Welcome to Mathematical Modelling FK (FRTN45)

Anders Rantzer

Department of Automatic Control, LTH

Mathematical modelling FK

Third modelling course in Pi-program

1st year: FMAA10 Matematisk modellering

2nd year: FMAF25 Matematisk modellering med statistiska tillämpningar

3rd year: FRTN45 Matematisk modellering FK

Idea: Start preparing for specialization

Models are Everywhere

- Natural sciences: Models for analysis (understanding)
- Engineering sciences: Models for synthesis (design)
- Economics and engineering: Models of our preferences

Outline

Thursday lecture

- Course introduction
- Ethics of modelling
- Static models from data (black boxes)

Friday lecture

- Dynamic models from data (black boxes)
- Models from physics (white boxes)
- Mixed models (grey boxes)

Matematisk Modellering FK (FRTN45)

Course homepage:

`http://www.control.lth.se/course/FRTN45`

- 4.5 högskolepoäng ; betyg U/G
- 4 h lectures
- 100 h project

Project

- Project supervision from
  - Mathematics, Mathematical Statistics, Automatic Control.
- Project plan. An A4-paper prepared after consulting the supervisor. Send to course responsible by February 6. Use email with subject line “FRTN45”.
- Written report
- Oral presentation (shared among all group members)
- Opposition (all team members together)
  Written opposition report
- 4 persons per project (possibly less)

Written report

See the website instructions:

- Cover sheet
- Summary
- Table of Contents
- Main Text
  - Presentation of problem: What is the purpose of the model?
  - Summary of used literature
  - Theory/Method
  - Implementation
  - Results
  - Evaluation/discussion: Does the model suit its purpose?
  - Reference list
- Description of how the work is distributed within the group

All Three Modelling Phases Must be Described

1. Problem structure
   - **Formulate purpose**, requirements for accuracy
   - Break up into subsystems — What is important?
2. Basic equations
   - Write down the relevant physical laws
   - Collect experimental data
   - Test hypotheses
   - Validate the model against fresh data
3. Model with desired features is formed
   - Put the model on suitable form.
     (Computer simulation or pedagogical insight?)
   - Document and illustrate the model
   - Evaluate the model: **Does it meet its purpose?**

Group 1: Vilken fågel sjunger?

Kan du skilja på en talgoxe och en gråsparv när du hör fågelsång utanför fönstret? "Kvitteromat" är en helt ny app som identifierar fågelarter baserat på sången. Den är dock, enligt utvärdering, känslig för störningar och ganska osäker i sitt beslut, då resultatet den presenterar är tre olika förslag på vilken art det är som sjunger. Detta projekts syfte är att identifiera några av våra vanligaste fågelarter genom att analysera deras sång, (lättare och svårare inspelningar), och hitta lämpliga kriterier för säker klassificering. Eventuellt kan en jämförelse och utvärdering göras mot kvitteromat. Verktyg för stationära stokastiska processer är användbara, tillsammans med information om signalens variation över tid. Data-material i mp3-format samt några mindre program för Matlab kommer att tillhandahållas.

Advisor: Maria Sandsten, Mathematical Statistics

Group 2: Modelling self-interacting random walks

This project deals with the modelling of a finite number of discrete particles performing a random walk on a certain (possibly, random) graph. The particles walk not independently, as the transition probabilities may depend both on the positions of other particles as well as the history of the process, thus making the resulting process a "marriage" between reinforced random walks and interacting random walks. Such processes are notoriously difficult to study analytically and hence simulations may be needed to predict their behaviour. They can, in principal, be used to model behaviour of e.g. ants or formation of social networks (virtual or real). This project will give some basic knowledge of probability theory and methods to simulate random phenomena using software. Some knowledge of random graph theory can be beneficial.

Advisor: Stanislav Volkov, Mathematical Statistics

Group 3: Modelling of Swedish Daily Temperature

This project considers the analysis of Swedish temperature data. Given three years of daily mean temperature at a number of locations we want to investigate which factors influence temperature and if they can be used to predict seasonal temperature variations at unobserved locations. The seasonal variability in daily temperature data can be modelled using a few sine and cosine functions. However, the amplitude and phase of the seasonality varies across space and we need to determine which factors (latitude / longitude / elevation / distance to coast / etc) affect temperature and how to include them in the model. Variations not captured by the seasonal structure could be modelled using tools from the stochastic process course. The models will be validated using temperature measurements at additional locations, and then used to predict temperature over all of Sweden.

Advisor: Johan Lindström, Mathematical Statistics

Group 4: Structure and motion for sound

Using several microphones it is possible to calculate the position of sound sources. If the microphone positions are known this is usually called trilateration. If neither the sound sources nor the microphone positions are known, the problem is more challenging. The purpose of this project is to study and develop mathematical models for sound and use them in experiments with real data for structure and motion for sound. There is a choice to focus more on the signal processing for the sound or to focus on the geometrical aspects of the positions of the microphones and the sounds sources.

Advisor: Kalle Åström, Mathematics LTH

Group 5: Hur uppfattar vi färg?

Färg är något som de flesta tycker att de vet vad det är, men vad menar vi egentligen när vi säger att något är blått? Och kan man bestämma avstånd mellan färger? I en dator kan man representera färgen i en pixel med tre värden, som beskriver hur mycket rött, grönt och blått som finns i pixeln. Tanken med projektet är att undersöka och modellera hur vi uppfattar skillnader i färger som visas pa en datorskärm. Kan man bestämma mått som beskriver hur mycket två färger skiljer sig åt? Hur kan man avgöra ifall detta mått stämmer överens med hur människor uppfattar skillnaderna?

Advisor: Magnus Oskarsson, Matematik LTH

Group 6: Stokastisk populationsdynamik

Ett mycket viktigt inslag i populationsmodeller är sk Markov Jump processes. Intuitivt, kan de beskrivas som processer där för det mesta händer ingenting på mycket korta tidsintervall, men då det händer något, är effekten "dramatiskt" (exempelvis antalet friska i en population ändras med +1). Man kan beskriva sådana processer med den sk Kolmogorov Forward Equation (1931) och den första numeriska algoritmen som implementerar idén gjordes av Kendall (1950), efter forskning av Feller från 1940. Syftet är att applicera sådana modeller på en lagom komplicerad populationsdynamisk process.

Advisor: Mario Natiello, Matematik LTH

Group 7: Bussar i rusningstrafik

Detta projekt handlar om ett fenomen som bland annat uppkommer i rusningstrafik när buss 171 på väg genom Lund plockar upp folk som ska till Malmö. Ju senare en buss kommer till en hållplats, ju fler personer har hunnit komma till hållplatsen och ju längre tid tar det för alla att gå ombord. Följaktligen kommer bussen att vara ännu senare vid nästa hållplats osv. En annan konsekvens är att nästa buss kommer ha färre personer att plocka upp så att den kommer ifrån hållplatsen snabbare och kanske kommer ifatt den föregående bussen. Resultatet blir ofta att en buss går till Malmö överfull och nästa går nästan tom. Uppgiften är att modellera fenomenet och komma med förslag på åtgärder som gör att bussarna blir mer jämnfulla.

Advisor: Johan Grönqvist, Reglerteknik

Group 8-9: En människas hjärtslagsfrekvens

En människas puls beror på många faktorer så som ansträngning, andningsfrekvens etc. Projektet syftar på att ta fram en dynamisk modell som beskriver dessa samband och kan användas för optimering. Exempelvis kan man optimera hastigheten för att ta sig en viss sträcka på minimal tid. Alternativt kan man försöka ta sig samma sträcka med ett minimalt antal hjärtslag. Resultaten ska valideras och kalibreras med mätdata från experiment. Utrustning för mätning och loggning av puls utnyttjas.

Advisor: Johan Grönqvist, Reglerteknik

Modelling in three phases:

1. Problem structure
   - **Formulate purpose**, requirements for accuracy
   - Break up into subsystems — What is important?
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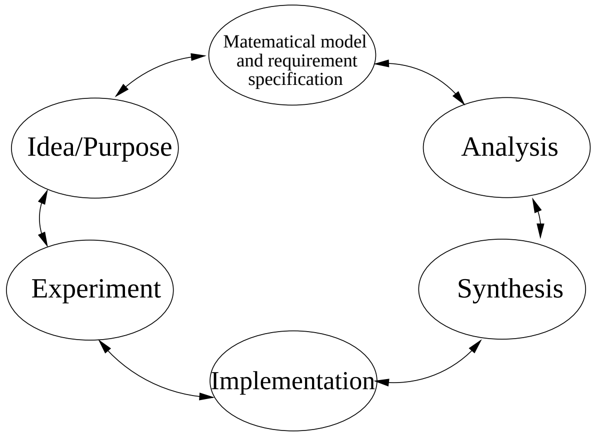
   - Put the model on suitable form. (Computer simulation or pedagogical insight?)
   - Document and illustrate the model
   - Evaluate the model: **Does it meet its purpose?**



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Engineering Ethics [1]

- Relevant for the Pi-program?
- Ethical linear algebra?
- Ethical mathematical modelling?

[1] Thanks to Maria Henningsson Pi-02 for suggesting this section.

"Our calculations show that..."

- What is behind the numbers?
- What assumptions are made?
- What limitations are there?

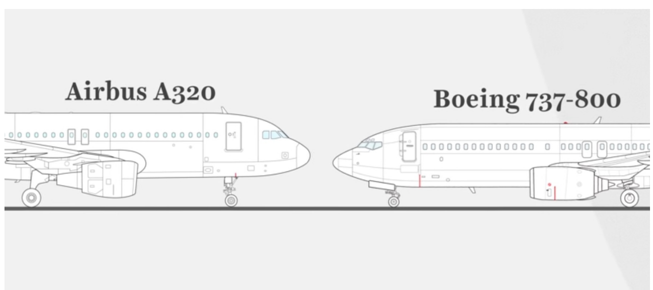
"Essentially, all models are wrong, but some are useful."
- George E. P. Box.

"Ethics is knowing the difference between what you have a right to do and what is right to do."
- Potter Stewart

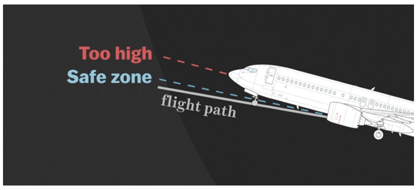
Example 1: Face Recognition

Example 1: Face Recognition

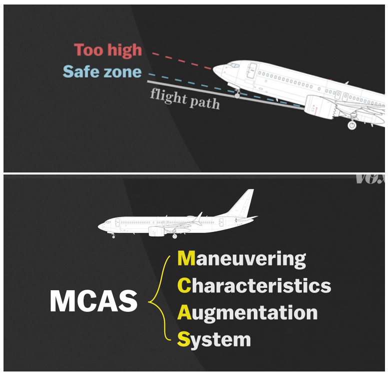
Example 2: Boeing 737 Max



Example 2: Boeing 737 Max

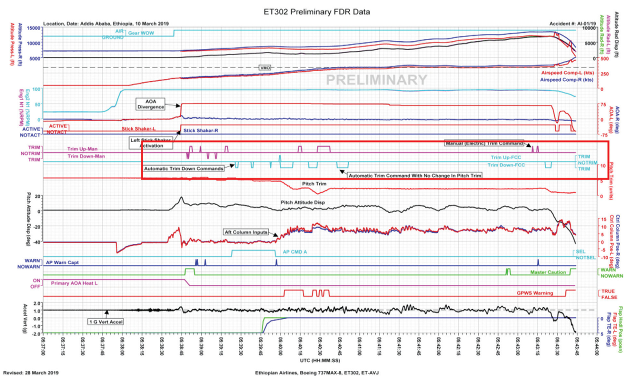


Example 2: Boeing 737 Max



With MCAS, models showed no need for new certification and pilot training!

Example 2: Boeing 737 Max



Example 3: The CitiCorp Building

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Thursday lecture

- Course introduction
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- Static models from data (black boxes)
  - **Singular Value Decomposition (SVD)**
  - Machine Learning

Friday lecture

- Dynamic models from data (black boxes)
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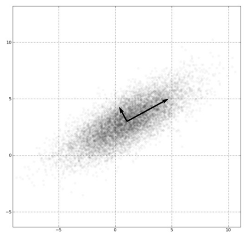
Principal Component Analysis (PCA)

Data from a bi-dimensional Gaussian distribution centered in $(1, 3)$:



Principal component $(0.878, 0.478)$ has standard deviation 3.

Next component has standard deviation 1.

[Source: Wikipedia]

Singular Value Decomposition (SVD)

A matrix M can always be factorized

$$M = U \begin{bmatrix} \Sigma & 0 \\ 0 & 0 \end{bmatrix} V^*$$

with Σ diagonal and invertible and U, V unitary:

$$\Sigma = \begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \end{bmatrix} \qquad U^*U = I \qquad V^*V = I$$

Diagonal elements of Σ are called singular values of M and correspond to the square roots of the eigenvalues of M^*M.

Computation of SVD is *very numerically stable*.

Example of SVD

$$M \quad = \quad U \quad \begin{bmatrix} \Sigma & 0 \\ 0 & 0 \end{bmatrix} \quad V^*$$

$$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} = \underbrace{\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}}_{U} \begin{bmatrix} 2 & 0 \\ 0 & 0 \end{bmatrix} \underbrace{\begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \frac{1}{\sqrt{2}}}_{V^*}$$

What does it mean if a singular value is zero?

What does it mean if it is near zero?

Good children can have many names

Collect all the data into a large matrix. Then compute the **SVD**:

$$\begin{bmatrix} y_1(1) & y_1(2) & \dots & y_1(N) \\ y_2(1) & y_2(2) & \dots & y_2(N) \\ \vdots & & & \\ y_p(1) & y_p(2) & \dots & y_p(N) \end{bmatrix} = U \underbrace{\begin{bmatrix} \sigma & & 0 \\ & \ddots & \\ 0 & & \sigma_p \end{bmatrix}}_{\Sigma} V^*$$

Singular values σ_i in decreasing order on the diagonal of Σ. The first columns of U give the direction of the main data area.

Principal Component Analysis: By replacing the small singular values σ_i with zeros focuses on the essential.

The name '**factor analysis**' is sometimes used as a synonymous, since large singular values σ_i highlight important factors.

Example: Image processing

What does this picture represent?

```
M =

     1     0     0     1     1     1     0     1     0     1
     1     0     0     0     1     0     0     1     0     1
     1     0     0     0     1     0     0     1     1     1
     1     0     0     0     1     0     0     1     0     1
     1     1     0     0     1     0     0     1     0     1
```

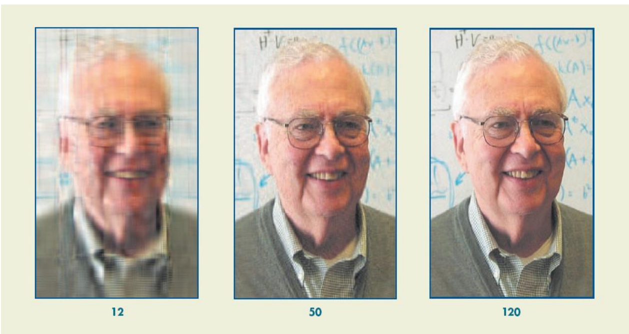
Example: Image processing with SVD

```
>> [U,S,V]=svd(M)

U =

   -0.4747    0.8662    0.0000   -0.1559    0.0000
   -0.4291   -0.1371   -0.0000    0.5450   -0.7071
   -0.4508   -0.3256   -0.7071   -0.4368   -0.0000
   -0.4291   -0.1371   -0.0000    0.5450    0.7071
   -0.4508   -0.3256    0.7071   -0.4368    0.0000

S =

4.5638 0      0      0      0      0      0      0      0      0
0      1.3141 0      0      0      0      0      0      0      0
0      0      1.0000 0      0      0      0      0      0      0
0      0      0      0.6670 0      0      0      0      0      0
0      0      0      0      0.0000 0      0      0      0      0
```

Example: Image processing with SVD

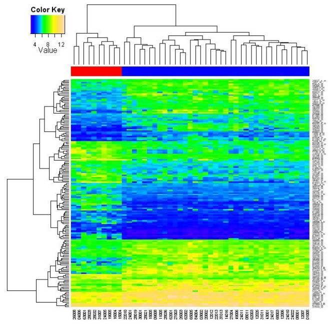
```
round(U*S1*V') =

     1     0     0     0     1     0     0     1     0     1
     1     0     0     0     1     0     0     1     0     1
     1     0     0     0     1     0     0     1     0     1
     1     0     0     0     1     0     0     1     0     1
     1     0     0     0     1     0     0     1     0     1

round(U*S2*V') =

     1     0     0     1     1     1     0     1     0     1
     1     0     0     0     1     0     0     1     0     1
     1     0     0     0     1     0     0     1     0     1
     1     0     0     0     1     0     0     1     0     1
     1     0     0     0     1     0     0     1     0     1
```

Example: Image processing



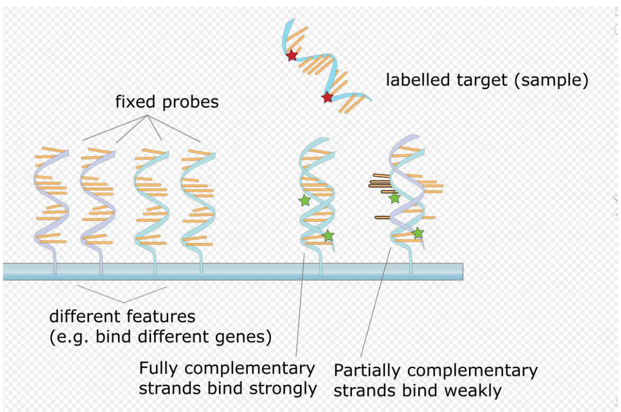
The original image has 897-by-598 pixels. Tacking red, green and blue vertically gives a 2691-by-598 matrix. Truncating all but 12 singular values gives the left picture. 120 gives the right.

Example: Correlations genes-proteines



Cancer research: microarrays (glass) with human genes are exposed to healthy cells, then to sick ones. Make a SVD of the data to find out which genes are important!

Example: Correlations genes-proteines



Research related to SVDs

How do you solve the following problems?

1. Given a matrix M find a matrix X of rank r that minimizes the spectral norm of $M - X$.
2. Given a matrix M find a matrix X with non-negative entries that minimizes the spectral norm of $M - X$.
3. Given a matrix M find a matrix X of rank r and non-negative entries that minimizes the spectral norm of $M - X$.

What if M has millions of rows and columns?

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Fun stuff before we get started

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Deep Dream version

4 / 24

Which one is Hemingway?

NO. 1:

Kilimanjaro is a snow-covered mountain 19,710 feet high, and is said to be the highest mountain in Africa. Its western summit is called the Masai "Ngaje Ngai," the House of God. Close to the western summit there is the dried and frozen carcass of a leopard. No one has explained what the leopard was seeking at that altitude.

NO. 2:

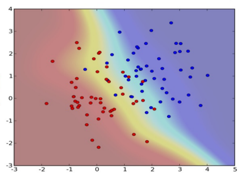
Kilimanjaro is a mountain of 19,710 feet covered with snow and is said to be the highest mountain in Africa. The summit of the west is called "Ngaje Ngai" in Masai, the house of God. Near the top of the west there is a dry and frozen dead body of leopard. No one has ever explained what leopard wanted at that altitude.

Before November 2016

Using language rule books:

Kilimanjaro is 19,710 feet of the mountain covered with snow, and it is said that the highest mountain in Africa. Top of the west, "Ngaje Ngai" in the Maasai language, has been referred to as the house of God. The top close to the west, there is a dry, frozen carcass of a leopard. Whether the leopard had what the demand at that altitude, there is no that nobody explained.

Components for deep lear



- One neuron
  - Example: Logistic regression
  - Classification model (x feature vector, (w,b) parameters, s smooth thresholding

    $x \in R^d, w \in R^d, b \in R, f(x) = s(w^T x + b)$
  - Logistic regression $s(z) = \frac{1}{1+e^{-x}}$
  - ML estimate of parameters (w,b) is a convex optimization problem

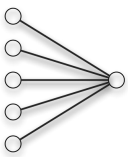
$$\min_{w} \quad \frac{1}{2} w^T w + C \sum_{i=1}^{l} \log(1 + e^{-y_i w^T x_i}).$$

LUND UNIVERSITY

Single Layer Neural Networks
One Neuron

- One neuron

  $x \in R^d, w \in R^d, b \in R, f(x) = s(w^T x + b)$



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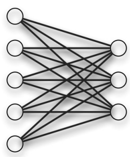
Single Layer Neural Networks
Several Neurons

- Several parallell neurons

  $x \in R^d, y \in R^k, B \in R^d, W - k \times \mathrm{dmatrix}$

  $y = s(Wx + B)$
- Elementwise smooth thresholding – s



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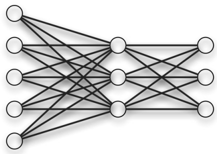
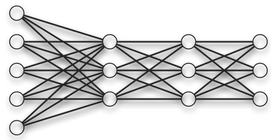
Artificial Neural Networks
One hidden layer

- Multi-class classification
- One hidden layer
- Trained by back-propagation
- Popular since the 1990ies



Deep Neural Networks
Many layers

- However
- Naively implemented would give to many parameters
- Example
- 1M pixel image
- 1M hidden layers
- 10^{12} parameters between each pairs of layers



Research related to deep learning

How do you solve the following problem:

Given convex functions $f_1(x), \ldots, f_N(x)$ of $x \in \mathbf{R}^n$, find x to minimize

$$\sum_{i=1}^{N} f_i(x).$$

What if the vector has millions of entries and the sum has millions of terms?

Exempel på kurser relevanta för modellering från data

FMSF15 Markovprocesser
EXTQ40 Introduktion till artificiella neuronnätverk och deep learning
FMSN45 Matematisk statistik, tidsserieanalys
FMSN20 Spatial statistik med bildanalys
FMSN35 Stationär och icke-stationär spektralanalys
FMAN60 Optimering
FMAF35 Linjär och kombinatorisk optimering
FMSN50 Monte Carlo-baserade statistiska metoder
FMNN01 Numerisk linjär algebra
FMAN20 Bildanalys
FMAN45 Maskininlärning
FRTN35 Systemidentifiering

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