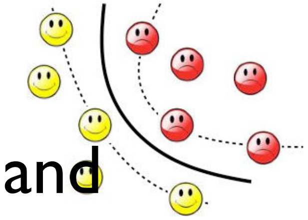
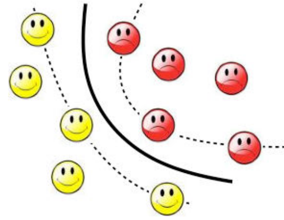


Machine Learning and Data Mining

Basic Matrix Analysis and Singular Value Decomposition

Nguyen Hoang Tran



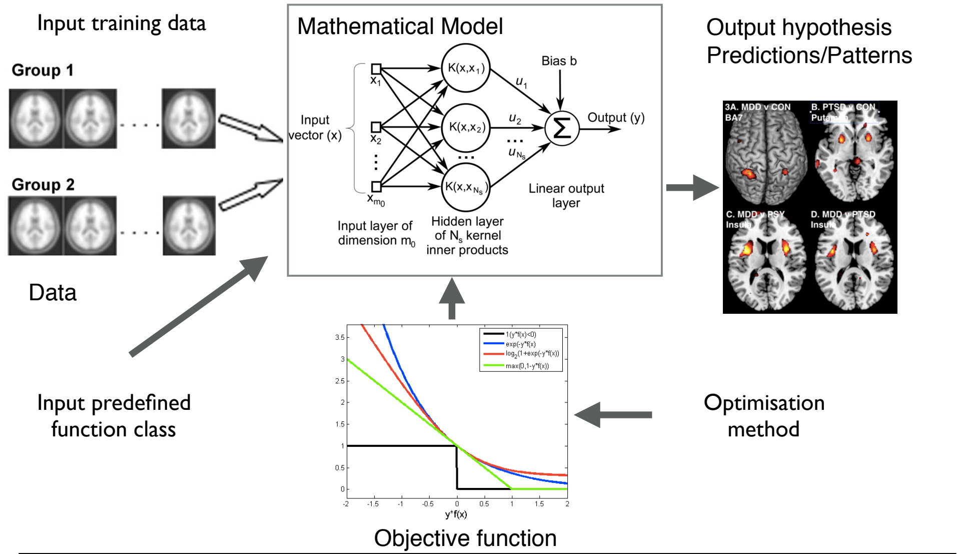
Review

What is Machine Learning?

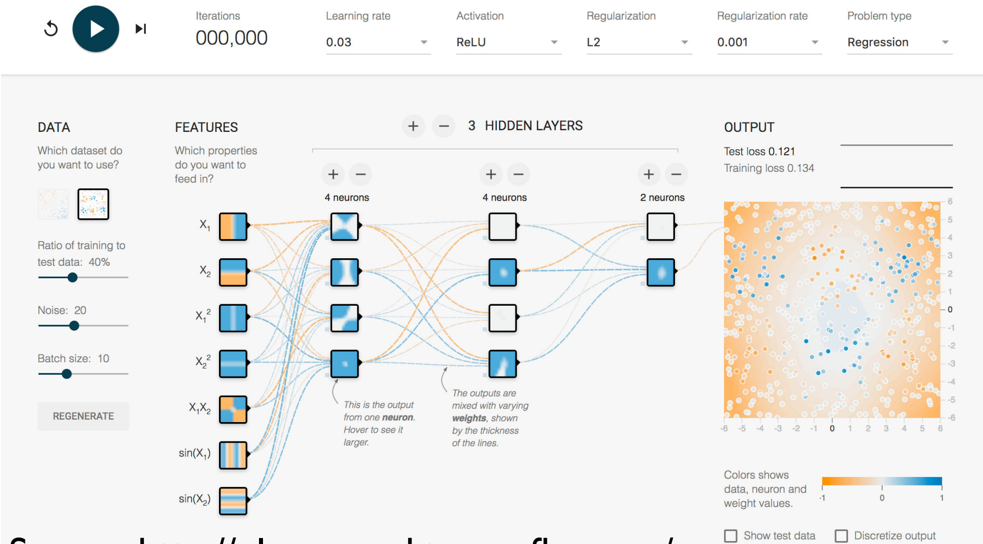
Informally: Making predictions from data

Formally: The construction of a statistical model that is an underlying distribution from which the data is drawn from, or using which we can classify the data into different categories.

Elements of Machine Learning

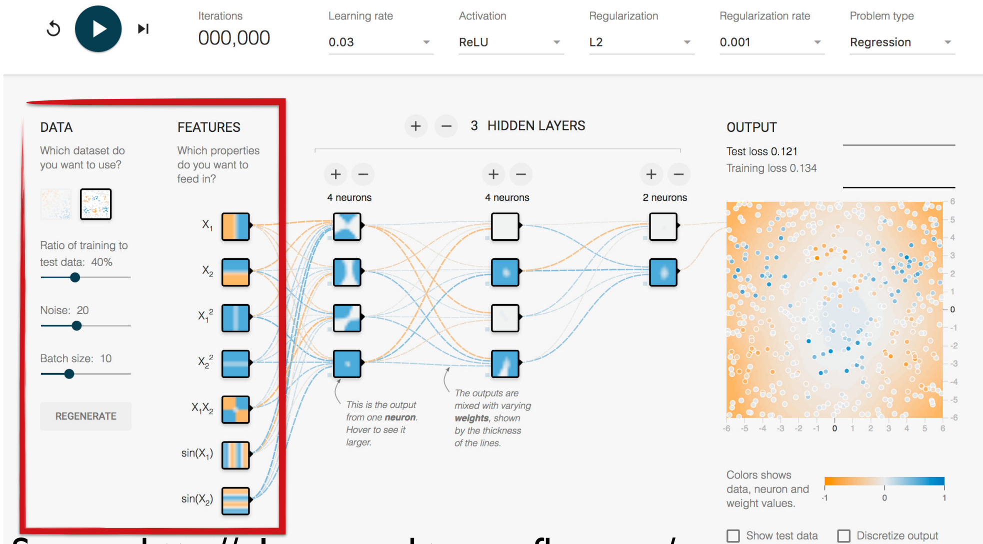


Neural Networks



Source: http://playground.tensorflow.org/

Neural Networks



Source: http://playground.tensorflow.org/

Common representation

IMAGE/ VIDEO	TEXT/ COMMENT	TIME SERIES
SYSTEM LOGS	NETWORK	TABULAR/ RATING

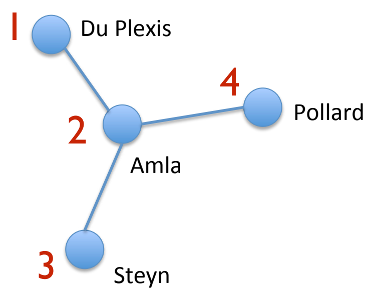
Is there a common way to represent data of different modalities ?

Text to matrix

- Document- Word Matrix
- Document 1:“AACCBBAAA”
- Document 2:“CCAABBDD”

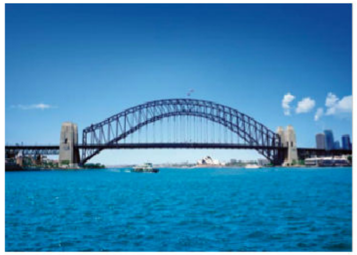
$$\begin{bmatrix} A & B & C & D \\ 5 & 2 & 2 & 0 \\ 2 & 2 & 2 & 2 \end{bmatrix}$$

Network data



$$
\begin{array}{cc}
 & \text{Nodes} \\
\text{Nodes} & \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}
\end{array}
$$

Image data


www.sydney.visitorsbureau.com.au

700 x 500

4	45	6
6	12	33
22	17	44

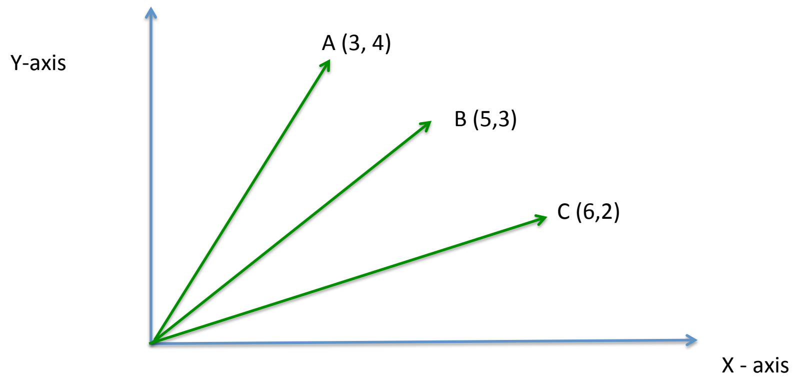
4	45	6	6	12	33	22	17	44

Similarity Computation

- We can now represent most data types as a matrix.
- A special case of a matrix is a vector.
- Now lets compute similarities with these objects.

Similarity Computation

How can we quantify
similarity between A, B and C ?



Similarity Computation

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- Dot product
  $x = (x_1, x_2, ..., x_n); \quad y = (y_1, y_2, ..., y_n);$
  $x.y = (x_1 y_1 + x_2 y_2 + ... + x_n y_n);$

- Norm (length) of a vector
  $\|x\| = (x.x)^{1/2} = (x_1.x_1 + x_2.x_2 + x_n.x_n)^{1/2}$

Similarity Computation

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- The similarity between two vectors x and y is given by

  $sim(x, y) = x.y/(\|x\| \, \|y\|)$

Similarity Computation

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- Can $sim(x, y) > 1$?
  $sim(x, y) = x.y/(\|x\| \, \|y\|)$

- No! Because of Cauchy-Schwarz inequality:

$$|x \cdot y| \leq \|x\| \|y\|.$$

Image search engine

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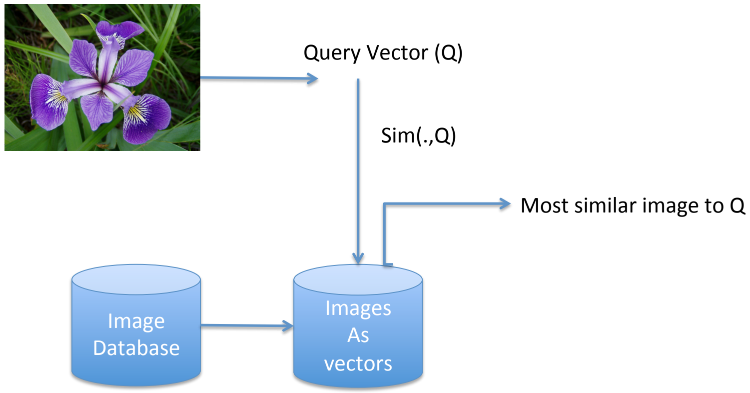

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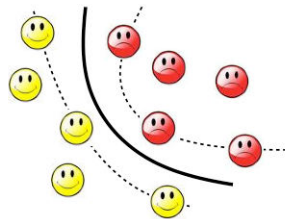

Matrix Algebra

Why Matrix Algebra?

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- Data Mining: Computation for large data sets
- Key idea: Data Reduction leads to "Knowledge Discovery"
- Matrix algebra provides simple algorithms with great power for data management, e.g., data reduction or data summarisation.

Why Matrix Algebra?

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- In database management, the fundamental entity is a *relation*.
  - SQL (relational algebra) is a collection of operations on relations – Select, project, join, group-by
- In machine learning and data mining, the fundamental entity is a *matrix*
  - We therefore need to know the basic operations on matrices
  - One important application is to summarise data or extract patterns from data or compress data
  - In SIT several people apply data mining for different domains: Chinese medicine, bioinformatics, student learning, multimedia, image processing, quality of cloud computing service, text analysis, medical imaging, robotics

Suggested book

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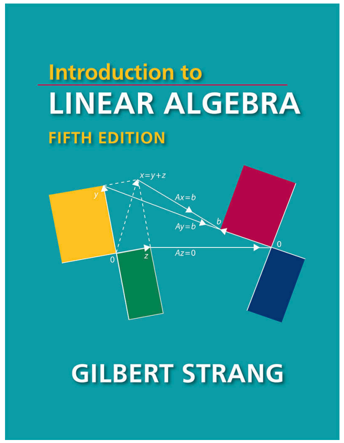

http://math.mit.edu/~gs/linearalgebra/

Numbers vs Matrices

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Numbers

- Can add and subtract numbers
- Multiply numbers
- Divide two numbers a/b as long as b is not equal to 0.
- Can factorise positive numbers into product of primes

Matrices

- Can add and subtract compatible metrics
- Multiply and divide matrices
- Division of matrices is complicated
- Can factorise any matrix to get data patterns (using a technique called Singular Value Decomposition)

Linear Algebra

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- Area in maths that deals with *vector spaces* and *linear mappings* between these spaces
- The generalisation of LA to infinite dimensions is known as *functional analysis*

2	4	7	3	6

D = 5

Linear algebra

2	4	7	3	6	9	…

D = ∞

Functional analysis

Definition for vector space: 8 Axioms

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- Associativity of addition: $(u+v)+w = u+(v+w)$
- Commutativity of addition: $u+v = v+u$
- Identity element of addition: $\exists 0, v+0 = v$
- Inverse elements of addition: $\forall v, \exists -v, v+(-v) = 0$
- Compatibility of scalar multiplication with field multiplication: (a and b are scalars) $a(bv) = (ab)v$
- Identity element of scalar multiplication: $\exists 1, 1v = v$
- Distributivity of scalar multiplication with respect to vector addition: (a is a scalar) $a(u+v) = au+av$
- Distributivity of scalar multiplication with respect to field addition: (a and b are scalers) $(a+b)v = av+bv$

Basics I

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$$S = \begin{bmatrix} 3 & 0 & 1 \\ 0 & 2 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

- This is a *3 x 3* matrix.
- In general $m \times n$.
  - m rows and n columns
  - Square matrix when $m = n$
- Each row or column could represent one object. If rows are objects then columns are features/attributes/components

Basics II

- Identity matrix I $\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

- If A is a square matrix, $AI = IA = A$
- I is an example of a **diagonal** matrix.

- If $A = [a_1, ...a_m]$ is matrix where a_i are the columns, then
  - A is orthogonal if $a_i.a_j = 0$ for $i \neq j$
  - A is orthonormal if above and $a_i.a_i = 1$

Basics III

- Every vector can be written as a linear combination of some finitely many "special" vectors.
- These are called basis-vectors.

$$S = \begin{bmatrix} 3 \\ 2 \\ 2 \end{bmatrix} = 3 \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} + 2 \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} + 2 \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

Linear independence

- Intuitively, a set of vectors is linearly independent if any element of the set cannot be expressed as a linear combination of the others.
- The columns are not linearly independent:

$$S = \begin{bmatrix} 3 & 0 & 1 \\ 0 & 2 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Exercise

Given $v = (1, 2, 3)$, calculate:

1. The length of v
2. A unit vector in the same direction as v
3. A set orthogonal bases for v
4. A vector perpendicular to v

Solution

Given $v = (1, 2, 3)$, calculate:

1. The length of v is $\sqrt{14}$
2. A unit vector in the same direction $(1/\sqrt{14}, 2/\sqrt{14}, 3/\sqrt{14})$
3. A set orthogonal bases: (1, 0, 0); (0, 1, 0), (0, 0, 1)
4. A vector perpendicular to $v = (-1, -1, 1)$

Determinant

- Matrix A maps the unit n-cube to the *n*-dimensional parallelotope defined by the column vectors
- The determinant gives the signed n-dimensional volume of this parallelotope
- For 2 by 2 matrix

$$|A| = \begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - bc$$

$$|A| = \begin{vmatrix} a & b & c \\ d & e & f \\ g & h & i \end{vmatrix} = a \begin{vmatrix} e & f \\ h & i \end{vmatrix} - b \begin{vmatrix} d & f \\ g & i \end{vmatrix} + c \begin{vmatrix} d & e \\ g & h \end{vmatrix}$$

$$= aei + bfg + cdh - ceg - bdi - afh.$$

Rank of a matrix I

- Given a matrix M, the **rank** of a matrix is the maximum number of linearly independent columns.
- A rank 2 matrix: $$S = \begin{bmatrix} 3 & 0 & 1 \\ 0 & 2 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Rank of a matrix II

- Can we automatically determine the rank of a matrix

$$S = \begin{bmatrix} 3 & 1 & 3.5 \\ 2 & 2 & 3 \\ 4 & 2 & 5 \end{bmatrix}$$

- Why is rank important anyways…?

Transpose of a matrix

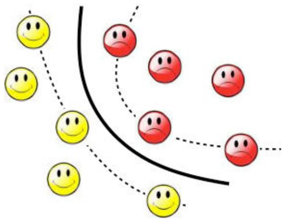
- The transpose of a matrix A, denoted A^T is another matrix B such that $B(i,j) = A(j,i)$ (just flip the matrix)
- The transpose of S is S^T

$$S = \begin{bmatrix} 3 & 3 & 1 \\ 0 & 2 & 4 \\ 0 & 0 & 0 \end{bmatrix} \qquad S^T = \begin{bmatrix} 3 & 0 & 0 \\ 3 & 2 & 0 \\ 1 & 4 & 0 \end{bmatrix}$$

Exercise

- What is the rank of the following matrix:

$$\begin{bmatrix} 1 & 2 & 3 \\ 3 & 4 & 5 \\ 5 & 4 & 3 \\ 0 & 2 & 4 \\ 1 & 3 & 5 \end{bmatrix}$$



Matrix Decompositions

Eigen Decomposition

- For any square matrix A we say that λ is an eigenvalue and $\mathbf{u}$ is its eigenvector if

$$A\mathbf{u} = \lambda\mathbf{u}, \quad \mathbf{u} \neq 0.$$

- Stacking up all eigenvectors/values gives

$$AU = U\Lambda = \begin{bmatrix} | & | & & | \\ \mathbf{u}_1 & \mathbf{u}_2 & \dots & \mathbf{u}_n \\ | & | & & | \end{bmatrix} \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n \end{bmatrix}$$

Eigen Decomposition

- If A is symmetric, all its eig-vals are real, and all its eig-vecs are orthonormal, $\mathbf{u}_i^T \mathbf{u}_j = \delta_{ij}$
- Hence $U^T U = U U^T = I, \quad |U|^2 = 1.$
- and $A = U \Lambda U^T = \sum_{i=1}^{n} \lambda_i \mathbf{u}_i \mathbf{u}_i^T$

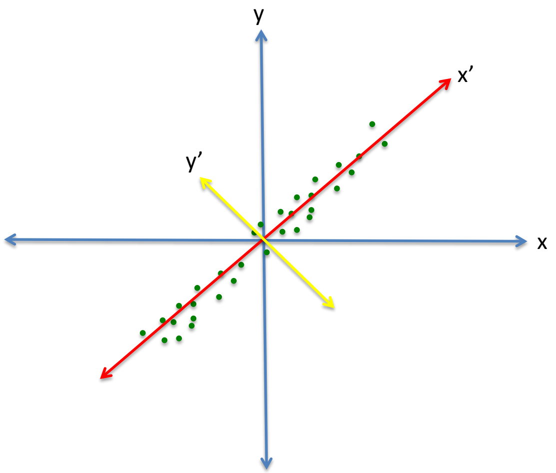
$$A = \begin{bmatrix} | & | & & | \\ \mathbf{u}_1 & \mathbf{u}_2 & \dots & \mathbf{u}_n \\ | & | & & | \end{bmatrix} \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n \end{bmatrix} \begin{bmatrix} — & \mathbf{u}_1^T & — \\ — & \mathbf{u}_2^T & — \\ & \vdots & \\ — & \mathbf{u}_n^T & — \end{bmatrix}$$

$$= \lambda_1 \begin{bmatrix} | \\ \mathbf{u}_1 \\ | \end{bmatrix} \begin{bmatrix} — & \mathbf{u}_1^T & — \end{bmatrix} + \dots + \lambda_n \begin{bmatrix} | \\ \mathbf{u}_n \\ | \end{bmatrix} \begin{bmatrix} — & \mathbf{u}_n^T & — \end{bmatrix}$$

Principal component

- Given a data matrix $X \in \mathbb{R}^{n \times d}$, the principle components of X are the eigenvectors of $X^\top X$
- Principal component analysis (PCA) for X is to find the eigenvectors and eigenvalues of the matrix $X^\top X$.

Geometric intuition



Exercise

- Find the eigenvectors and eigenvalues for the following matrix

$$\begin{bmatrix} 3 & 2 \\ 2 & 6 \end{bmatrix}$$

Singular Value Decomposition

- Given **any** real matrix X of size (m, n) it can be expressed as:

$$X = \underbrace{U}_{m \times r}\underbrace{\Sigma}_{r \times r}\underbrace{V^T}_{r \times n}$$

- r is the rank of matrix X
- U is a (m, r) column-orthonormal matrix
- V is a (n, r) column-orthonormal matrix
- Σ is diagonal r x r matrix

Singular Value Decomposition

$$X = \underbrace{U}_{m \times r}\underbrace{\Sigma}_{r \times r}\underbrace{V^T}_{r \times n}$$

$$X = \lambda_1 \mathbf{u}_1 \times \mathbf{v}_1^t + \lambda_2 \mathbf{u}_2 \times \mathbf{v}_2^t + \cdots + \lambda_r \mathbf{u}_r \times \mathbf{v}_r^t$$

SVD in Python

- One line command:

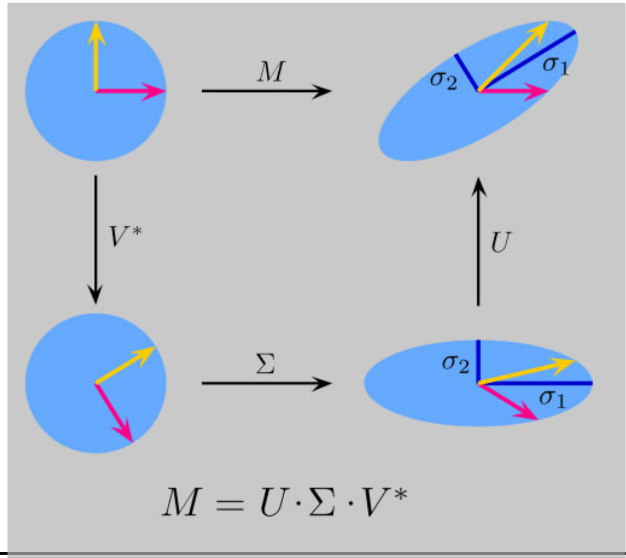
```
>>> U, s,V = np.linalg.svd(a, full_matrices = True)
```

$X =$

	Wed	Thur	Friday	Sat	Sun
ABC Ltd	1	1	1	0	0
DEF Ltd	2	2	2	0	0
GHI Inc	1	1	1	0	0
KLM Co	5	5	5	0	0
Smith	0	0	0	2	2
Johnson	0	0	0	3	3
Thompson	0	0	0	1	1

$$X = \begin{bmatrix} 0.18 & 0 \\ 0.36 & 0 \\ 0.18 & 0 \\ 0.90 & 0 \\ 0 & 0.53 \\ 0 & 0.80 \\ 0 & 0.27 \end{bmatrix} \times \begin{bmatrix} 9.64 & 0 \\ 0 & 5.29 \end{bmatrix} \times \begin{bmatrix} 0.58 & 0.58 & 0.58 & 0 & 0 \\ 0 & 0 & 0 & 0.71 & 0.71 \end{bmatrix}$$

SVD as a sequence of operations



Qualitative use of SVD

$$X = \begin{bmatrix} 0.18 & 0 \\ 0.36 & 0 \\ 0.18 & 0 \\ 0.90 & 0 \\ 0 & 0.53 \\ 0 & 0.80 \\ 0 & 0.27 \end{bmatrix} \times \begin{bmatrix} 9.64 & 0 \\ 0 & 5.29 \end{bmatrix} \times \begin{bmatrix} 0.58 & 0.58 & 0.58 & 0 & 0 \\ 0 & 0 & 0 & 0.71 & 0.71 \end{bmatrix}$$

- Two kinds of customers (businesses and individuals)
- Two kinds of days (weekday and weekends)
- U is a customer-pattern matrix
- V is a day-pattern matrix
- $V(1,2) = 0$ means Wednesday has zero similarity with the "weekend pattern."

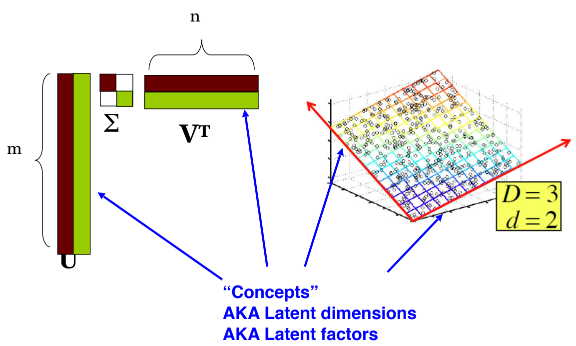
Data reduction with SVD

- Now how can we use an SVD decomposition…
- The first way is **qualitative**…
  - Customer-day pattern; or Customer-Pattern-day matrix…
- The second way is **quantitative**…
  - When X is very large, we can compress X into a smaller matrix but still retain important information…

Example: Users to Movies

- $A = U\Sigma V^T$ - example: Users to Movies

$$\begin{array}{cc} & \begin{array}{ccccc} \text{Matrix} & \text{Alien} & \text{Serenity} & \text{Casablanca} & \text{Amelie} \end{array} \\ \begin{array}{c} \text{SciFi} \\ \\ \\ \\ \text{Romance} \\ \\ \\ \end{array} & \begin{bmatrix} \mathbf{1} & \mathbf{1} & \mathbf{1} & 0 & 0 \\ \mathbf{3} & \mathbf{3} & \mathbf{3} & 0 & 0 \\ \mathbf{4} & \mathbf{4} & \mathbf{4} & 0 & 0 \\ \mathbf{5} & \mathbf{5} & \mathbf{5} & 0 & 0 \\ 0 & \mathbf{2} & 0 & \mathbf{4} & \mathbf{4} \\ 0 & 0 & 0 & \mathbf{5} & \mathbf{5} \\ 0 & \mathbf{1} & 0 & \mathbf{2} & \mathbf{2} \end{bmatrix} \end{array} =$$



Example: Users to Movies

- $A = U\Sigma V^T$ - example: Users to Movies

***U* is "user-to-concept" similarity matrix**

SciFi-concept

Romance-concept

"strength" of the SciFi-concept

$$\begin{array}{cc} \text{Matrix} & \begin{array}{ccccc} \text{Alien} & \text{Dr Strange} & \text{American} & \text{Capt} & \text{Amelie} \end{array} \\ \begin{array}{c} \text{SciFi} \\ \\ \\ \\ \text{Romance} \\ \\ \\ \end{array} & \begin{bmatrix} \mathbf{1} & \mathbf{1} & \mathbf{1} & 0 & 0 \\ \mathbf{3} & \mathbf{3} & \mathbf{3} & 0 & 0 \\ \mathbf{4} & \mathbf{4} & \mathbf{4} & 0 & 0 \\ \mathbf{5} & \mathbf{5} & \mathbf{5} & 0 & 0 \\ 0 & \mathbf{2} & 0 & \mathbf{4} & \mathbf{4} \\ 0 & 0 & 0 & \mathbf{5} & \mathbf{5} \\ 0 & \mathbf{1} & 0 & \mathbf{2} & \mathbf{2} \end{bmatrix} \end{array} = \begin{bmatrix} \mathbf{0.13} & 0.02 & -0.01 \\ \mathbf{0.41} & 0.07 & -0.03 \\ \mathbf{0.55} & 0.09 & -0.04 \\ \mathbf{0.68} & 0.11 & -0.05 \\ 0.15 & \mathbf{-0.59} & \mathbf{0.65} \\ 0.07 & \mathbf{-0.73} & \mathbf{-0.67} \\ 0.07 & \mathbf{-0.29} & \mathbf{0.32} \end{bmatrix} \times \begin{bmatrix} \mathbf{12.4} & 0 & 0 \\ 0 & \mathbf{9.5} & 0 \\ 0 & 0 & \mathbf{1.3} \end{bmatrix} \times$$

$$\begin{bmatrix} \mathbf{0.56} & \mathbf{0.59} & \mathbf{0.56} & 0.09 & 0.09 \\ 0.12 & -0.02 & 0.12 & \mathbf{-0.69} & \mathbf{-0.69} \\ 0.40 & \mathbf{-0.80} & 0.40 & 0.09 & 0.09 \end{bmatrix}$$

Example: Users to Movies

- $A = U\Sigma V^T$ - example:

SciFi-concept

V is "movie-to-concept" similarity matrix

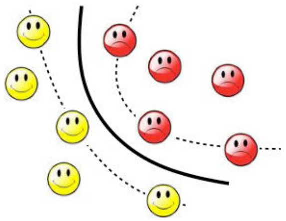
$$
\begin{array}{c|c}
 & \text{Matrix} \quad \text{Alien} \quad \text{Serenity} \quad \text{Casablanca} \quad \text{Amelie} \\
\begin{array}{c}\text{SciFi}\\ \\ \\ \\ \text{Romance}\\ \\ \\ \end{array} &
\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 2 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 1 & 0 & 2 & 2 \end{bmatrix}
\end{array}
=
\begin{bmatrix} \mathbf{0.13} & 0.02 & -0.01 \\ \mathbf{0.41} & 0.07 & -0.03 \\ \mathbf{0.55} & 0.09 & -0.04 \\ \mathbf{0.68} & 0.11 & -0.05 \\ 0.15 & \mathbf{-0.59} & \mathbf{0.65} \\ 0.07 & \mathbf{-0.73} & \mathbf{-0.67} \\ 0.07 & \mathbf{-0.29} & \mathbf{0.32} \end{bmatrix}
\times
\begin{bmatrix} \mathbf{12.4} & 0 & 0 \\ 0 & \mathbf{9.5} & 0 \\ 0 & 0 & \mathbf{1.3} \end{bmatrix}
\times
\begin{bmatrix} \mathbf{0.56} & \mathbf{0.59} & \mathbf{0.56} & 0.09 & 0.09 \\ 0.12 & -0.02 & 0.12 & \mathbf{-0.69} & \mathbf{-0.69} \\ 0.40 & \mathbf{-0.80} & 0.40 & 0.09 & 0.09 \end{bmatrix}
$$

SciFi-concept

Interpretation

'**movies**', '**users**' and '**concepts**':

- ***U***: user-to-concept similarity matrix
- ***V***: movie-to-concept similarity matrix
- Σ: its diagonal elements: 'strength' of each concept



Data Reduction and Matrix compression

Spectral representation

- Matrix X can also be written as:

$$X = \lambda_1 \mathbf{u}_1 \times \mathbf{v}_1^t + \lambda_2 \mathbf{u}_2 \times \mathbf{v}_2^t + \cdots + \lambda_r \mathbf{u}_r \times \mathbf{v}_r^t$$

- The above is called **spectral** representation.

$$X = 9.64 \times \begin{bmatrix} 0.18 \\ 0.36 \\ 0.18 \\ 0.90 \\ 0 \\ 0 \\ 0 \end{bmatrix} \times \begin{bmatrix} 0.58 & 0.58 & 0.58 & 0 & 0 \end{bmatrix} + 5.29 \times \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0.53 \\ 0.80 \\ 0.27 \end{bmatrix} \times \begin{bmatrix} 0 & 0 & 0.71 & 0.71 \end{bmatrix}$$

Example: compression of X

$$X = \underbrace{U}_{m \times r}\underbrace{\Sigma}_{r \times r}\underbrace{V^T}_{r \times n}$$

- Size of $X = mn$
- Size of $U + \Sigma + V$ is $mr + r + nr$
- Thus compression ratio is

$$\frac{mr + r + nr}{mn} = \frac{r(m+1+n)}{mn} \approx \frac{rm}{mn} = \frac{r}{n}$$

- Can we do better?

Example: compression of X

- To get better compression we should look at the λ values.
  - These are called **singular values**.
- We can arrange them in descending order:

$$\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_r > 0$$

- Now recall….

$$X = \lambda_1 \mathbf{u}_1 \times \mathbf{v}_1^t + \lambda_2 \mathbf{u}_2 \times \mathbf{v}_2^t + \cdots + \lambda_r \mathbf{u}_r \times \mathbf{v}_r^t$$

Example: compression of X

- Now a compact way of writing the spectral representation is:

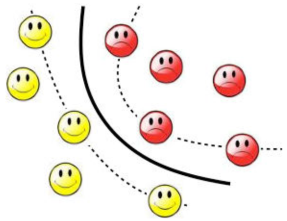
$$X = \sum_{i=1}^{r} \lambda_i \mathbf{u}_i \times \mathbf{v}_i^t$$

- However, can approximate it as:

$$\hat{X} = \sum_{i=1}^{k} \lambda_i \mathbf{u}_i \times \mathbf{v}_i^t$$

- This new compression ratio is:

$$\frac{mk + k + nk}{mn} = \frac{k(m+1+n)}{mn} \approx \frac{km}{mn} = \frac{k}{n} \leqslant \frac{r}{n}$$



Thanks!