MA 580; Numerical Analysis I

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Version of October 23, 2016

NCSU, Fall 2016
Part I: Management

Contents

Management: MA 580

- Call me "Tim"
  Dr. Kelley is my brother, the physician.
- Are you enrolled in this class?
- Check the Moodle page early and often.
  https://moodle-courses1617.wolfware.ncsu.edu/course/view.php?id=2823
- Use the forums on the moodle page
  We follow the forums.
- Reread this lecture on the House Rules.
  Posted on the Moodle page as Part I

Lectures, Notes, Books

- 2016 Lectures captured by DELTA
  https://delta.online.ncsu.edu/online/Catalog/catalogs/import-ma-580-c-t-kelley
- 2015 Lectures on Moodle page, updated as we go.
- I go fast. Feel free to tell me to slow down.
- Notes $\subset$ Lectures $\subset$ Books (mostly)
- Exams $\subset$ Lectures + Homework

MA 1160

- I travel a lot for work
  Dates I know about: Aug 29, Oct 3, 5, 26, 28.
- We will have exams on Aug 29 and Oct 3.
- We will do double sessions at most four times during the term.

Highlights of House Rules

- Prerequisites: Linear Algebra + MATLAB + calculus
- Books are free online
- Three exams + homework + final(?)
  - Exam Dates: Aug 29, Oct 3, Nov 18
  - Optional Final Exam: Dec 14, 8:00 AM
- In-class and Delta courses are different:
  Different purpose, different grading.

Three kinds of students

- In-class: boot camp for prelims in math; you get me. See Moodle page for office hours.
- Delta: distance learning, not for math majors; you get distance support from the Moodle forum.
- Internet surfers: no support

Objectives: In-class

- Preparation for written prelims in this field.
  - in-class timed exams
  - tough grading for both homework and exams
- Preparation for research career in mathematics.
  - understanding both theory and practice well
  - writing clear mathematics (TEX is part of this)

Objecives: Delta

- Learn to use this technology wisely
- Learn to use the methods in practice
- Professional development
  Engineers tend to be ahead of mathematicians at this level.
- Master theory well enough to
  - pick correct tools
  - diagnose failures
- Homework and exams focus on practice more than theory.
- Proctored exams in DELTA space

Delta students are not responsible for lengthy proofs.

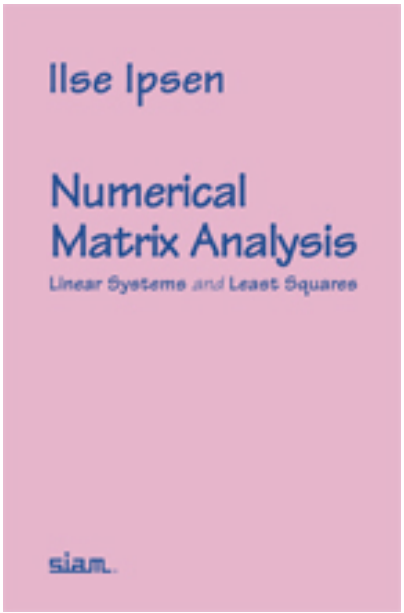
Objectives: Internet

Have fun.

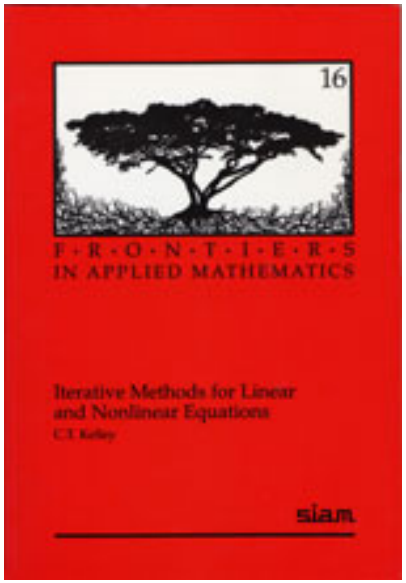
Books

- I. C. F. Ipsen, Numerical Matrix Analysis, SIAM, 2009.
  http://catalog.lib.ncsu.edu/record/NCSU2514760
- C. T. Kelley,
  Iterative Methods for Linear and Nonlinear Equations, SIAM, 1995.
  http://catalog.lib.ncsu.edu/record/NCSU2512957
- Desmond J. Higham and Nicholas J. Higham,
  Matlab Guide: Second Edition, SIAM, 2005
  http://catalog.lib.ncsu.edu/record/NCSU3108706
- Registered students download for free from NCSU library.

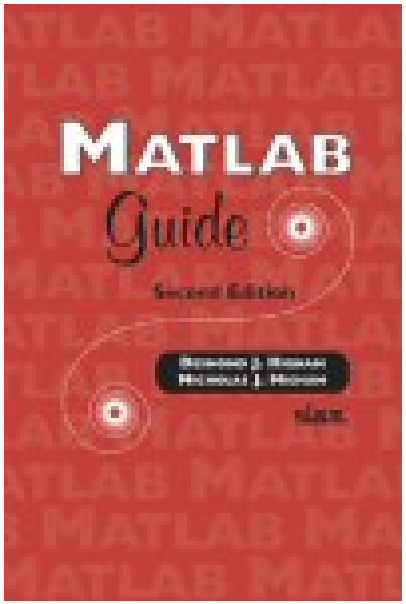
Books



Pink Book



Red Book



Matlab Book

Draft 580 Text

https://drive.google.com/file/d/0B5o2V29F0a7kaFdRWi1BbVE4WTQ/view?usp=sharing

- Written as we teach.
- Continously updated.
- For now, focus on chapters 1, 2, 3.

Notation in Books and Lectures

You're graduate students, so differences in notation should not be a problem.

- Notation in lecture notes will be the same as the tests.
- Most differences in notation are in the fonts (**bold** vs *italics* vs Roman . . .)
- When in doubt, ask!

Grades

- Grades: based on 350 (or 550) points
  - Three exams: $50 + 100 + 100 = 250$ points
    50 point exam on prerequisities coming soon.
  - Take-home programming in Exam 3!!!
  - Optional 200 point final exam.
  - Homework + Programming, five assignments: 100 points
    Must be typeset (LaTeX, word, . . .)
    I encourage you to work in teams of ≤ 5.
    You'll get the homework assignments early, so . . .
    No late homework!!!
- Programming language is MATLAB
  If you are good at C or Fortran, you can easily learn MATLAB.

Neatness Counts in MA 580!

You must

- Typeset and neatly format your homework.
  Turn it in via Moodle in pdf.
- Discuss your results in clear English.
  Returning only numbers and plots is not enough.
- Label axes and curves in figures.
  The Matlab `xlabel`, `ylabel`, `legend` commands are useful.
- Tables should only present useful and informative data.
  Don't report 16 digits when only the exponent is of interest.

Learning and Using LaTeX

- NCSU supports LaTeX.
- I will give you both the LaTeXand pdf files for exams/homework.
- There are some very useful resources out there.
  - MATLAB and LaTeX and U. Houston
    http://www.math.uh.edu/~torok/math_6298/
  - The WikiBook is pretty complete
    http://en.wikibooks.org/wiki/LaTeX
  - Tutorial from Ireland
    http://www.maths.tcd.ie/~dwilkins/LaTeXPrimer

Prerequisites

- Linear algebra/matrix theory
- Calculus + DEs
- Good programming and computer skills
  Typesetting assignments, MATLAB, editing . . .

Prerequisites: Calculus and DEs

- Integration and differentiation of elementary functions.
- Methods of integration (eg parts)
- Series and summation. Taylor series for simple functions.
- Taylor's theorem with remainder.
- Multiple integrals, partial derivatives.

Prerequisites: Linear Algebra

- Matrix and vector manipulation
- Gaussian elimination
  Solve 2×2 linear systems by hand
- Eigenvalues and eigenvectors
  Find eigenvalues/vectors of 2×2 matrices by hand

Prerequisites: Programming

Class motto: *Tim does not ask you to debug his programs, so . . .*

- Good programming skills in a scientific language:
  C, C++, Fortran, Matlab, Java . . .
  "Good" does not have to mean great.
- Ability to learn Matlab on your own.
- Ability to learn the NCSU computing environment.
- Can you write a program that takes two matrices as input and prints their product on the screen?

Calculus You Should Know

- Differentiation and integration
- Taylor's formula and the remainder term
- Manipulation of infinite series

Examples of Series Tricks

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!} \text{ so } e^{x^2} = \sum_{n=0}^{\infty} \frac{x^{2n}}{n!}$$

$$\frac{1}{1-x} = \sum_{n=0}^{\infty} x^n \text{ for } |x| < 1.$$

Integrate termwise to get

$$\begin{aligned} \ln(1-x) &= -\int_0^x \tfrac{1}{1-\xi} d\xi = -\int_0^x \textstyle\sum_{n=0}^{\infty} \xi^n d\xi \\ &= -\textstyle\sum_{n=0}^{\infty} \int_0^x \xi^n d\xi = -\sum_{n=1}^{\infty} x^n/n. \end{aligned}$$

Taylor's Theorem

Assume: $c, x \in (a, b)$ and

$f \in C^{n+1}(a, b) =$
$n+1$ times continuously differentiable functions on (a, b)

Then

$$f(x) = \sum_{k=0}^{n} \frac{f^{(k)}(c)(x-c)^k}{k!} + \frac{f^{(n+1)}(\xi)(x-c)^{n+1}}{(n+1)!}.$$

where ξ is between c and x.

Taylor's Theorem Trick I

How many terms in the Taylor series for e^x do you need to get an error $< 10^{-6}$ for all $x \in [0,1]$.
In this case $(a,b) = [0,1]$. Expand about $c = 0$.
Since $f(x) = e^x = f^{(k)}(x)$ for all k. The error after the nth order term is (worst case for $x \in [0,1]$)

$$|E| \leq \frac{e^1}{(n+1)!}.$$

Do some matlab and find that $n = 9$ will do the job, so the answer is 10.

Trick II: Finite Difference Approximations to Derivatives

Assume that $f \in C^2$.

$$f(x \pm h) = f(x) \pm f'(x)h + f''(\xi_\pm)h^2/2$$

So

$$\frac{f(x+h) - f(x)}{h} = f'(x) + f''(\xi_+)h/2 = f'(x) + O(h)$$

Expand to 4th order and there's more

Second Order Accurate Difference

$$f(x \pm h) = f(x) \pm f'(x)h + f''(x)h^2/2 \pm f'''(x)h^3/6 + O(h^4)$$

What is that $O(h^4)$ stuff?

So

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

Gaussian Elimination for Small Systems

Solve two linear equations in two unknowns.

$$\begin{aligned} \text{(I)} \quad & 2x_1 + x_2 = 1 \\ \text{(II)} \quad & x_1 + x_2 = 2 \end{aligned}$$

Elimination of x_1 from (II):
Multiply (I) by $1/2$ and subtract from (II) to turn (II) into

$$\text{(II)'} \quad x_2/2 = 1.5$$

Gaussian Elimination for Small Systems

So now we have

$$\begin{aligned} &\text{(I)} && 2x_1 + x_2 = 1 \\ &\text{(II)'} && x_2/2 = 1.5 \end{aligned}$$

Solve for $x_2 = 3$. Plug into (I) to get

$$2x_1 + 3 = 1$$

and so $x_1 = -1$.
Which is correct (check it!).

Matrix Form

$$\mathbf{A}\mathbf{x} = \mathbf{b}$$

where

$$\mathbf{A} = \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix}, \mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, \text{ and } \mathbf{b} = \begin{pmatrix} 1 \\ 2 \end{pmatrix}.$$

Do all linear systems have solutions?

What about

$$\begin{aligned} &(\mathrm{I}) \quad x_1 + x_2 = 1 \\ &(\mathrm{II}) \quad x_1 + x_2 = 2 \end{aligned}$$

You get a solution for all right hand sides if $\det(\mathbf{A}) \neq 0$.

Eigenvalues and Eigenvectors

λ is an **eigenvalue** of a square matrix $\mathbf{A}$ with eigenvector $\mathbf{x} \neq 0$ if

$$\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$$

The eigenvectors of a square matrix are the roots of the **characteristic polynomial**

$$p_C(z) = \det(z\mathbf{I} - \mathbf{A})$$

So there are N eigenvalues if $\mathbf{A}$ is $N \times N$.

Example I

Find the eigenvalues and eigenvectors of

$$\mathbf{A} = \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}.$$

Step 1: find the roots of

$$p_C(z) = \det(z\mathbf{I} - \mathbf{A}) = \det \begin{pmatrix} z-2 & 1 \\ 1 & z-2 \end{pmatrix} = z^2 - 4z + 3.$$

Use the quadratic formula to find $\lambda = 1$ and $\lambda = 3$

How about the vectors?

Fact: if $\mathbf{x}$ is an eigenvector for λ, the so is $a\mathbf{x}$ for any scalar $a \neq 0$.
I'll pick the $\mathbf{x}$ with $x_1 = 1$ (which works most of the time).
So, for $\lambda = 3$ and $x_1 = 1$, $\mathbf{Ax} = 3\mathbf{x}$ means

$$2 - x_2 = 3 \text{ and } -1 + 2x_2 = 3x_2$$

Both equations agree that $x_2 = -1$. So

$$\mathbf{x} = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

does the job.

And now for $\lambda = 1$

Same story. Let $x_2 = 1$. Then $\mathbf{Ax} = \mathbf{x}$ means

$$2x_1 - 1 = 1 \text{ and } -x_1 + 2 = 1,$$

and both equations agree that $x_1 = 1$, so

$$\mathbf{x} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

A little about multiplicity

How about

$$\mathbf{A} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

Do the math to get

$$p_C(z) = z^2$$

so the only eigenvalue is $\lambda = 0$ and it has **algebraic multiplicity** 2. Vectors? If $x_1 = 1$ and $\mathbf{Ax} = 0$, that means

$$x_2 = 0 \text{ so } \mathbf{x} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

Can $x_2 \neq 0$?

Can you find another eigenvector with $x_2 = 1$?

- $\mathbf{Ax} = 0$ and $x_2 = 1$ imply that $1 = 0$, so you can't.
- The dimension of the null space of $\lambda\mathbf{I} - \mathbf{A} = -\mathbf{A}$ (**geometric multiplicity**) is one.
- If the algebraic multiplicity and the geometric multiplicity of an eigenvalue are not the same, ...
  - that's numerical trouble, and
  - things can get very weird.
- So, it's an opportunity.

Wisdom on weirdness

When the going gets weird, the weird turn pro.
H. S. Thompson

But Tim, how do I know I'm in command of the prerequisites?

I'm here to help, so . . .

- I'm giving a 50 point test on them very soon.
  - This test counts for real.
  - Most of you will do very, very well and start off right.
  - Some of you will find that you need to review a few things.
- See the review test on the Moodle page or at
  - http://www4.ncsu.edu/~ctk/Resources_580/review.pdf
  - http://www4.ncsu.edu/~ctk/Resources_580/review.tex

What about the exam?

- Taylor series you should know
- Integrals; double integrals; differentiation
- 2×2 and easy 3×3
- Very simple programming
  Take some input; do something; return a result

What is this course about?

Big Picture:

- Numerical Analysis is about getting useful answers with algorithms:
  - numbers,
  - yes-no decisions,
  - pictures and movies,
- and understanding what you did and what the limitations are.

This is the best stuff there is.

This is the best time in human history to learn it.

What is MA 580 about?

Details:

- 580 is the entry-level course for all of our NA courses.
- Solution of Linear Equations: $\mathbf{Ax} = \mathbf{b}$
- Linear Least Squares Problems: $\min \|\mathbf{Ax} - \mathbf{b}\|_2^2$
- Eigenvalue problems: $\mathbf{Ax} = \lambda \mathbf{x}$
- Nonlinear equations: $\mathbf{F}(\mathbf{x}) = 0$

Things you need to do.

- Read Pages 1–36 of the pink book (Ipsen).
- Read Chapters 1–4 of the Matlab book.
  Play with the examples to get comfortable.
- Read pages 1–7 of the red book (Kelley).
- Learn LaTeX. Play with the sample file
  http://www4.ncsu.edu/~ctk/Resources_580/sample.tex
- Review the prerequisites and prepare for the first exam.
  The review.tex and review.pdf files will help.
  http://www4.ncsu.edu/~ctk/Resources_580/review.tex
  http://www4.ncsu.edu/~ctk/Resources_580/review.pdf