Numerical Analysis and Computing

Lecture Notes #01 — First Meeting

Joe Mahaffy,
⟨mahaffy@math.sdsu.edu⟩

Department of Mathematics
Dynamical Systems Group
Computational Sciences Research Center
San Diego State University
San Diego, CA 92182-7720

http://www-rohan.sdsu.edu/~jmahaffy

Spring 2010

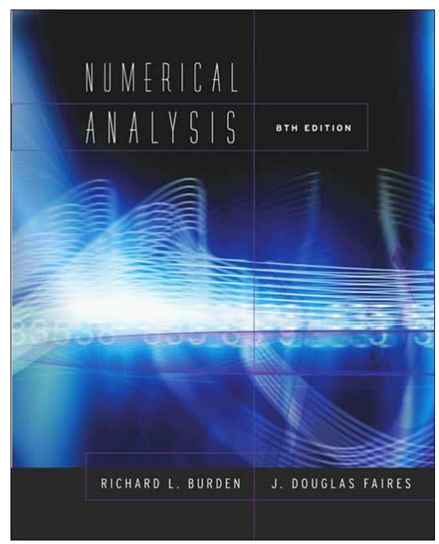
Outline

1. The Professor
   - Contact Information, Office Hours
2. The Class — Overview
   - Literature & Syllabus
   - Grading
   - CSU Employee Furloughs
   - Expectations and Procedures
3. The Class...
   - Resources
   - Formal Prerequisites
4. Introduction
   - The What? Why? and How?
5. Application
   - Analysis

Contact Information

Office	GMCS-593
Email	mahaffy@math.sdsu.edu
Web	http://www-rohan.sdsu.edu/~jmahaffy
Phone	(619)594-3743
Office Hours	MW: 1 – 2, 3 – 4), and by appointment

Basic Information: The Book



Title:
"Numerical Analysis,"
8th Edition

Authors:
Richard L. Burden &
J. Douglas Faires

Publisher:
Thomson – Brooks/Cole

ISBN:
0-534-39200-8

Basic Information: Syllabus

Chapter	Title
1	Mathematical Preliminaries
2	Solutions of Equations in One Variable
3	Interpolation and Polynomial Approximation
4	Numerical Differentiation and Integration
6	Direct Methods for Solving Linear Systems
8	Approximation Theory
7	Iterative Techniques in Matrix Algebra
Math 542: Numerical Solutions of Differential Equations	
5	Initial-Value Problems for ODEs
11	Boundary Value Problems for ODEs
Math 543: Numerical Matrix Analysis	
7	Iterative Techniques in Matrix Algebra
9	Approximating Eigenvalues
Math 693a: Advanced Numerical Analysis (Numerical Optimization)	
10	Numerical Solution of Nonlinear Systems of Equations
Math 693b: Advanced Numerical Analysis (Numerics for PDEs)	
12	Numerical Solution of PDEs

Basic Information: Grading

Approximate Grading

Homework*	40%
Midterm+	30%
Final×	30%

* Both theoretical, and implementation (programming) — Matlab will be the primary programming language. However, you can program in other languages if desired, but the instructor may not be able to help.

\+ The midterm is likely to be part take-home and part in-class.

× Scheduled time: Wednesday, May 19, 15:30am – 17:30pm. (Again likely to be part take-home and part in-class.)

CSU Employee Furloughs - AY 2009–2010

Due to extraordinary budget cuts to the CSU, student fees have *increased 32%*, many sections have been cut and faculty will be required to take *nine (9) unpaid furlough days* each semester.

This is the result of a dramatic cut to the CSU by the state after years of under-funding the system.

Expectations and Procedures, I

- Most class attendance is OPTIONAL — Homework and announcements will be posted on the class web page. If/when you attend class:
  - Please be on time.
  - Please pay attention.
  - Please turn off mobile phones.
  - Please be courteous to other students and the instructor.
  - Abide by university statutes, and all applicable local, state, and federal laws.

Expectations and Procedures, II

- Please, turn in assignments on time. (The instructor reserves the right not to accept late assignments.)
- The instructor will make special arrangements for students with documented learning disabilities and will `try` to make accommodations for other unforeseen circumstances, *e.g.* illness, personal/family crises, etc. in a way that is fair to all students enrolled in the class. **Please contact the instructor EARLY regarding special circumstances.**
- Students are expected **and encouraged** to ask questions in class!
- Students are expected **and encouraged** to to make use of office hours! If you cannot make it to the scheduled office hours: contact the instructor to schedule an appointment!

Expectations and Procedures, III

- Missed midterm exams: Don't miss exams! The instructor reserves the right to schedule make-up exams, make such exams oral presentation, and/or base the grade solely on other work (including the final exam).
- Missed final exam: Don't miss the final! Contact the instructor ASAP or a grade of incomplete or F will be assigned.
- **Academic honesty**: submit your own work — but feel free to discuss homework with other students in the class!

Honesty Pledges, I

- The following **Honesty Pledge** must be included in all programs you submit (as part of homework and/or projects):
  - I, (your name), pledge that this program is completely my own work, and that I did not take, borrow or steal code from any other person, and that I did not allow any other person to use, have, borrow or steal portions of my code. I understand that if I violate this honesty pledge, I am subject to disciplinary action pursuant to the appropriate sections of the San Diego State University Policies.
- Work missing the honesty pledge **may not be graded!**

Honesty Pledges, II

- Larger reports must contain the following text:
  - I, (your name), pledge that this report is completely my own work, and that I did not take, borrow or steal any portions from any other person. Any and all references I used are clearly cited in the text. I understand that if I violate this honesty pledge, I am subject to disciplinary action pursuant to the appropriate sections of the San Diego State University Policies. `Your signature`.
- Work missing the honesty pledge `may not be graded!`

Computer Resources

- Access to a (somewhat) current release of Matlab is highly recommended.
- Class accounts for the GMCS-422/428 labs will be available (username/password next class meeting).
- You can also use the Rohan Sun Enterprise system or another capable system.
- How to open a ROHAN account: **http://www-rohan.sdsu.edu/raccts.shtml**
- You may also want to consider buying the student version of Matlab: **http://www.mathworks.com/**

Math 541: Formal Prerequisites

Math 254, or Math 342A

254 ⇒ **Introduction to Linear Algebra**

- Matrix Algebra, Gaussian elimination, determinants, vector spaces, linear transformations, orthogonality, eigenvalues and eigenvectors.

342A ⇒ **Methods of Applied Mathematics, I**

- Vector analysis, divergence and Stokes' theorem, integral theorems. Matrix analysis, eigenvalues and eigenvectors, diagonalization. Introduction to ODEs. Computer software for matrix applications, solving, and graphing differential equations.

Math 541: Formal Prerequisites

CS 106, CS 107 or CS 205

106 ⇒ **Intro to Programming: FORTRAN**

- Problem solving using a computer, design of algorithms.

107 ⇒ **Intro to Programming: JAVA**

- Programming methodology and problem solving. Basic concepts of computer systems, algorithm design and development, data types, program structures.

205 ⇒ **Intro to Programming and Visualization**

- Problem solving skills for science, computing/software tools of computational science, computer communications, programming and visualization.

Math 541: Course Design

- Professor Joe Mahaffy thanks Professors Peter Blomgren and Don Short for extensive access to their experience and notes for this course.
- I will borrow heavily, edit, and post on the web the notes and homework assignments created from these past instructors, especially Peter Blomgren.

Math 541: Introduction — What we will learn

- Numerical tools for problem solving:

⇒ `powertool` Newton's Method for $f(x) = 0$.

⇒ `powertool` Least squares approximation.

⇒ `powertool` The Fast Fourier Transform (FFT).

⇒ `tool` Polynomial Interpolation.

⇒ `tool` Numerical differentiation and integration.

⇒ `foundation` Taylor's Theorem.

⇒ `foundation` Weierstrass' Theorem.

Math 541: Introduction — Why???

`Q:` Why are numerical methods needed?

`A:` To accurately approximate the solutions of problems that cannot be solved exactly.

`Q:` What kind of applications can benefit from numerical studies?

`A:` Engineering, physics, chemistry, computer, biological and social sciences.

Image processing / computer vision, computer graphics (rendering, animation), climate modeling, weather predictions, "virtual" crash-testing of cars, medical imaging (CT = Computed Tomography), AIDS research (virus decay vs. medication), financial math...

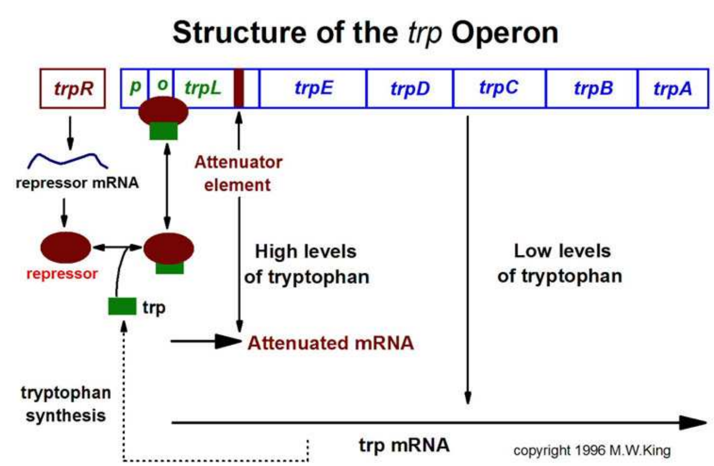
Math 541: Introduction — Computing Efficiency

Numerical tools for problem solving:

- Computers are getting faster, but the computer's speed is only one (a big one for sure!) part of the overall performance for a computation...
- Computing speed depends on **FLOPS** (floating-point operations or number of additions and multiplications) and **memory accesses**. These are largely questions of computer architecture and won't be examined in this course much.
- Numerical Algorithms are the center of this course, and their efficiency affects performance.

Research Problem from my Work

Genetic Control by Repression



Model for Conrol by Repression

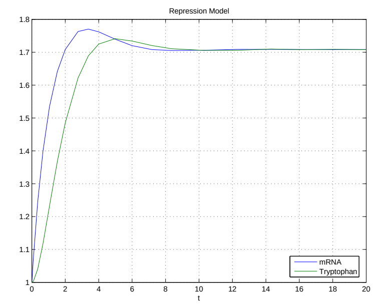
Let $x_1(t)$ be the concentration of mRNA and $x_2(t)$ be the concentration of the tryptophan (endproduct). This process is often called endproduct inhibition, and it is a negative feedback system. These systems, especially with delays, can result in oscillatory behavior.

$$\begin{aligned} \frac{dx_1(t)}{dt} &= \frac{a_1}{1+kx_2^n(t-R)} - b_1x_1(t) \\ \frac{dx_2(t)}{dt} &= a_2x_1(t) - b_2x_2(t) \end{aligned}$$

This is a system of first order delay differential equations, which is infinite dimensional because of the need for initial data including a history of the solution on the interval $[-R, 0]$.

Simulation of Repression Model

Simulated model with $a_1 = 2$, $a_2 = b_1 = b_2 = 1$, $n = 4$, and $R = 2$.
MatLab simulation uses package DDE23. You will study a related algorithm in Math 542, the Runge-Kutta-Felberg method for integrating ordinary differential equations (numerically solving the ODE).



Equilibrium Analysis

- Qualitative analysis of any differential equation begins with finding all equilibria for the system.
- The equilibria are found by solving the derivatives equal to zero.

$$\begin{aligned} \frac{a_1}{1+k\bar{x}_2^n} - b_1\bar{x}_1 &= 0 \\ a_2\bar{x}_1 - b_2\bar{x}_2 &= 0 \end{aligned}$$

- This gives a system of nonlinear equations equal to zero, which usually require numerically methods to approximate the equilibria. Here it easily reduces to a nonlinear scalar equation, $f(x) = 0$, which early in this course, we learn to solve.

$$\frac{a_1}{1+k\bar{x}_2^n} - \frac{b_1b_2}{a_2}\bar{x}_2 = 0 \quad \text{with} \quad \bar{x}_1 = \frac{b_2}{a_2}\bar{x}_2$$

Characteristic Equation

- The characteristic equation is used to study the local (linear) behavior near an equilibrium.
- The characteristic equation for delay differential equations is found like one does for ordinary differential equations (Math 537), but the result is an exponential polynomial with an infinite number of solutions.

$$\begin{vmatrix} -b_1-\lambda & f'(\bar{x}_2)e^{-\lambda R} \\ a_2 & -b_2-\lambda \end{vmatrix} = 0$$

$$(\lambda+b_1)(\lambda+b_2) - a_2f'(\bar{x}_2)e^{-\lambda R} = 0$$

Need to find complex solutions to this equation.

Characteristic Equation–Finding Eigenvalues

- The numerical simulation showed damped oscillations which suggests that all eigenvalues have negative real part.
- The characteristic equation is studied by letting $\lambda = \mu + i\nu$, which gives

$$(\mu+i\nu+b_1)(\mu+i\nu+b_2)-a_2f'(\bar{x}_2)e^{-\mu R}(\cos(\nu R)-i\sin(\nu R)) = 0$$

- This is solved numerically by simultaneously finding the real and imaginary parts equal to zero. Solving two nonlinear equations in two unknowns uses vector and matrix methods to extend our technique for solving $f(x) = 0$. We may get to these algorithms in this class, but they certainly appear in Math 693A.

Characteristic Equation–Numerical Eigenvalues

- This course examines some of the basics behind the packages for solving these problems. **MatLab** allows users to examine the coding algorithm, so knowledge from this course helps you better choose amongst different packages.
- We employed Maple's **fsolve** routine, and the first three pairs of eigenvalues with the largest imaginary parts are found.

$$\begin{aligned}
\lambda_{1,2} &= -0.19423 \pm 0.98036i \\
\lambda_{3,4} &= -0.55573 \pm 3.9550i \\
\lambda_{5,6} &= -0.0.68084 \pm 7.07985i
\end{aligned}$$

These eigenvalues show the damped oscillatory behavior and indicate the intervals between maxima are about 2π time units.

Maple code available from Website.