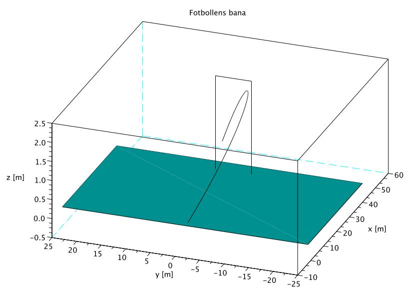
TANA09 Datatekniska beräkningar



Fredrik Berntsson, Linköping University

TANA09 Aims and Content

The aims for the course is

- Give insight into difficulties that occur when mathematical problems are solved on computers.
- Give an overview of modern methods for solving mathematical problems using computers.
- Show how computational methods can be analyzed with respect to efficiency, sensitivity with respect to errors,. . . .

The areas that are covered are

- Computer arithmetic. Error analysis.
- Non-linear equations.
- Linear systems and least squares problems.
- Interpolation. Curve and surface representation.

TANA09 Organisation

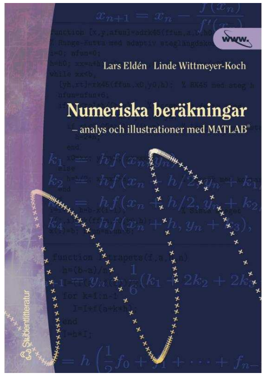
The course consisis of

- Lectures
  - Presentation of theory and examples.
- Lessons
  - Problem demonstration and individual work.
- Computer Laborations
  - Groups of two students. Three laborations.
  - Leave in the teachers mail box and collect in the course box.

Teachers are Fredrik Berntsson och Andrew Ross Winters

We are located in the B-building, 23-25, 2:nd floor.

TANA09 Litterature



L. Eldén and L. Wittmeyer-Koch,
Student Litteratur, 2001.
The book contains

- an overview of modern numerical methods.
- mathematical analysis of the methods.
- applications and implementation.

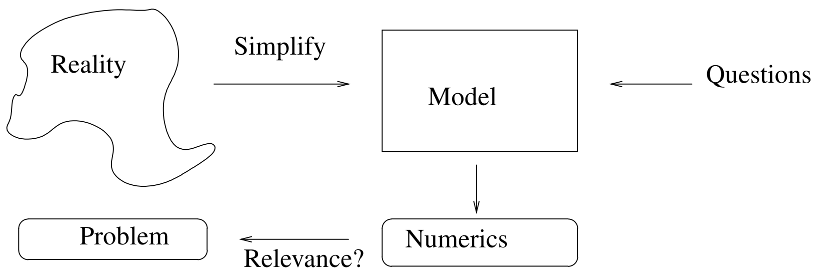
Sometimes seen as a bit difficult to read. There is an english translation.

Lessons Problem collection as a PDF for each lesson

Lecture 1

- Introduction. Simulation of a soccer ball.
- Sources of Error. Computation of an integral.
- Definitions. Basic concepts.
- Error propagation. Arithmetic operations. Catastrophic cancellation.

Engineering problem solving



Mathematics is the language used to fomulate engineering problems!

Exemple - How does a soccer ball move?

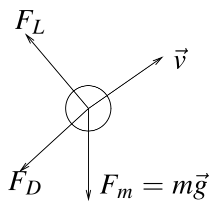
Variables The movement of a ball is specified by giving its *position* $p(t)$ and its velocity $v(t)$. We define the *state vector*

$$S(t) = (\, p(t) \;\; v(t) \,)^T.$$

We have the following

> **Theorem** If the initial state $S_0 = S(t_0)$ is known at $t = t_0$ then the balls trajectory is obtained by solving the initial value problem
>
> $$\frac{dS(t)}{dt} = f(t, S(t)), \qquad S(t_0) = S_0.$$

Newtons law of motion is $v'(t) = F/m$. Find the forces!



The forces acting on the ball are the *drag force*,

$$F_D(t) = -\frac{1}{2}\rho A C_D |\vec{v}(t)| \vec{v}(t),$$

and the *Magnus force*,

$$F_L(t) = \rho A C_L (\vec{\omega} \times \vec{v}(t)),$$

where $\vec{\omega}$ is the angular momentum.

Numerical solution

We need to

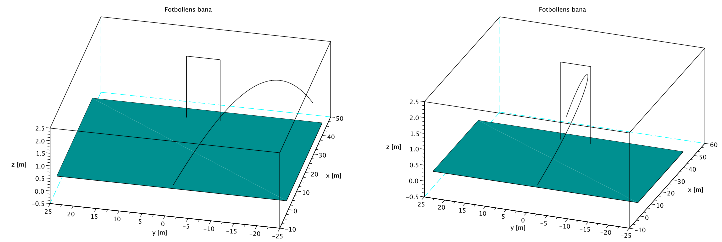
- Write a function that computes the derivative $S'(t)$ given $S(t)$.
- Solve the initial value problem using `ode45`.

We obtain a Matlab function

```
>> [t,P]=FindTrajectory(V0,P0,Omega);
```

What can we do with this function?

We simulate the trajectory with initial velocity $v(0) = (35.4\,,\ -14.9\,,\ 4.13\,)^T$ and different vectors ω.



To the left is a pure back-spin $\vec{\omega} = (0.0\,,\ -6.9\,,\ 0.0)^T$. To the right a side spin has been added so that the ball hits the goal!

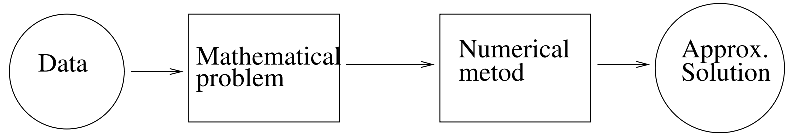
This is a famous free kick by Roberto Carlos, 1997.

What will we do in the course?

- How to plot the trajectory given $\{p(t_i)\}_{i=0}^N$? What distance does the ball travel? Use parametric curves and *spline interpolation*.
- Suppose we know where the ball hits the ground but can't measure the drag coefficient. Solve a *non-linear equation* $f(C_D) = |p_{end}(C_D) - p^*| = 0$.
- Suppose we have a measurement error in $v(0)$ and $\vec{\omega}$. How to estimate the error in the result? The *Error propagation formula*.

Remark Using numerical software is **easy**! Need to know whats available and also how the algorithms behave.

Error analysis and error sources



Definition The different *Sources of error* are classified as

- R_X - Errors in the used data.
- R_{XF} - Errors in used function values.
- R_B - Rounding error.
- R_T - Truncation error.

It is important to be able to estimate the size of the different errors in a calculation.

Example We want to compute an integral

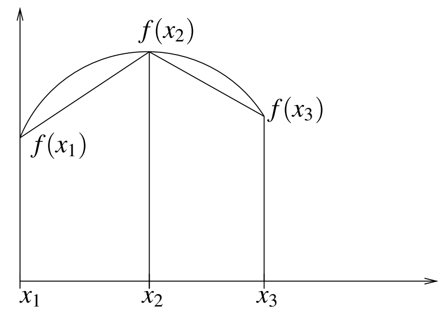
$$I = \int_{x=0}^{1} f(x)dx,$$

using a table of function values

x	0.00	0.20	0.40	0.60	1.00
$f(x)$	1.31	1.93	1.82	1.56	0.87

How to proceed?

Numerical method Approximate $f(x)$ by a piecewise linear function and find the area



We obtain

$$I \approx T = h\left(\frac{f(x_1)}{2} + f(x_2) + \frac{f(x_3)}{2}\right), \qquad h = x_2 - x_1.$$

This is called the *trapezoidal method*. What are the error sources?

The result is

$$I \approx T = 0.2\left(\frac{1.31}{2} + 1.93 + 1.82 + 1.56 + \frac{0.87}{2}\right) = 1.28 \approx 1.3.$$

The following sources of error are identified

- The function $f(x)$ is approximated by straight lines. This gives a *truncation error*,

$$|R_T(h)| = |I - T(h)|.$$

  The error should depend on both $f(x)$ and the step size h.
- Errors in the function values $\{f(x_k)\}$ gives an error R_{XF}.
- Final rounding of the answer gives an error R_B.

How to estimate the magnitude of the errors?

Basic concepts

Definition Let a denote the *exact* and $\bar{a}$ be an *approximate value*. Then

$$\Delta a = \bar{a} - a,$$

is the *absolute error* in the approximation$\bar{a}$ and

$$\frac{\Delta a}{a}, \qquad (a \neq 0),$$

is the *relative error* in $\bar{a}$.

Exemple Let $a = \sqrt{3}$ and $\bar{a} = 1.732$.

> **Definition** If the absolute error satisfies
>
> $$|\Delta a| \leq 0.5 \cdot 10^{-t},$$
>
> then $\bar{a}$ has t *correct decimals*.

> **Definition** If $\bar{a}$ has $t > 0$ correct decimals then all digits in positions with unit $\geq 10^{-t}$ are called *significant digits*, except leading zeroes.

Exempel Let $a = \sqrt{3}$ and $\bar{a} = 1.732$. How many significant digits does the approximate value have?

Error propagation

Problem We want to compute $f(a)$ but only an approximate value $\bar{a}$ is available. How do we estimate the resulting error

$$|\Delta f(a)| = |f(\bar{a}) - f(a)|.$$

Solution Use the *Mean value theorem.*

> **Theorem** Suppose $f(x)$ is differentialbe. Then there is a $\xi \in (a, \bar{a})$ such that
>
> $$f(\bar{a}) - f(a) = f'(\xi)(\bar{a} - a) = f'(\xi)\Delta a.$$

If Δa is small then $f'(\xi) \approx f'(a)$ and we obtain

$$|\Delta f| \lesssim |f'(a)||\Delta a|.$$

This is called the *error propagation formula*.

Exemple Suppose that

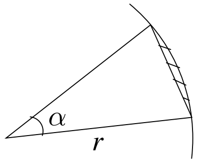
$$f(x) = (A - x)^2,$$

where $A = 2.6 \pm 0.05$. Compute $f(1)$ with error bound.

> **Question** What if $f(x)$ is not differentiable?
>
> **Answer** The copurse is based on approximating functions locally by Taylor expansions. Thus functions **have** to be differentiable!

We can generalize to many variables. We obtain

> **Definition** Suppose $f(x_1, x_2, \ldots, x_n)$ is differentiable and only approximate values
>
> $$\bar{x}_k = x_k + \Delta x_k, \qquad k = 1, 2, \ldots, n,$$
>
> are known. The *general error propagation formula* states that
>
> $$|\Delta f| \lesssim |\frac{\partial f}{\partial x_1}||\Delta x_1| + \cdots + |\frac{\partial f}{\partial x_n}||\Delta x_n|.$$



$r = 1.12 \pm 0.5 \cdot 10^{-2}$

$\alpha = 0.073 \pm 0.5 \cdot 10^{-3}$

Example Calculate the area $A = \frac{r^2}{2}(\alpha - \sin(\alpha))$ and an error bound.

Exemple Suppose we want to compute a/b, and only approximate values $\bar{a}$ and $\bar{b}$ are known. What is the error bound for the division? What happens if we instead calculate the sum $a + b$?

Error propagation at arithmetic operations

Lemma Let $\bar{a}$ and $\bar{b}$ be approximations of a and b.
If $c = a + b$ or $c = a - b$ then

$$|\Delta c| \leq |\Delta a| + |\Delta b|.$$

If instead $c = a \cdot b$ or $c = a/b$ then

$$\frac{|\Delta c|}{|c|} \leq \frac{|\Delta a|}{|a|} + \frac{|\Delta b|}{|b|}.$$

Question Is this good or bad? What happens if $a = 101 \pm 1$ och $b = 100 \pm 1$.

Cancellation

Definition Subtraction of two almost equal numbers $\bar{a}$ och $\bar{b}$ leads to a loss of accuracy. This is called *cancellation*.

Exemple The polynomial equation $x^2 - 18x + 1 = 0$ has the roots $x_{1,2} = 9 \pm \sqrt{80}$. Suppose we know $\sqrt{80}$ with 4 correct decimals. How accurate can we determine the roots?

Exemple We know that

$$f(x) = \frac{1 - \cos(x)}{\sin(x)} = \frac{\sin(x)}{1 + \cos(x)}.$$

For small x we have $\cos(x) \approx 1$ and cancellation occurs in the first expression. Avoid the cancellation by rewriting the expression.

> Mathematically equivalent expressions are not numerically equivalent.