Numerical Methods & Scientific Computing: lecture notes

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Numerical Methods & Scientific Computing

A new syllabus in 2017 — a revision of MAST30028 Numerical & Symbolic Mathematics.

We study how to solve mathematical problems that cannot be done by hand using **numerical** methods.

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Example

solve a large linear system of equations

Example

solve a complicated differential equation to give numerical values of solution at certain times, not formulae

- **Demo**

New topics

Since this subject now covers only numerical methods, not symbolic software, we get to cover more topics:

Example

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use computer simulation to explore the behaviour of stochastic (probabilistic) models

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Example

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fit data to linear and nonlinear models

Example

an introduction to useful software engineering tools

What are Numerical Methods?

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Numerical Methods also called

- Computational Mathematics 620-381 before 2010
- Numerical Analysis (includes proof of error properties)
- Scientific Computing

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As a software platform, we use MATLAB. We also briefly show NumPy. Alternatives include: Octave, SciPad, Julia, C, Fortran, ...

From ‘Trefethen’s Maxims’

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- *There are three great branches of science: theory, experiment, and computation.*

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- *As technology advances, the ingenious ideas that make progress possible vanish into the inner workings of our machines, where only experts may be aware of their existence. Numerical algorithms, being exceptionally uninteresting and incomprehensible to the public, vanish exceptionally fast.*

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L.N.Trefethen, Oxford

Discrete or continuous?

Some mathematical problems are naturally discrete

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Example

algebra (inc. linear algebra), graph theory, combinatorics, bioinformatics, pattern matching ...

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Some mathematical problems are naturally continuous

Example

analysis, integrals, limits, differential equations ....

More from Trefethen... ..

The big gulf in the mathematical sciences is between the continuous problems (and people) and the discrete ones. Most scientists and engineers are in the continuous group, and most computer scientists are in the discrete one.

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Definition

Numerical analysis is the study of algorithms for the problems of continuous mathematics

$\Longrightarrow$ not for the problems of discrete mathematics (graph theory, pattern matching, discrete optimization etc. $\rightarrow$ Computer Science)

What is it for?

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Many BIG problems:

- climate change modeling
- drug design
- salinity/pollution monitoring

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require heavy 'scientific computing'.
NOT (typically) bioinformatics — more discrete.

Where to find more...

Numerical methods are covered briefly in several other UoM subjects.

Example

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BMEN20001, COMP20005, PHYC20013

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and more fully in one other subject:
ENGR30003 Numerical Programming for Engineers

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More specialized subjects e.g. PDEs, optimization, CFD exist at Masters level.

Example

MAST90026 Computational Differential Equations

Week 1: aim to cover

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- Errors in scientific computing (now)
- Programming in MATLAB; 1D arrays (vectors) in MATLAB (Lab 1)
- Output in MATLAB; variable scope in MATLAB (Lecture 2)

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Goals

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We need mathematics to

1. understand the problem
2. construct an algorithm
3. prove it gives the answer (in principle)
4. estimate how long/ how much memory it takes **complexity**

For many discrete problems, that's all.

For continuous problems, also need to

- approximate the continuous problem by a discrete one
  — this produces **truncation error**
- show that resultant errors stay small enough for a useful result
  — this property is called **stability**

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Sources of error in scientific computing

- Modeling error: does the model capture reality?
- Measurement error: are the experiments/observations accurate?
- Programming errors: does the program do what was intended?
- Computational error: do the numerical results approximate the true mathematical solution?
- Statistical error: for stochastic problems, there is unavoidable error due to randomness; how do we deal with that?

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For deterministic models, we focus on Truncation error and Roundoff errors which together are the Computational error . Usually one of these is dominant.

Truncation error

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arises because we need to approximate continuous objects (functions, integrals, DEs ..) by discrete ones (sums ...)

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Example

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the dominant error in solving IVPs

Roundoff error

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arises because we need to approximate real numbers by numbers we can store in computer

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Example

the only error in solving linear systems by direct methods

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A good algorithm minimizes computational error and maximizes efficiency (possibly a tradeoff here).

Statistical error

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- Arises because of randomness in stochastic models
- Every realization of a stochastic process produces a different result

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- We have to average over many realizations to get average or distributional information. Then we can use statistical methods to estimate the statistical error.

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- The computational error is still present but may be dominated by statistical error, depending on the noise level.

Measures of error

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Let $\hat{x}$ be approximate value of x

- **absolute error**: $e = \hat{x} - x$
- **relative error**: $r = (\hat{x} - x)/x = e/x$
  not useful if $x = 0$
  a better measure if x can be large

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Note: $\hat{x} = x(1 + r)$

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How many significant figures do we need?

According to Trefethen:

> *No physical constants are known to more than* **around 11 digits***, and no truly scientific problem requires computation with much more precision than this. (OK, throw in another 5 or 6 digits to counter the slow accumulation of rounding errors in very long calculations – using numerically stable algorithms, of course, without which you're sunk in any precision.)*

By contrast **engineering accuracy** = 2–3 digits

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End of Lecture 1

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