k-dimensional space and preserve most of the information
- (Ideally) The k dimensions reveal latent features/aspects/topics of the term (document) space.
- (Ideally) The A_k approximation of matrix A, contains all the useful information, and what is discarded is noise

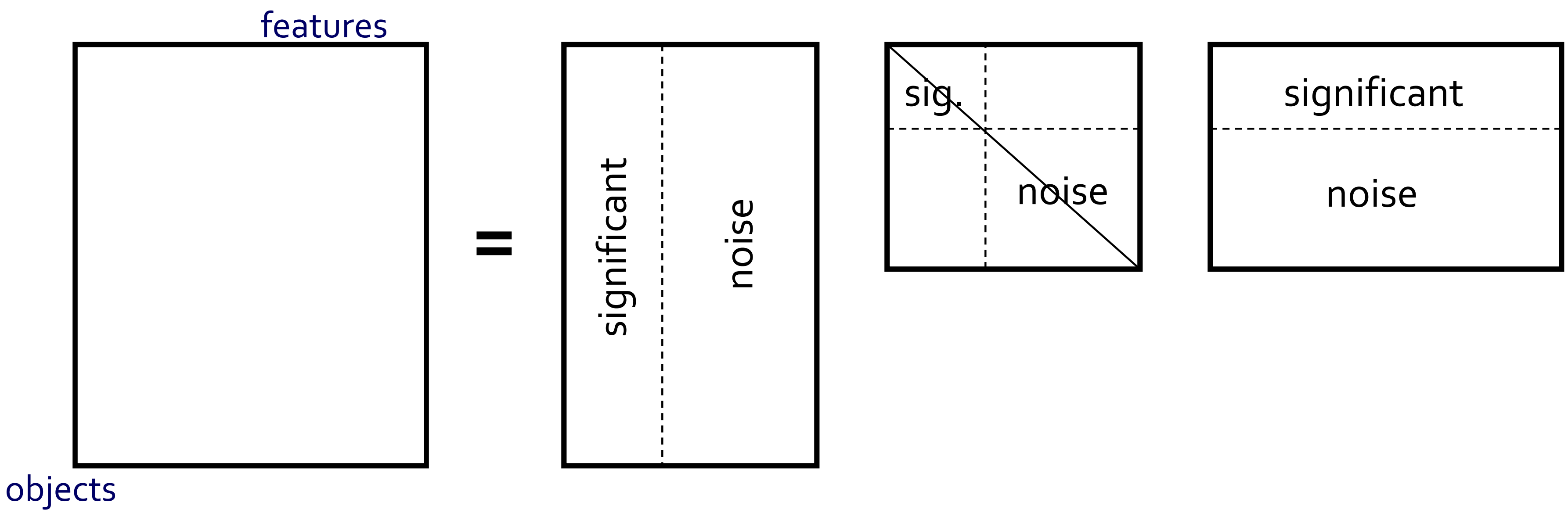
Latent factor model

- Rows (columns) are linear combinations of k latent factors
  - E.g., in our extreme document example there are two factors
- Some noise is added to this rank-k matrix resulting in higher rank

- SVD retrieves the latent factors (hopefully).

k

$$A \quad = \quad U \quad \Sigma \quad V^T$$



Application: Recommender systems

- Data: Users rating movies
  - Sparse and often noisy
- Assumption: There are k basic user profiles, and each user is a linear combination of these profiles
  - E.g., action, comedy, drama, romance
  - Each user is a weighted cobination of these profiles
  - The "true" matrix has rank k
- What we observe is a noisy, and incomplete version of this matrix $\tilde{A}$
  - The rank-k approximation $\tilde{A}_k$ is provably close to A_k
- Algorithm: compute $\tilde{A}_k$ and predict for user u and movie m, the value $\tilde{A}_k[m, u]$.
  - Model-based collaborative filtering

SVD and PCA

- PCA is a special case of SVD on the centered covariance matrix.

Covariance matrix

- Goal: reduce the dimensionality while preserving the "information in the data"
- Information in the data: variability in the data
  - We measure variability using the covariance matrix.
  - Sample covariance of variables X and Y

$$\sum_i (x_i - \mu_X)^T (y_i - \mu_Y)$$

- Given matrix A, remove the mean of each column from the column vectors to get the centered matrix C
- The matrix $V = C^T C$ is the covariance matrix of the row vectors of A.

PCA: Principal Component Analysis

- We will project the rows of matrix A into a new set of attributes (dimensions) such that:
  - The attributes have zero covariance to each other (they are orthogonal)
  - Each attribute captures the most remaining variance in the data, while orthogonal to the existing attributes
    - The first attribute should capture the most variance in the data

- For matrix C, the variance of the rows of C when projected to vector x is given by $\sigma^2 = ||Cx||^2$
  - The right singular vector of C maximizes σ^2!

PCA Algorithm

The PCA algorithm consists of 5 main steps:

1. Subtract the mean: subtract the mean from each of the data dimensions. The mean subtracted is the average across each dimension. This produces a data set whose mean is zero.
2. Calculate the covariance matrix:

   $$C^{n\times n} = (c_{i,j}, c_{i,j} = cov(Dim_i, Dim_j))$$

   where $C^{n\times n}$ is a matrix which each entry is the result of calculating the covariance between two separate dimensions.

3. Calculate the eigenvectors and eigenvalues of the covariance matrix.
4. Choose components and form a feature vector: once eigenvectors are found from the covariance matrix, the next step is to order them by eigenvalue, highest to lowest. So that the components are sorted in order of significance. The number of eigenvectors that you choose will be the number of dimensions of the new data set. The objective of this step is construct a feature vector (matrix of vectors). From the list of eigenvectors take the eigenvectors selected and form a matrix with them in the columns:

   FeatureVector = (eig_1, eig_2, ..., eig_n)

5. Derive the new data set. Take the transpose of the FeatureVector and multiply it on the left of the original data set, transposed:

   FinalData = RowFeatureVector x RowDataAdjusted

   where RowFeatureVector is the matrix with the eigenvectors in the columns transposed (the eigenvectors are now in the rows and the most significant are in the top) and RowDataAdjusted is the mean-adjusted data transposed (the data items are in each column, with each row holding a separate dimension).

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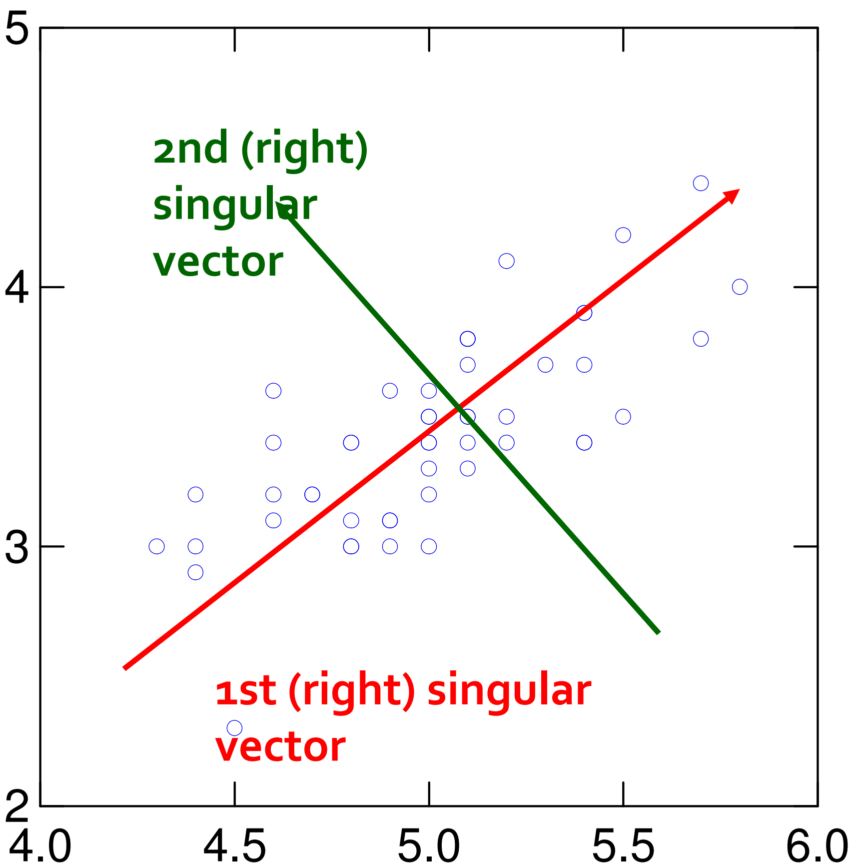
Input: 2-d dimensional points

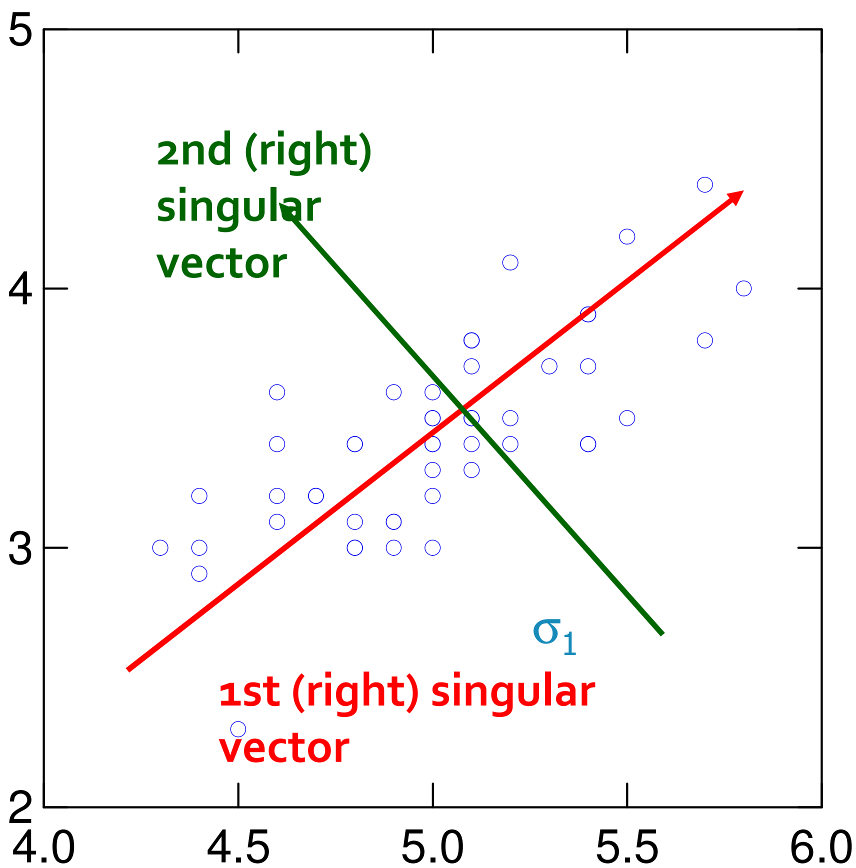
Output:



1st (right) singular vector:
direction of maximal variance,

2nd (right) singular vector:
direction of maximal variance, after removing the projection of the data along the first singular vector.

[redacted]



σ_1: measures how much of the data variance is explained by the first singular vector.

σ_2: measures how much of the data variance is explained by the second singular vector.

Singular values tell us something about the variance

- The variance in the direction of the k-th principal component is given by the corresponding singular value σ_k^2

- Singular values can be used to estimate how many components to keep

- ***Rule of thumb:*** keep enough to explain ***85%*** of the variation:

$$\frac{\sum_{j=1}^{k} \sigma_j^2}{\sum_{j=1}^{n} \sigma_j^2} \approx 0.85$$

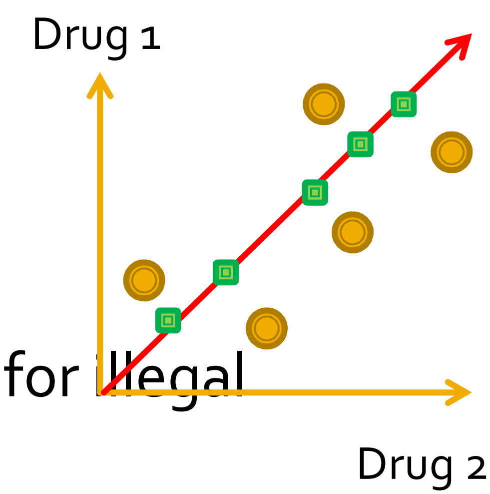
Example

$$\begin{array}{cc} A = \begin{bmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{nn} \end{bmatrix} & \text{students} \\ \text{legal} \qquad \text{illegal} & \end{array}$$

a_{ij}: usage of student i of drug j

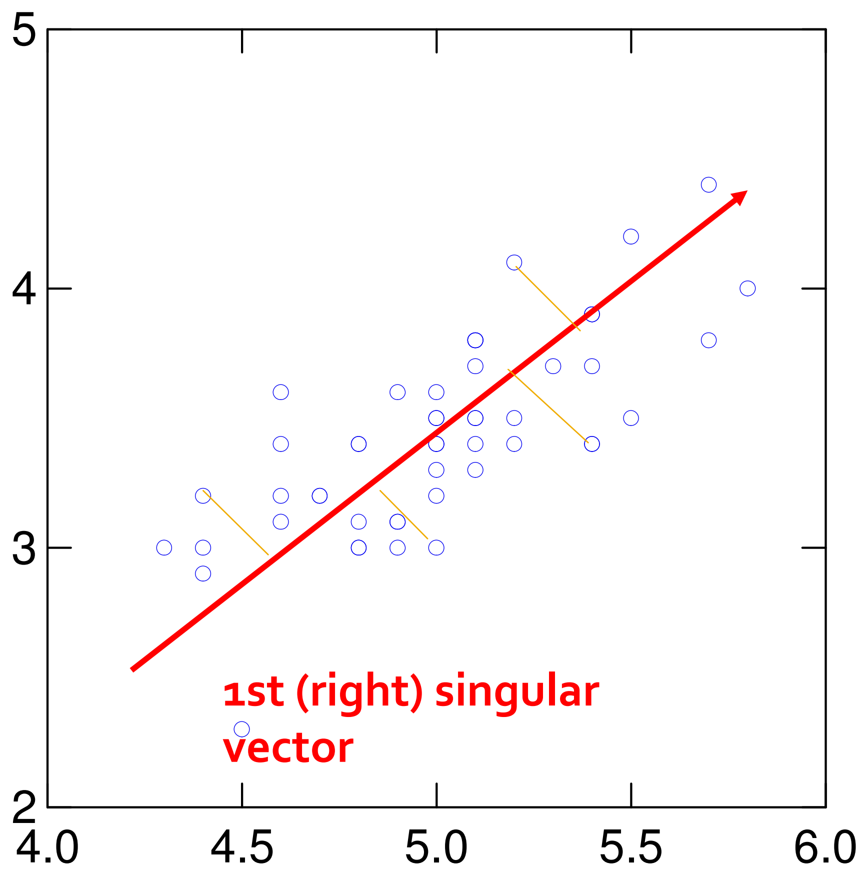
$$A = U\Sigma V^T$$

- First right singular vector v_1
  - More or less same weight to all drugs
  - Discriminates heavy from light users
- Second right singular vector
  - Positive values for legal drugs, negative for illegal



Another property of PCA/SVD

- The chosen vectors are such that minimize the sum of square differences between the data vectors and the low-dimensional projections



Application

- Latent Semantic Indexing (LSI):
  - Apply PCA on the document-term matrix, and index the k-dimensional vectors
  - When a query comes, project it onto the k-dimensional space and compute cosine similarity in this space
  - Principal components capture main topics, and enrich the document representation

SVD in R

```
# SVD
dat = seq(1,240,2)
X = matrix(dat,ncol=12)
s = svd(X)
A = diag(s$d)
s$u %*% A %*% t(s$v) #  X = U A V'

dat = seq(1,240,2)
X = matrix(dat,ncol=12)
s = svd(X, nu = nrow(X), nv = ncol(X))
A = diag(s$d)
A = cbind(A, 0)  # Add two columns with zero, in order to A have the same dimensions of X.
A = cbind(A, 0)p
s$u %*% A %*% t(s$v) #  X = U A V'

install.packages("jpeg")
library(jpeg)
tux = readJPEG("tux.jpg")
tux = imagematrix(tux,type='grey')
plot(tux)
```

SVD in R

```
reduce <- function(A,dim) {
   #Calculates the SVDprincomp
   sing <- svd(A)

   #Approximate each result of SVD with the given dimension
   u<-as.matrix(sing$u[, 1:dim])
   v<-as.matrix(sing$v[, 1:dim])
   d<-as.matrix(diag(sing$d)[1:dim, 1:dim])

   #Create the new approximated matrix
   return(imagematrix(u%*%d%*%t(v),type='grey'))
}

tux_d = svd(tux)
length(tux_d$d)
plot(reduce(tux,1))
# 90% reduction
plot(reduce(tux,35))

plot(pc$scores[,2], pc$scores[,1])
```

PCA in R

```
# PCA
pc = princomp(iris2)
summary(pc)
pc$scores
pc$loadings
```