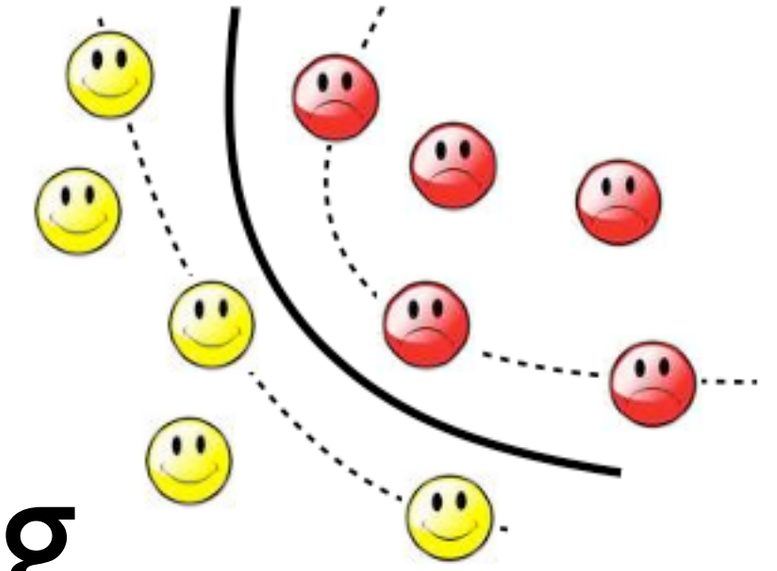
THE UNIVERSITY OF SYDNEY



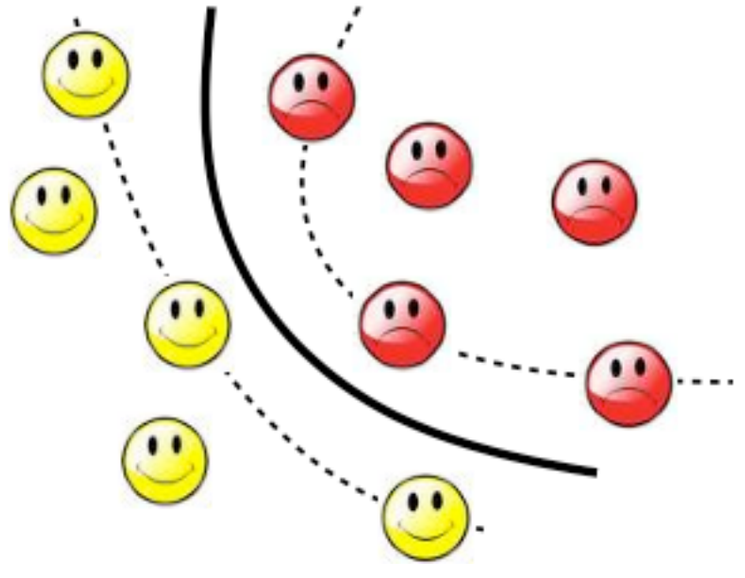
Machine Learning and Data Mining

(COMP 5318)

Basic Matrix Analysis and Singular Value Decomposition

A/Prof Fabio Ramos
Dr Roman Marchant

THE UNIVERSITY OF SYDNEY



Review

What is Machine Learning?

THE UNIVERSITY OF SYDNEY

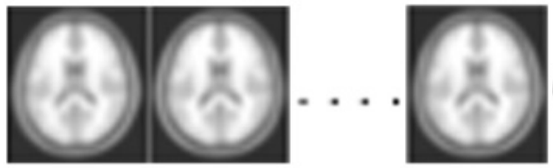
Informally: Making predictions from data

Formally: The construction of a statistical model that is an underlying distribution from which the data is drawn from.

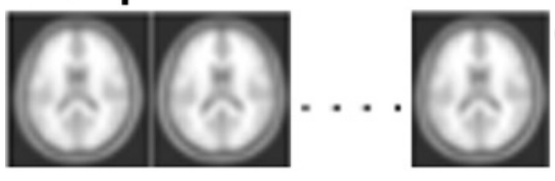
Elements of Machine Learning

THE UNIVERSITY OF SYDNEY

Group 1

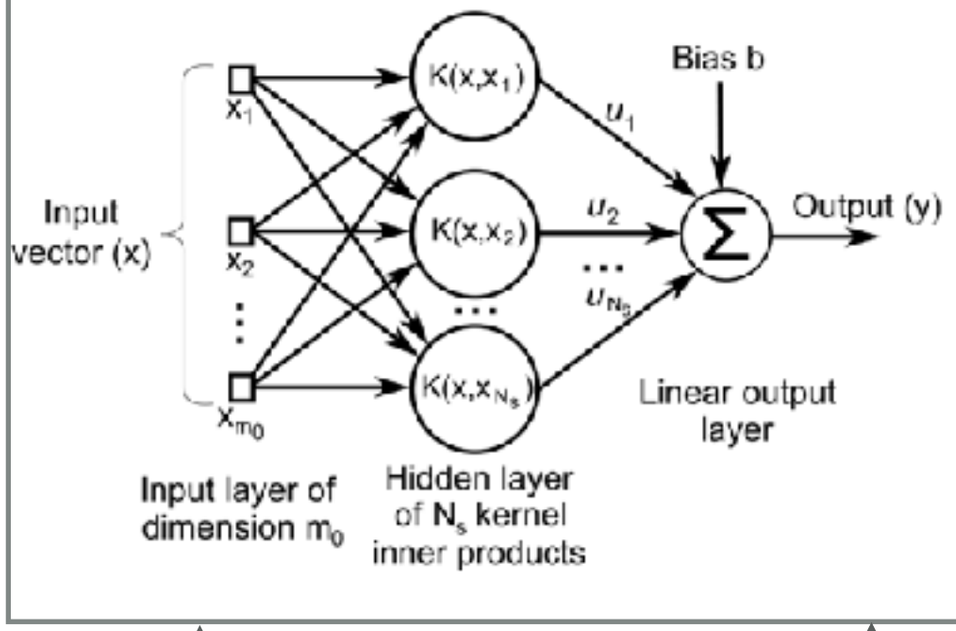


Group 2

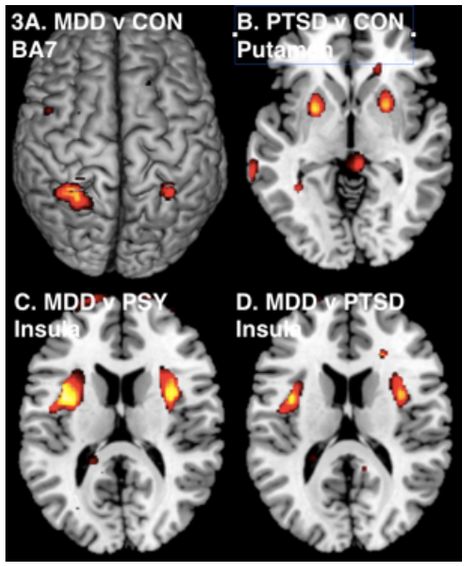


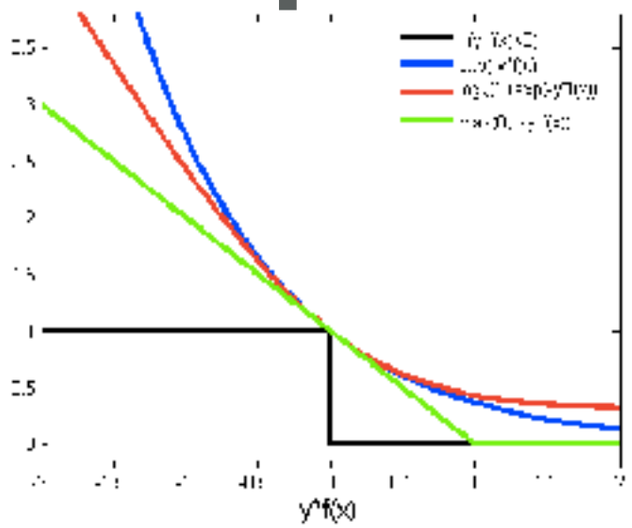
Data

Mathematical Model

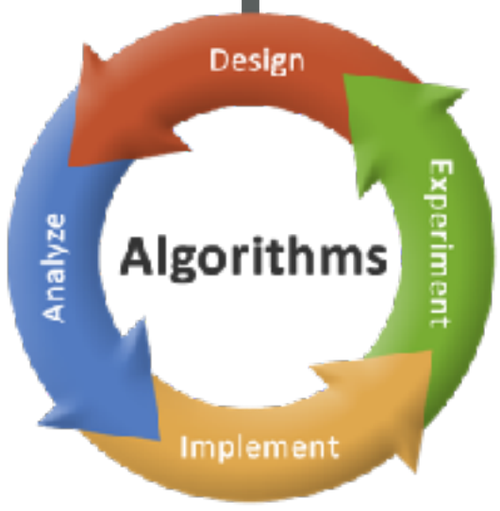


Predictions/Patterns



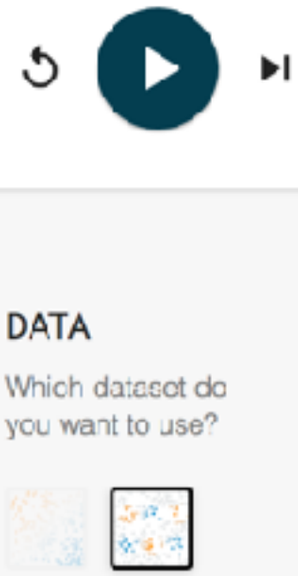


Objective function



Neural Networks

THE UNIVERSITY OF SYDNEY



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

Common representation

THE UNIVERSITY OF SYDNEY

IMAGE/ VIDEO

TEXT/ COMMENT

TIME SERIES

SYSTEM LOGS

NETWORK

TABULAR/ RATING

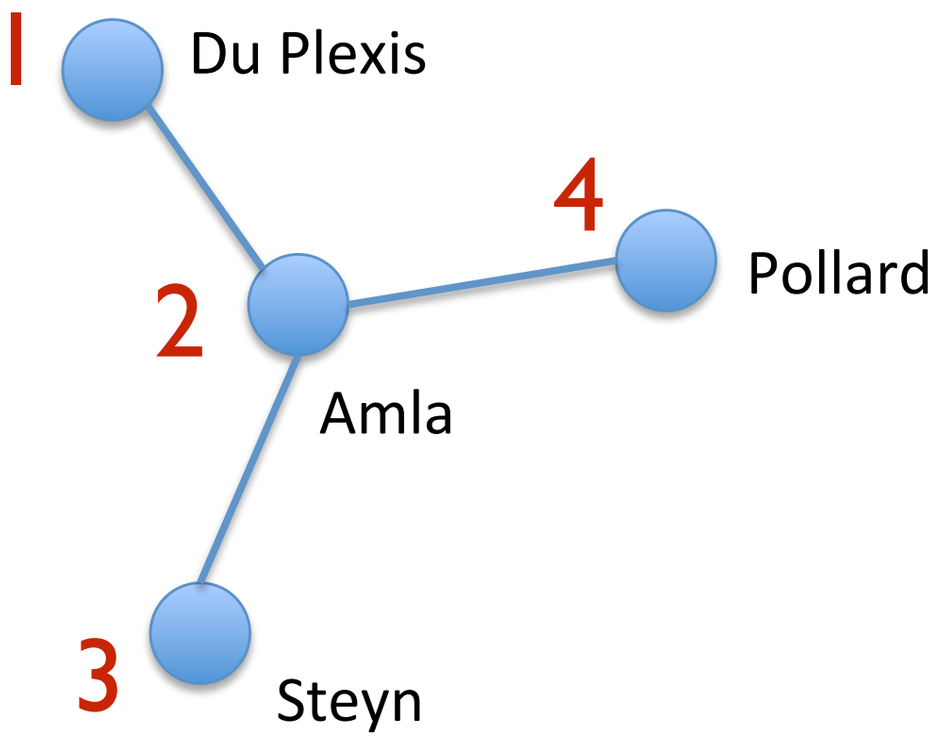
Is there a common way to represent data of different modalities ?

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



Nodes

Nodes

$$\begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

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

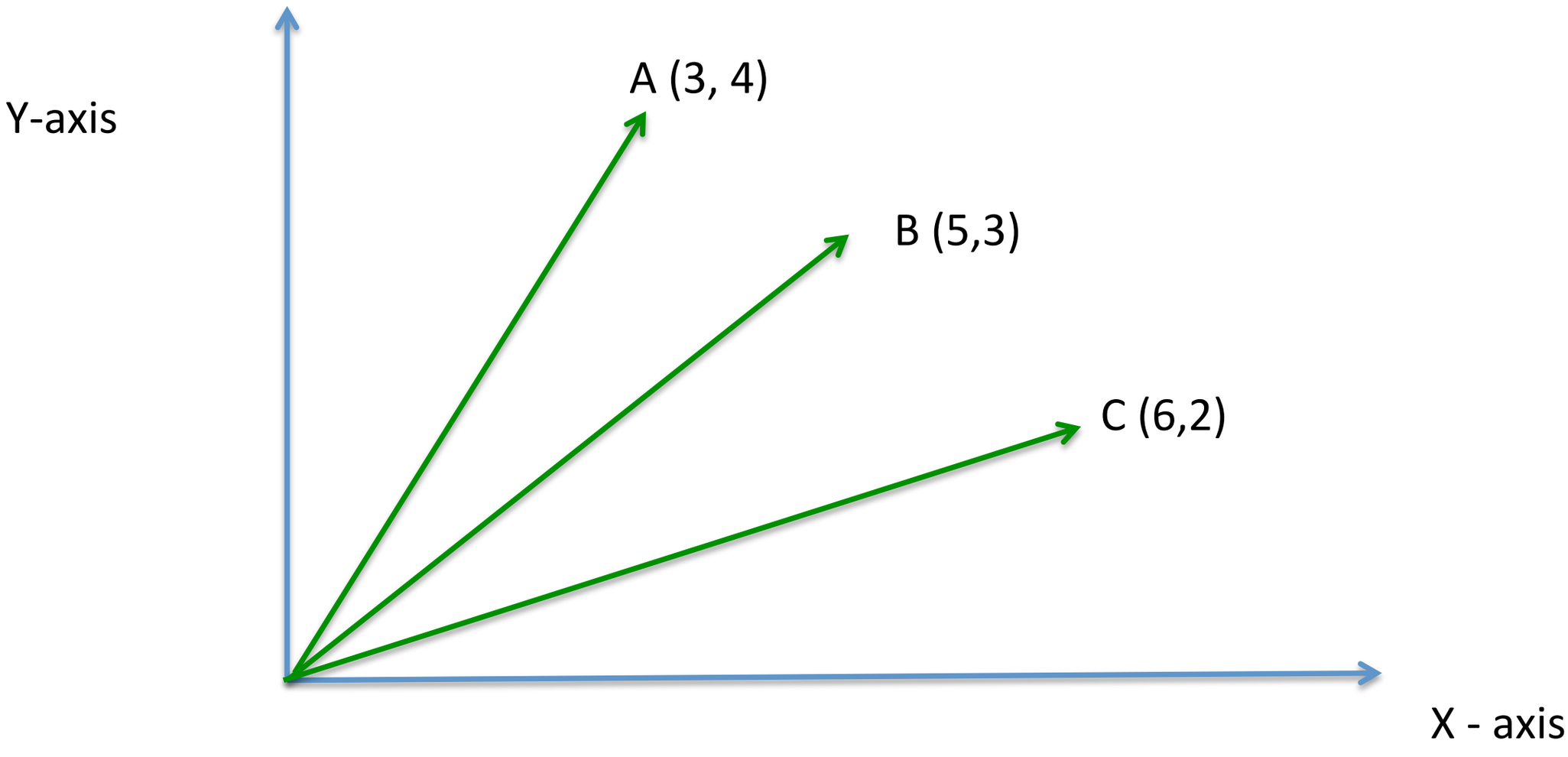
Similarity Computation

THE UNIVERSITY OF SYDNEY

- 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

- 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

$$\|x\| = (x.x)^{1/2} = (x_1.x_1 + x_2.x_2 + x_n.x_n)^{1/2}$$

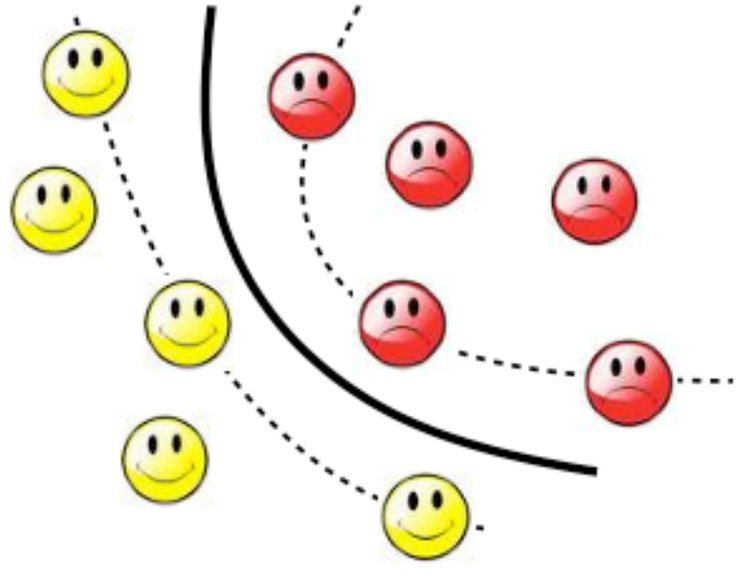
Similarity Computation

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

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

Image search engine

THE UNIVERSITY OF SYDNEY



Matrix Algebra and Decompositions

Why Matrix Algebra?

THE UNIVERSITY OF SYDNEY

- 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 reduction or data summarisation.

ML algorithms as linear algebra operations

input: X (inputs), $\mathbf{y}$ (targets), k (covariance function), σ_n^2 (noise level), $\mathbf{x}_*$ (test input)

2: $L := \text{cholesky}(K + \sigma_n^2 I)$

$\boldsymbol{\alpha} := L^\top \backslash (L \backslash \mathbf{y})$

4: $\bar{f}_* := \mathbf{k}_*^\top \boldsymbol{\alpha}$ } predictive mean eq. (2.25)

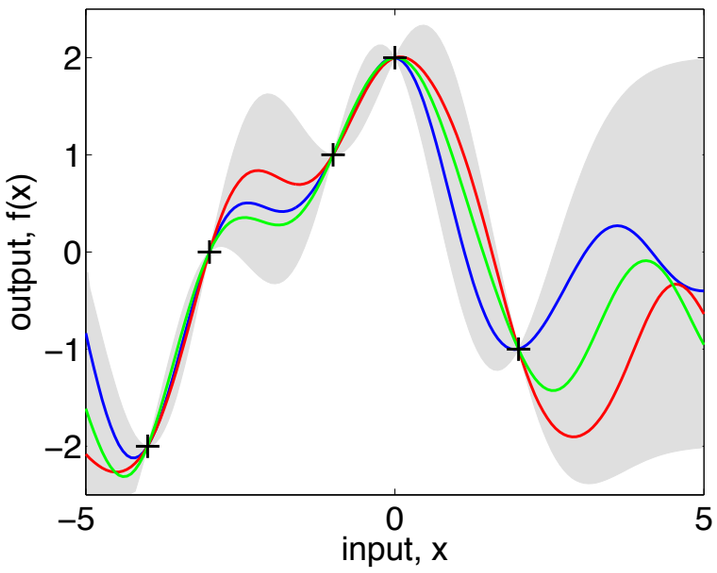
$\mathbf{v} := L \backslash \mathbf{k}_*$

6: $\mathbb{V}[f_*] := k(\mathbf{x}_*, \mathbf{x}_*) - \mathbf{v}^\top \mathbf{v}$ } predictive variance eq. (2.26)

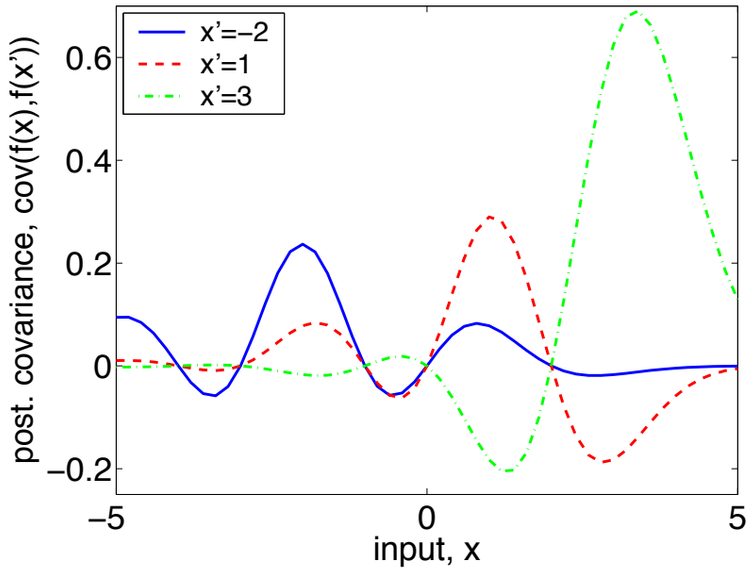
$\log p(\mathbf{y}|X) := -\frac{1}{2}\mathbf{y}^\top \boldsymbol{\alpha} - \sum_i \log L_{ii} - \frac{n}{2}\log 2\pi$ eq. (2.30)

8: **return**: $\bar{f}_*$ (mean), $\mathbb{V}[f_*]$ (variance), $\log p(\mathbf{y}|X)$ (log marginal likelihood)

Algorithm 2.1: Predictions and log marginal likelihood for Gaussian process regression. The implementation addresses the matrix inversion required by eq. (2.25) and (2.26) using Cholesky factorization, see section A.4. For multiple test cases lines 4-6 are repeated. The log determinant required in eq. (2.30) is computed from the Cholesky factor (for large n it may not be possible to represent the determinant itself). The computational complexity is $n^3/6$ for the Cholesky decomposition in line 2, and $n^2/2$ for solving triangular systems in line 3 and (for each test case) in line 5.



(a), posterior

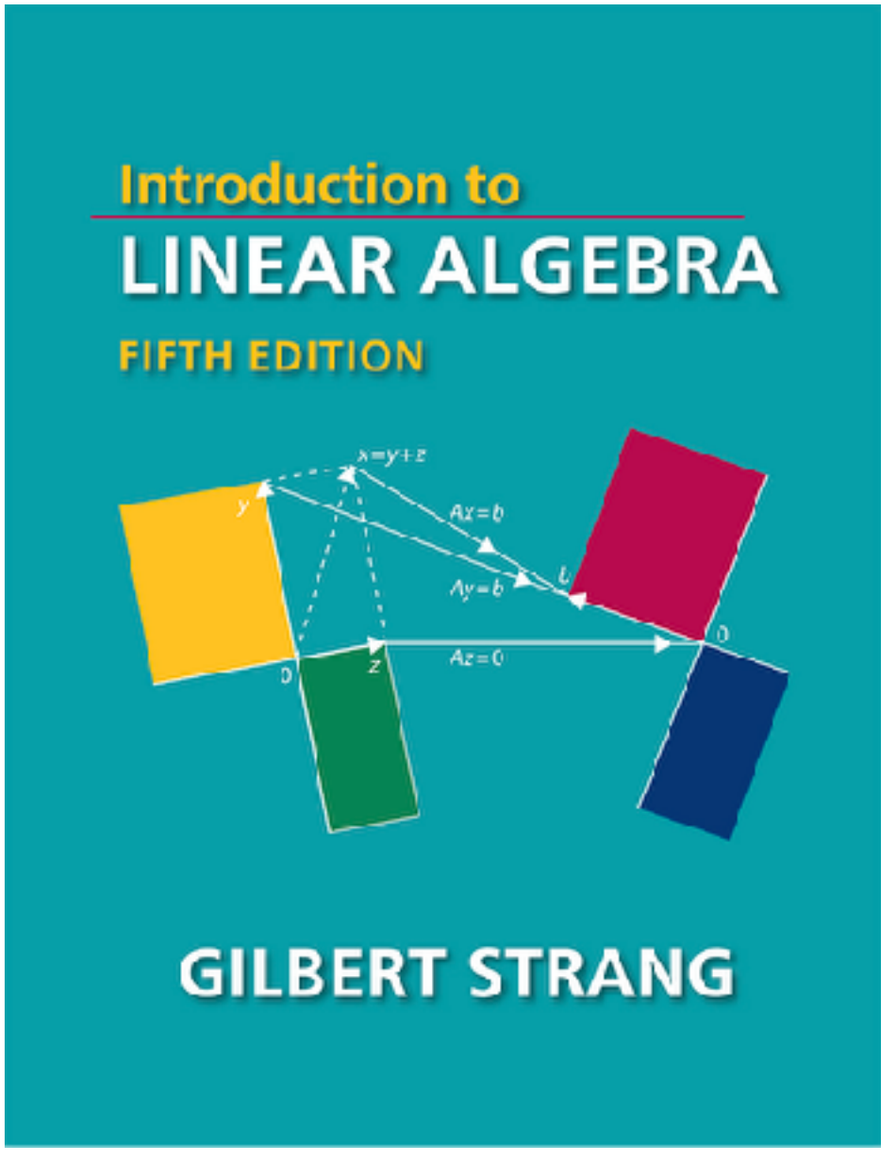


(b), posterior covariance

Matrix Algebra

- 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, the fundamental entity is a *matrix*
  - We therefore need to know the basic operations on matrices
  - Our goal 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



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

Numbers vs Matrices

THE UNIVERSITY OF SYDNEY

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

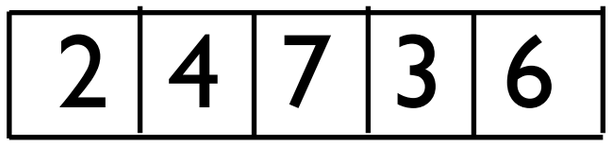
Matrices

- 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

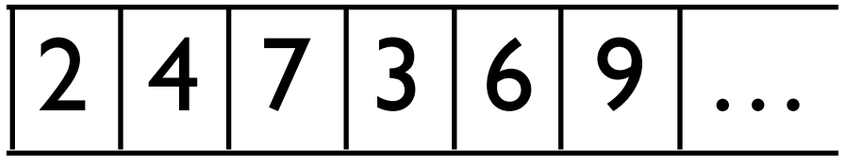
- Area in maths that deals with *vector spaces* and *linear mappings* between these spaces

- The generalisation of LA to infinite dimensions is known as *functional analysis*



D = 5

Linear algebra



D = ∞

Functional analysis

Basics I

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

- 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 <u>orthogonal</u> if $a_i.a_j = 0$ for $i \neq j$
  - A is <u>orthonormal</u> 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. An orthogonal basis for v
4. A vector perpendicular to v

Determinant

- The determinant of a square matrix is a single number telling us if the matrix is invertible, $detA^{-1} = 1/(detA)$
- For 2 by 2 matrix

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

- For 3 by 3 matrix

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

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

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:

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

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

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

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

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:

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

$m \times r$ $\quad$ $r \times r$ $\quad$ $r \times n$

- 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

SVD in Python

- One line command:

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

	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

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

Advice Querying on X

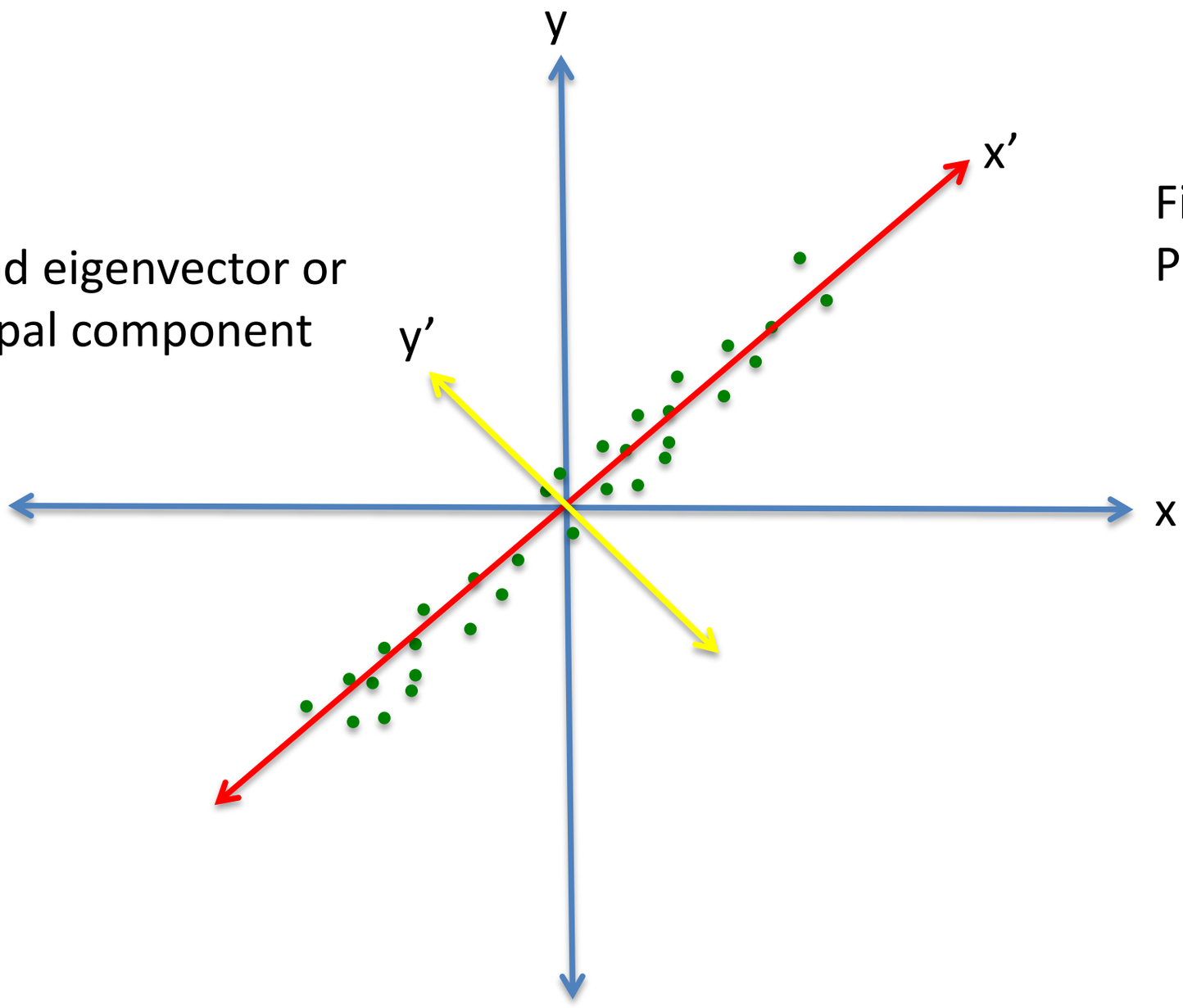
- Suppose X was very very large… (all mobile users in China)
- Now the query is "Find the amount spent by Jack Ma on Friday"
  - The original answer $X(JackMa, Friday)$
  - The approximate answer $\hat{X}(JackMa, Friday)$
  - Is it a good approximation?

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."

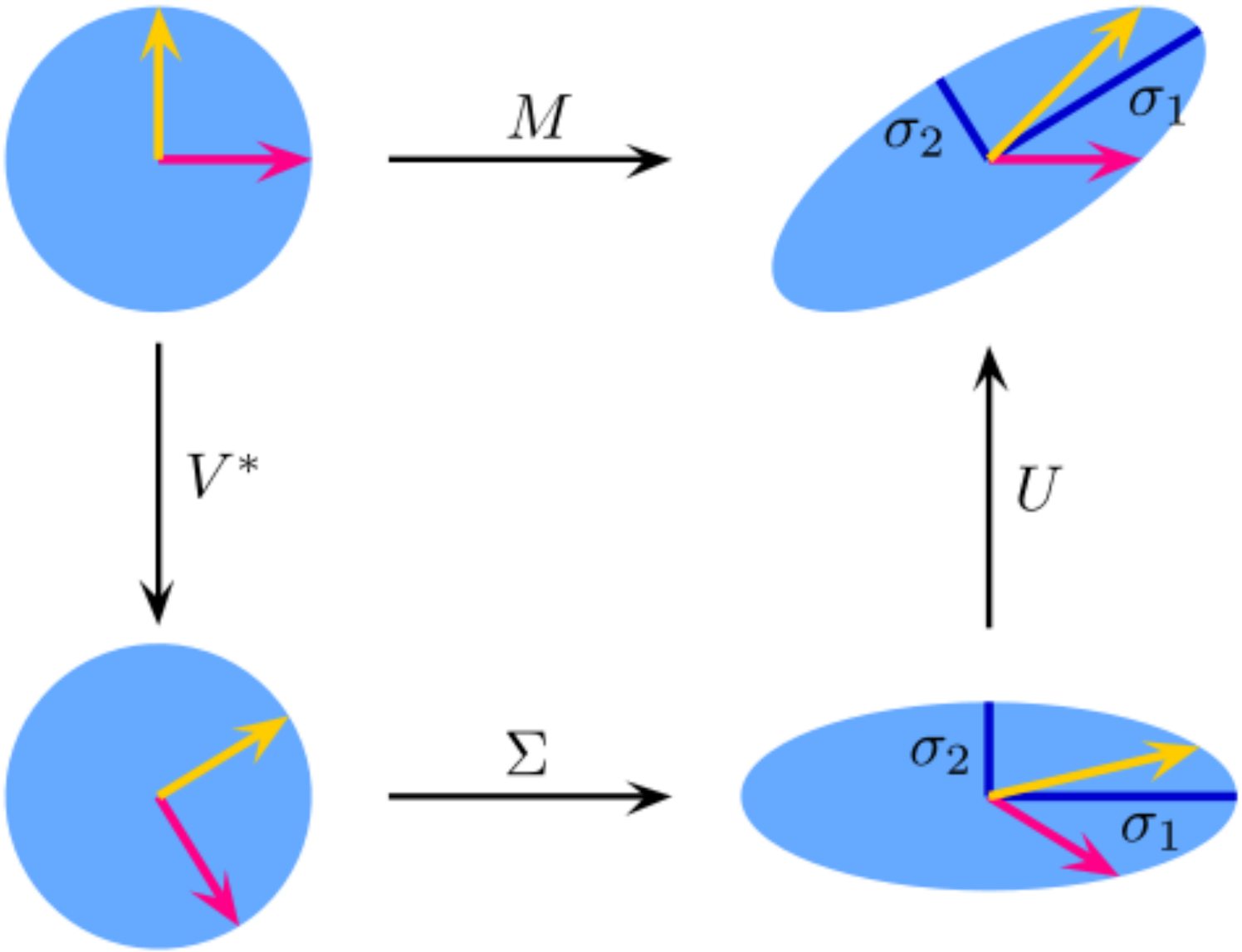
Geometric intuition



Second eigenvector or
Principal component

First eigenvector or
Principal component

SVD as a sequence of operations



$$M = U \cdot \Sigma \cdot V^*$$

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.

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

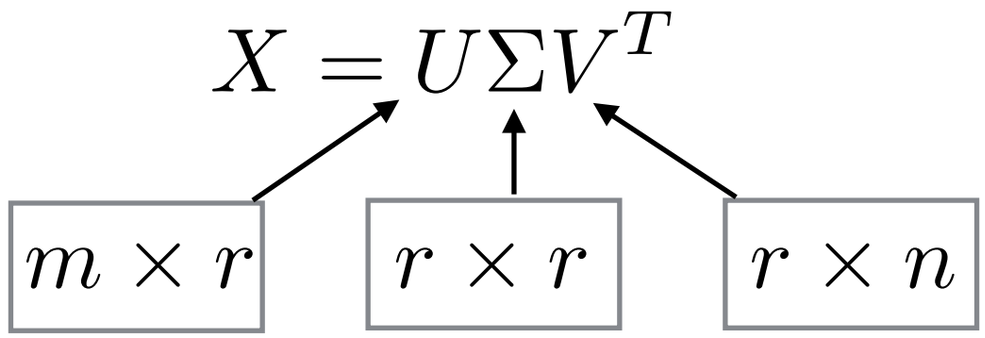
Data reduction with SVD

- 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: compression of X



- 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:

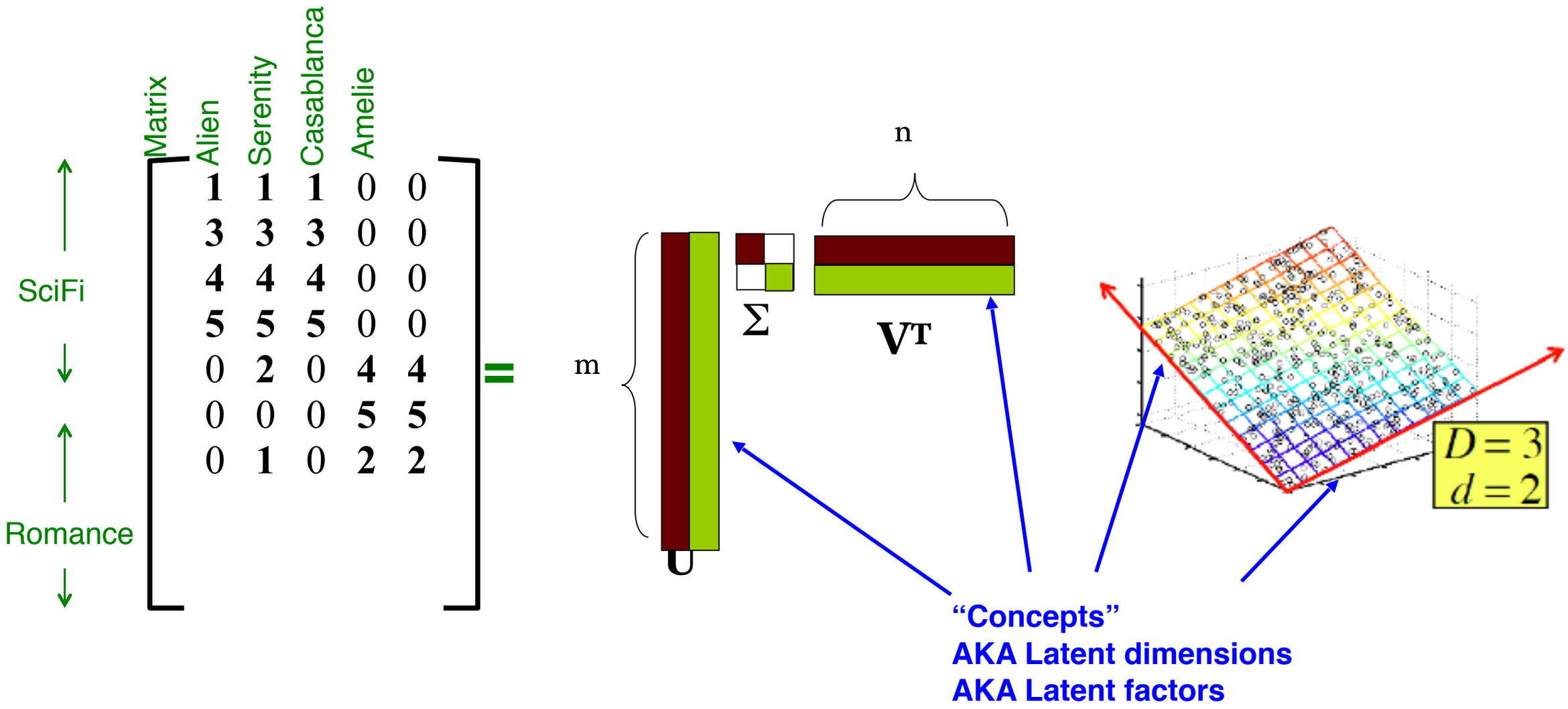
$$\hat{X} = \sum_{i=1}^{k} \lambda_i \mathbf{u}_i \times \mathbf{v}_i^t$$

- This new compression ratio is:

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

Example: Users to Movies

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



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

SciFi ↑

Romance ↑

	Matrix	Alien	Serenity	Casablanca	Amelie
	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

=

0.13	0.02	-0.01
0.41	0.07	-0.03
0.55	0.09	-0.04
0.68	0.11	-0.05
0.15	**-0.59**	**0.65**
0.07	**-0.73**	**-0.67**
0.07	**-0.29**	**0.32**

x

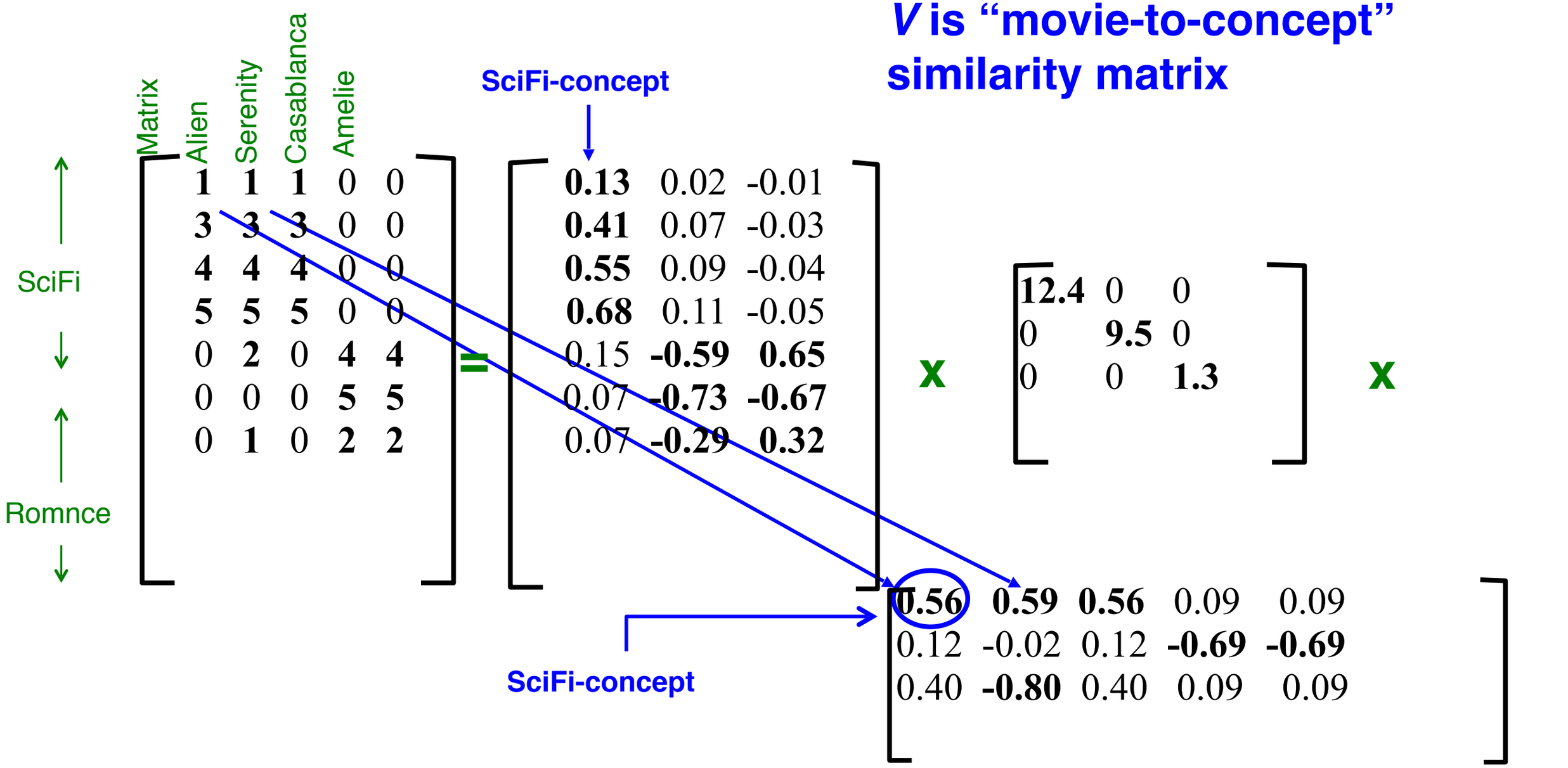
12.4	0	0
0	**9.5**	0
0	0	**1.3**

x

0.56	**0.59**	**0.56**	0.09	0.09
0.12	-0.02	0.12	**-0.69**	**-0.69**
0.40	**-0.80**	0.40	0.09	0.09

Example: Users to Movies

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



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

Tutorials: Mondays 8-9pm

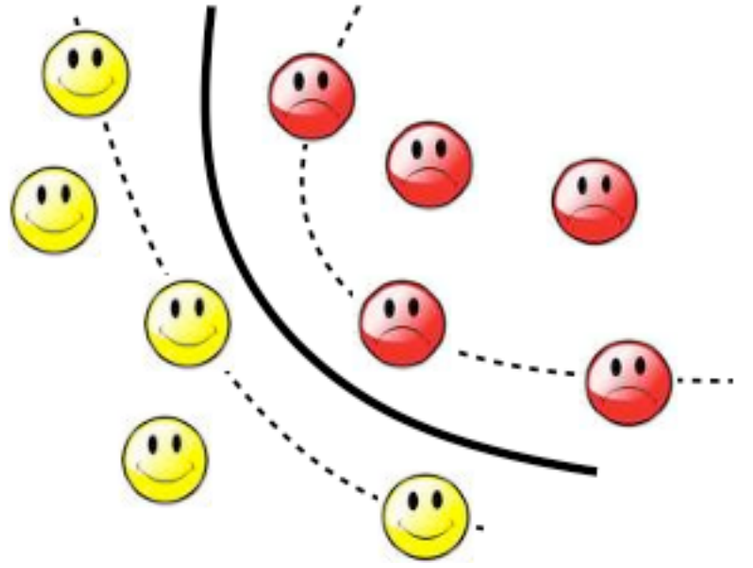
THE UNIVERSITY OF SYDNEY

- Madsen Computer Lab 211 — Tutor: Sean
- Madsen Computer Lab 226 — Tutor: Rafael
- New Law, Seminar 100 — Tutor: Kelvin & Anthony
- New Law, Seminar 105 — Tutor: Nick & Philippe
- New Law, Seminar 107 — Tutor: Harrison & Mr XXX

Tutorials: Tuesdays 5-6pm

- SIT Lab 118 — Tutor: Nick
- SIT Lab 116 — Tutor: Harrison
- SIT Lab 115 — Tutor: Sean

THE UNIVERSITY OF SYDNEY



Research Topics