1 OVERVIEW / NUMERICAL APPROXIMATION

1.1 ORGANIZATION (http://www.nada.kth.se/kurser/kth/2D1240)

1.1.1 Who's who

Lecturer André Jaun (jaun@nada.kth.se, tel: 7908130), Fri 9:15-10:00 in room 1519.

Assistants Mikael Huss (gr1, hussm@nada.kth.se), André Jaun (gr2, jaun@nada.kth.se), Erik von Schwerin (gr3, schwerin@nada.kth.se), Pål Westermark (gr4, paal@nada.kth.se).

Lab assistants David Möller and others when needed.

1.1.2 Course material

Package (Nada exp Mon–Fri 9:45–11:30, Mon–Thu 12:45–14:15)	100 kr =
G. Eriksson, *Numeriska algoritmer med Matlab* (NAM), 2002	40 kr +
L. Edsberg, *Exempelsamling i numeriska methoder* (EX), 2002	40 kr +
2D1240 package, incl. *Matlab-övningar* (MÖ), program, plan, Matlab user manual, collection of formulas, hederskodex, theory questions, example of former exams	20 kr

Web News, slides, etc → http://www.nada.kth.se/kurser/kth/2D1240

Book M.T. Heath, *Scientific Computing*, 2nd edition, 2002, 630 kr

1.1.3 Timetable (careful – some exceptions)

Lectures Tue 8–10, Thu 10–12. Note 5+19 sep are **Thursdays.**

Exercises Tue 13–15

Lab gr1,gr2 (Fri 10-12) and gr3,4 (Fri 13–15)

Report (2p) Oral presentation of lab1 (16–20 oct) and lab2 (7–10 oct)

Exam (2p) Written 3h incl. theory + problems (Sat 19 oct, 8-11 hours)

Extra (2p) Oral exam with presentation of lab3+4

1.1.4 Organization

Lectures
Follow NAM in Swedish (or an approximation) with slides in English.

Q&A (use a white A4 paper sheet between you and your hand)

> **Language.** Who prefers that I speak: ↑Swedish ↓English

Questions
In the classroom: formulate questions clearly for everyone, rise your hand.
Between / after lectures: step forward.
Fri 9–10 room 1519 at Nada, 10–12, 13–15 room XQ3-8

Peer Teaching (2×1 minute to think, explain to your neighbour and vote)

> **Archimedes.** Henrik sits with a big rock in a boat floating in a swimming pool; he lifts the rock out into the water. Does the water level in the pool:
> ↑rise ↔stay the same ↓drop

Exercises
Create four groups: gr1,gr3,gr4 (in Swedish), gr2 (in English).

Computer labs
Create groups of 2 helping each other; everyone has to be able to report!

1.1.5 Register

res checkin nume02
Follow the link from the course webpage

res show nume02
To verify the status of your accreditation

1.2 INTRODUCTION

1.2.1 Review: what you should remember / revise from last years

Geometry
Equations for a line, plane, parabola, circle

Analysis
Functions, trigonometry, derivation, integration, Taylor series, l'Hospital

Algebra
Vectors, matices, system of linear equations, Gaussian elimination.

Science
Lots of nice applications

1.2.2 Goal: what you will learn in this course

Foundations of numerical analysis
Use a computer instead of analytical formulas, rely on the result.

Programing with Matlab
Solve simple problems in preparation for more advanced engineering.

Present your work
Explain your ideas to your friends, report orally and in document.

1.2.3 Overview: what you will learn today

Course layout
Who's who, timetable, material, organization.

Approximation
Uncertainty, error, propagation, finite differences.

Matlab (this afternoon)
Vector operations, plotting, MÖ-exercises.

1.3 Numerical approximation (NAM 1.2, H 1.2)

Illustration Calculate the volume of the Earth $V = \frac{4}{3}\pi R^3$

The sphere is only a model of the true shape

The radius $R \approx 6370$ km has been measured with a limited precision

The value $\pi \approx 3.1415$ is a truncation of $\pi = 4\arctan(1)$

The calculation is probably performed on a calculator with at most 15 digits

Within reasonable doubt, the volume is $V \approx 1.1 \cdot 10^{21} m^3$

Error analysis Define an approximation $\hat{x} \approx x$ — $\hat{x} = 3.1415 \approx \pi = x$

Absolute error $e_x = \hat{x} - x$ — $e_x = 3.1415 - \pi = -9.27 \cdot 10^{-5}$

Relative error $r_x = (\hat{x} - x)/x = e_x/x$ — $r_x = e_x/\pi = -2.9 \cdot 10^{-5}$

Error bounds $E_x = |e_x|, R_x = |r_x|$

Uncertainty from a measurement $V = x \pm E_x$ — $g = 9.81 \pm 0.005$

Number of significant digits $|r_x| \leq 10^{-d}$ — $d \geq -\log_{10}|r_x| = 4.53 \simeq 5$

Keep only relevant figures and specify the main source of uncertainty.

Exercise Leading order approx. $\hat{x} = a \approx \sin(a) = a - \frac{1}{3!}a^3 + \ldots, \forall |a| < 0.5 \simeq 28^o$

We get $E_x < 0.021$, $R_x < 0.043$ (4.3 percent), more than $d \geq 3.1 \simeq 3$ digits!

Examples EX 8.2 + 8.4

Error propagation through an operation $\hat{y} = f(\hat{x})$

With $(+, -)$ add the absolute error

With $(\cdot, \div)$ add the relative error

If f' exists, substract Taylor expansion

$$\begin{array}{rcl} \hat{y} & = & f(\hat{x}) \\ f(x) = y & = & f(\hat{x}) + (x - \hat{x})f'(\hat{x}) + \ldots \\ \hline \hat{y} - y & \approx & (\hat{x} - x)f'(\hat{x}) \end{array}$$

which can be generalized to functions of more than one variables.

Otherwise, estimate $[\min f(x); \max f(x)]$ from a set of samples $x \in \{x_k\}$

Peer Teaching $(2 \times 1$ minutes to think, explain to your neighbour and vote)

> **Cancellation.** Which operation yields the largest error amplification?
>
> ↖ $+$ ↗ $-$ ↘ $\times$ ↙ $\div$

Illustration Formulas for the quadratic equation $ax^2 + bx + c = 0$

Avoid overflows by rescaling a, b, c by the largest in magnitude.

Avoid cancellation between $-b$ and $\sqrt{\cdot}$ by using one of the two

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \quad \text{or} \quad x = \frac{2c}{-b \mp \sqrt{b^2 - 4ac}}$$

Condition number of an operator $f(\cdot)$ and loss of precision

$$\kappa = \frac{|\text{rel error out}|}{|\text{rel error in}|} = \frac{|\epsilon_r(y)|}{|\epsilon_r(x)|} = \frac{|(\hat{y}-y)/y|}{|(\hat{x}-x)/x|} \approx \left|\frac{xf'(x)}{f(x)}\right|$$

An operation with a condition number $\kappa = 10^d$ looses d significant digits!

Illustration Sensitivity of $y = \tan(x)$ for $x = (1.57079 \pm 0.00001) \approx \pi/2$

Derivative: $y' = 1 + tan^2(x)$

Condition number: $\kappa = \left|\frac{x(1+\tan^2(x))}{\tan(x)}\right| \simeq 3 \cdot 10^5 \Rightarrow$ loose at least 5 digits

High precision input: $x = 1.57079 \pm 0.00001$

Low precision output: $\tan\begin{pmatrix} 1.57078 \\ 1.57079 \\ 1.57080 \end{pmatrix} = \begin{pmatrix} 6.125 \cdot 10^4 \\ 1.581 \cdot 10^5 \\ -2.722 \cdot 10^5 \end{pmatrix}$

Solution cannot be written in the $y \pm dy$ format: the error is not bounded!

Rather, use intervals $y \in]-\infty; -2.722 \cdot 10^5] \cup [6.125 \cdot 10^4; +\infty[$

$\tan(x)$ is very sensitive around $x = \pi/2$; $\arctan(x)$ is very insensitive.

1.4 Finite difference (NAM 1.3, H example 1.3)

Illustration

Use $f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$ to calculate $[\exp(x)]'$ at $x = 1$

Using a calculator with 8 significant digits, we get:

h	$[\exp(1+h) - \exp(1)]/h$
1	4.6707743
0.1	2.8588418
0.01	2.7319190
0.001	2.7196400
0.0001	2.7184000
0.00001	2.7200000
0.000001	2.7700000
0.0000001	3.0000000
0.00000001	0.0000000

The cancellation error from the difference becomes very large: with $h = 10^{-7} \Rightarrow e^{1.0000001} - e^{1} = 2.7182821 - 2.7172818 = 0.0000003$, showing that nearly all the precision is lost!

Finite difference approximations

Use a Taylor expansions of $f_n \equiv f(x_n)$ around x_0 assuming that the function is know on a homogeneous grid $x_n = x_0 + nh$:

$$
\begin{aligned}
f(x+2h) = f_2 &= f(x) + 2hf'(x) + \frac{4h^2}{2!}f''(x) + \dots \\
f(x+h) = f_1 &= f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \dots \\
f(x) = f_0 &= f(x) \\
f(x-h) = f_{-1} &= f(x) - hf'(x) + \frac{h^2}{2!}f''(x) - \dots \\
\text{etc}
\end{aligned}
$$

Substract $(f_1 - f_0)$ or $(f_1 - f_{-1})$ to approximate $f'(x)$:

$f(x+h) - f(x) = hf'(x) + \mathcal{O}(h^2) \Rightarrow$ $\boxed{f'(x) = \frac{f(x+h)-f(x)}{h} + \mathcal{O}(h^2)}$

$f(x+h) - f(x-h) = 2hf'(x) + \mathcal{O}(h^3) \Rightarrow$ $\boxed{f'(x) = \frac{f(x+h)-f(x-h)}{2h} + \mathcal{O}(h^3)}$

A centered difference in $\mathcal{O}(h^3)$ is more precise!

Combine $(f_1 - 2f_0 + f_{-1})$ to approximate $f''(x)$:

$f(x+h) - 2f(x) + f(x-h) = h^2 f''(x) + \mathcal{O}(h^3)$

$$\Rightarrow \boxed{f''(x) = \frac{f(x+h)-2f(x)+f(x-h)}{h^2} + \mathcal{O}(h^3)}$$

Try the combination $(-3f_0 + 4f_1 - f_2)$...