Numerical Solutions to Differential Equations

Lecture Notes #1 — Introduction

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Outline

- KTH MSc. Engineering Physics, Royal Institute of Technology (KTH), Stockholm, Sweden. Thesis Advisers: Michael Benedicks, Department of Mathematics KTH, and Erik Aurell, Stockholm University, Department of Mathematics. Thesis Topic: *"A Renormalization Technique for Families with Flat Maxima."*

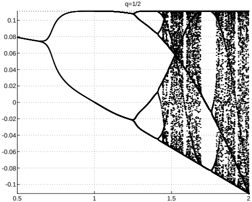

Figure: Bifurcation diagram for the family $f_{a,\frac{1}{2}}$ [Blomgren-1994]

- PhD. UCLA Department of Mathematics. Adviser: Tony F. Chan. PDE-Based Methods for Image Processing. Thesis title: *"Total Variation Methods for Restoration of Vector Valued Images."*

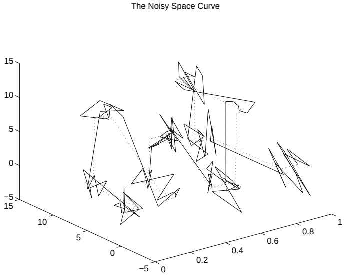

Figure: The noisy (SNR $= 4.62\,$dB), and recovered space curves. Notice how the edges are recovered. [BLOMGREN-1998]

- Research Associate. Stanford University, Department of Mathematics. Main Focus: Time Reversal and Imaging in Random Media (with George Papanicolaou, *et. al.*)

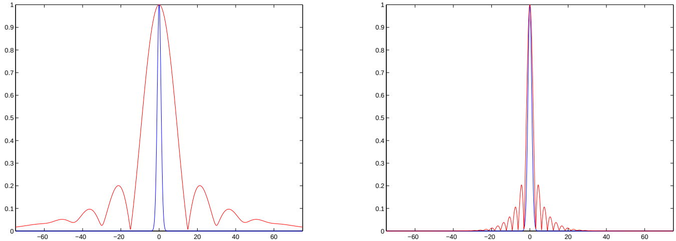

Figure: Comparison of the theoretical formula for a medium with $L = 600\,m$, $a_e = 195\,m$, $\gamma = 2.12 \times 10^{-5}\,m^{-1}$. [LEFT] shows a homogeneous medium, $\gamma = 0$, with $a = 40\,m$ TRM (in red / wide Fresnel zone), and a random medium with $\gamma = 2.12 \times 10^{-5}$ (in blue). [RIGHT] shows $\gamma = 0$, with $a = a_e = 195\,m$ (in red), and $\gamma = 2.12 \times 10^{-5}$, with $a = 40\,m$ (in blue). The match confirms the validity of [the theory]. [BLOMGREN-PAPANICOLAOU-ZHAO-2002]

- SDSU Professor, San Diego State University, Department of Mathematics and Statistics. Projects: Computational Combustion, Biomedical Imaging (Mitochondrial Structures, Heartcell Contractility, Skin/Prostate Cancer Classification).

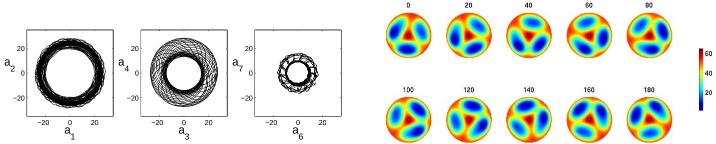

Figure: [LEFT] Phase-space projections produced by the time coefficients of the POD decomposition of the rotating pattern shown in [RIGHT]. [BLOMGREN-GASNER-PALACIOS-2005]

Contact Information

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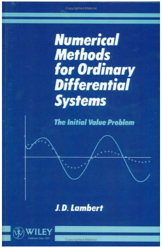
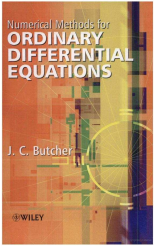
Phone	(USE EMAIL)
Office Hours	Tu: 9:00am – 10:30am, Th 2:00pm – 3:30pm and by appointment

Fun Times... $\Rightarrow$ Endurance Sports

- Triathlons:
  - (11) Ironman distance $(2.4 + 112 + 26.2)$ — 11:48:57
  - (16) Half Ironman distance — 5:14:20
- Running
  - (1) Trail Double-marathon (52 miles) — 10:59:00
  - (4) Trail 50-mile races — 9:08:46
  - (6) Trail 50k (31 mile) races — 5:20:57
  - (12) Road Marathons — 3:26:19 (7:52/mi)
  - (20) Road/Trail Half Marathons — 1:36:25 (7:21/mi)

- The following books are listed as "optional" for the class:
    - *Numerical Methods for Ordinary Differential Systems: The Initial Value Problem*, J.D. Lambert, John Wiley & Sons, 1991.
    - *Numerical Methods for Ordinary Differential Equations* (2nd Edition), J.C. Butcher, John Wiley & Sons, 2003.





The class is largely defined by the class notes and web-page; think of Lambert's book as the initial condition for the class, and Butcher's book as the limit as $t \to \infty$.

I recommend Butcher's book as an excellent reference, and if you have too much money get Lambert's book as well...

Goals

- Solve simple model equations to **illustrate** numerical solution of differential equations; **understand** the analysis behind derivation of schemes. (For modeling issues: see `Math 336` & `Math 636`: Mathematical Modeling.)
- **Main Focus: ODEs** — Differential equations involving only one independent variable. ODEs are classified according to their order, linearity (or non-linearity), and boundary conditions.
- **Some, but more in** `Math 693B`: **PDEs** — Differential equations involving more than one independent variable. PDEs are classified in various ways, the ODE classifications apply, and additionally they are divided into Elliptic, Parabolic and Hyperbolic equations.

2015 Goals

"Refresh" the course — some new material added (some old deleted).

More emphasis on practical computing to (1) illustrate the theory; and (2) work on programming skills.

Goals

"The purpose of computing is insight, not numbers."
— Richard Hamming (1962).

Grading

- `50.0%` **Homework:** — both theoretical, and implementation (programming) — Matlab is the recommended and supported environment, but feel free to program in 6510 assembler, Java, Fortran, C/C++, M$-D$^\flat$...
- `50.0%` **Project:** — details to be discussed (including in-class presentation).

Subject to revisions...

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!`

- Access to a (somewhat) current release of Matlab is highly recommended.
- The GMCS-422/428 labs will be available.
- 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/**
- **SDSU students can download a copy of matlab from http://www-rohan.sdsu.edu/~download/matlab.html**

- `Math 541`, Introduction to Numerical Analysis and Computing:
    - Solution of equations of one variable, direct methods in numerical linear algebra, least squares approximation, interpolation and uniform approximation, quadrature.
    - $\Rightarrow$ Linear Algebra, Intro to Programming.

- `Math 337`, Elementary Differential Equations:
    - Integration of first-order differential equations, initial and boundary value problems for second order equations, series solutions and transform methods, regular singularities.
    - $\Rightarrow$ Calculus.

The “Why?”

- Why solve Differential Equations (ODEs / PDEs)?
  - Frequently used to model Real World^{TM} physics / science / engineering problems.
- Why solve Differential Equations Numerically?
  - Closed-form solutions to most interesting problems are not available.

Ordinary Differential Equations — Order

Example: First order linear ODE —

$$\underbrace{y'(t)}_{\text{1st derivative}} + ay(t) = f(t).$$

Example: Second order linear ODE —

$$\underbrace{y''(t)}_{\text{2nd derivative}} + ay'(t) + by(t) = f(t).$$

Example: Second order non-linear ODE —

$$y''(t) + a \underbrace{y(t)y'(t)}_{\text{Nonlinear term}} + by(t) = f(t).$$

An n^{th} order ODE can be written on the form

$$F\left(t, y, \frac{dy}{dt}, \frac{d^2y}{dt^2}, \ldots, \frac{d^ny}{dt^n}\right) = 0.$$

It is **linear** if the function F is linear in the variables $\{y, \frac{dy}{dt}, \frac{d^2y}{dt^2}, \ldots, \frac{d^ny}{dt^n}\}$, *i.e.* a general linear ODE of order n can be written

$$\sum_{k=0}^{n} a_k(t) y^{(k)}(t) = f(t).$$

If this is not true (*i.e* the function F contains products of the dependent variables), the ODE is said to be **non-linear**.

ODEs — Homogeneous / Non-Homogeneous

The ODE

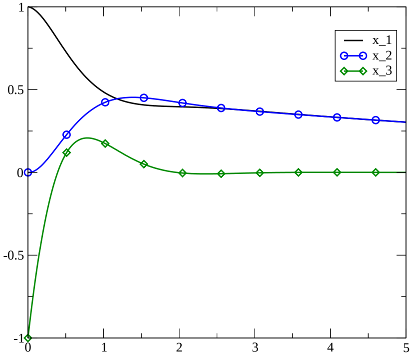
$$\sum_{k=0}^{n} a_k(t) y^{(k)}(t) = f(t)$$

is **homogeneous** (unforced) if and only if $f(t) \equiv 0$, otherwise it is **non-homogeneous** (forced).

If the coefficients $a_k(t)$ are constant we have a **constant coefficient ODE**, otherwise we have a **variable coefficient ODE**.

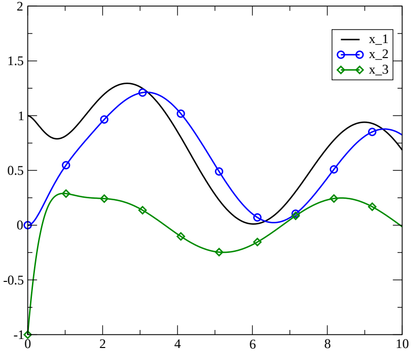
ODEs — Example: Linear Unforced ($f(t) = 0$) 3D ODE

$$\frac{d\tilde{\mathbf{x}}}{dt} = \frac{1}{20}\begin{bmatrix} -21 & 19 & -20 \\ 19 & -21 & 20 \\ 40 & -40 & -40 \end{bmatrix}\tilde{\mathbf{x}}, \quad \tilde{\mathbf{x}}(0) = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}.$$



ODEs — Example: Linear 3D ODE

$$\frac{d\tilde{\mathbf{x}}}{dt} = \frac{1}{20}\begin{bmatrix} -21 & 19 & -20 \\ 19 & -21 & 20 \\ 40 & -40 & -40 \end{bmatrix}\tilde{\mathbf{x}} + \begin{bmatrix} \sin(t) \\ 0 \\ 0 \end{bmatrix}, \quad \tilde{\mathbf{x}}(0) = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}.$$



ODEs — Initial / Boundary Value Problems

The preceding two examples illustrate **Initial Value Problems** — the dependent variables (and appropriate derivatives) are known at the initial values of the independent variable.

Sample problem: At time $t = 0$, you fire off a missile with a speed of 1000mph, at an angle of 10°. — Track the trajectory.

In **Boundary Value Problems** the values of the dependent variables (and appropriate derivatives) are known at the terminating values of the independent variable.

Sample problem: At time $t = T$, you want your dart to hit the center of the dart board. How (speed and angle) should you throw the dart to accomplish this?

If some values (dependent variables / derivatives) are known at the initial boundary, and some at the terminating point, the problem is called a **two-point boundary value problem.**

The canonical (standard) form of an ODE is a system of simultaneous first order ODEs:

$$\begin{aligned}
\frac{dy_1}{dt} &= f_1(y_1, y_2, \dots, y_n, t) \\
\frac{dy_2}{dt} &= f_2(y_1, y_2, \dots, y_n, t) \\
&\vdots \\
\frac{dy_n}{dt} &= f_n(y_1, y_2, \dots, y_n, t).
\end{aligned}$$

We can transform *any* n^{th} order ODE into canonical form...

Transformation into Canonical Form

Given a general n^{th} order ODE of the form

$$\frac{d^n y}{dt^n} = F\left(y, \frac{dy}{dt}, \frac{d^2 y}{dt^2}, \ldots, \frac{d^{n-1} y}{dt^{n-1}}, t\right)$$

Introduce, and identify:

$$\begin{array}{ccccccc}
 & & y & = & y_1 & & \\
\frac{dy}{dt} & = & \frac{\mathbf{dy_1}}{\mathbf{dt}} & = & y_2 & = & \mathbf{f_1}\left(\mathbf{y_1}, \mathbf{y_2}, \mathbf{y_3}, \ldots, \mathbf{y_n}, \mathbf{t}\right) \\
 & & \vdots & & & & \\
\frac{d^{n-1}y}{dt^{n-1}} & = & \frac{\mathbf{dy_{n-1}}}{\mathbf{dt^{n-1}}} & = & y_n & = & \mathbf{f_{n-1}}\left(\mathbf{y_1}, \mathbf{y_2}, \mathbf{y_3}, \ldots, \mathbf{y_n}, \mathbf{t}\right) \\
\frac{d^n y}{dt^n} & = & \frac{\mathbf{dy_n}}{\mathbf{dt}} & = & & & F\left(y_1, y_2, y_3, \ldots, y_{n-1}, t\right) \\
 & & & = & & & \mathbf{f_n}\left(\mathbf{y_1}, \mathbf{y_2}, \mathbf{y_3}, \ldots, \mathbf{y_n}, \mathbf{t}\right).
\end{array}$$

Example: A Very Geocentric View of the Universe, I

The equations of motion of a body moving in earth's gravitational field (ignoring the existence of the sun and the moon for simplicity) are

$$\begin{aligned} x'' &= -G\frac{x}{(x^2+y^2+z^2)^{3/2}} \\ y'' &= -G\frac{y}{(x^2+y^2+z^2)^{3/2}} \\ z'' &= -G\frac{z}{(x^2+y^2+z^2)^{3/2}} \end{aligned}$$

where G is the gravitational constant (which we will set to 1 for further simplicity).

Example: A Very Geocentric View of the Universe, II

By defining

$$x_1 = x, \quad x_2 = \frac{dx}{dt}, \quad x_3 = y, \quad x_4 = \frac{dy}{dt}, \quad x_5 = z, \quad x_6 = \frac{dz}{dt}$$

we can write the ODEs in canonical form...

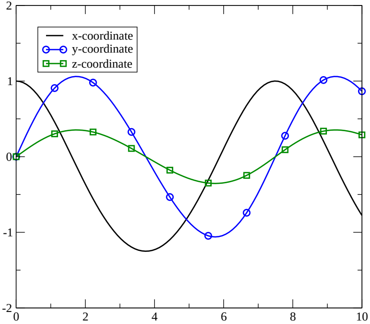
$$\frac{d}{dt}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{bmatrix} = \begin{bmatrix} x_2 \\ -G\frac{x_1}{(x_1^2+x_3^2+x_5^2)^{3/2}} \\ x_4 \\ -G\frac{x_3}{(x_1^2+x_3^2+x_5^2)^{3/2}} \\ x_6 \\ -G\frac{x_5}{(x_1^2+x_3^2+x_5^2)^{3/2}} \end{bmatrix}$$

Example: A Very Geocentric View of the Universe, III

With initial conditions (below) the solutions for (x, y, z) are:

$$x = x_1 = 1, \quad y = x_3 = 0, \quad z = x_5 = 0$$

$$\frac{dx}{dt} = x_2 = 0, \quad \frac{dy}{dt} = x_4 = 1, \quad \frac{dz}{dt} = x_6 = 1/3,$$



Let us consider the single first order ODE

$$\frac{dy}{dt} = f(t, y), \quad y(t_0) = y_0.$$

There are two approaches to numerically solving this ODE:

Computing Solutions, II

Approach #1: Integrate the function $f(t, y)$ using a numerical integration scheme (like the ones discussed in **Math 541**.) We rewrite the equation as:

$$dy = f(t, y)dt$$

and integrate

$$y_{i+1} - y_i = \int_{y_i}^{y_{i+1}} dy = \int_{t_i}^{t_{i+1}} f(t, y)dt,$$

and apply a numerical integration scheme on the right-hand-side.

Notice that $y = y(t)$, so that the integral on the right-hand-side depends on the quantity $y(t)$ we are trying to compute...

Approach #2: Instead of viewing the problem in terms of integration, we find a numerical (*finite difference*) approximation to the derivative (the left-hand-side)

$$\frac{dy}{dt} = f(t, y).$$

If we use the *forward difference*, we get

$$\frac{y_{i+1} - y_i}{t_{i+1} - t_i} = f(t_i, y).$$

In this class we are going to use methods based on approach #2.

The forward difference method shown on the previous slide is known as **Euler's Method**. It is not the best method, but is a natural starting point for our discussion on numerical solutions of ODEs.

Usually the time points t_i are uniformly spaced, *i.e.* $t_i = t_0 + ih$. We write

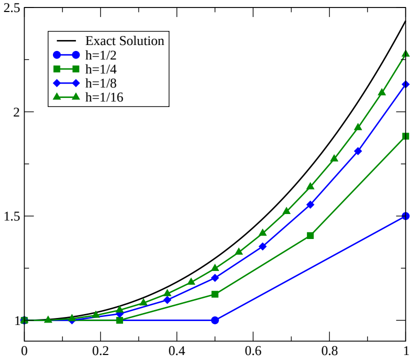
Euler's method

$$\mathbf{y_{i+1} = y_i + h\,f(t_i, y)}, \quad \mathbf{y(t_0) = y_0}, \quad \mathbf{t_i = t_0 + i\,h}$$

Euler's Method — Example, $y' = y + 2t - 1$

Exact Solution: $y(t) = 2e^t - 2t - 1$

Euler's method on the interval $[0, 1]$, with $h \in \{1/2, 1/4, 1/8, 1/16\}$.



Euler's Method — Things to Quantify

Accuracy:

We have seen that the quality of the numerical solution depends on the step size h.

Some of the concepts we need to define in order to analyze numerical methods for ODEs:

Consistency:

Is the numerical scheme solving the right problem?

Stability:

Is the numerical scheme robust with respect to propagation of round-off errors?

Convergence:

Do we get the right numerical solution as $h \searrow 0$???