MATH 350: Introduction to Computational Mathematics

Chapter I: Mathematical Modeling, Taylor Series, Floating-Point Numbers, and MATLAB

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Outline

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What is "computational mathematics"?

Possible answer:

Definition

"Computational mathematics is concerned with the study of algorithms (or numerical methods) for the solution of computational problems in science and engineering."

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Desirable properties of algorithms:

- accuracy
- efficiency (speed and memory use)
- reliability/stability

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- numerical algorithms can contain truncation errors
- programming errors

Physical Problem

A skydiver jumps out of an airplane (from sufficiently high altitude). What is his *terminal velocity*? (picture below taken from [Prof. Kallend's website])

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This leads to the first model we will use:

$$\frac{dv}{dt}(t) = \frac{F_g + F_d(t)}{m} = g - \frac{c}{m}v(t). \tag{1}$$

Approximate Solutions

- The ODE

$$\frac{\mathrm{d}v}{\mathrm{d}t}(t) = g - \frac{c}{m}v(t)$$

is linear first-order (also separable) and has the analytical solution (assuming $v(0) = v_0 = 0$)

$$v(t) = \frac{gm}{c}\left(1 - \mathrm{e}^{-(c/m)t}\right). \tag{2}$$

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Note: Terminal velocity is obtained by taking $t \to \infty$, so $v_T = \frac{gm}{c}$.
- The simplest method for obtaining a numerical solution of any first-order ODE $y'(t) = f(t, y)$ is Euler's method (approximate $y'(t) \approx \frac{y(t+h)-y(t)}{h}$, where h is some *stepsize* for the time step):
$$y'(t) = f(t, y) \quad \longrightarrow \quad y(t+h) \approx y(t) + hf(t, y)$$

Euler's Method

For our problem the general Euler formulation results in

$$v'(t) = \underbrace{g - \frac{c}{m}v(t)}_{=f(t,v)} \quad \longrightarrow \quad v(t+h) \approx v(t) + h\left(g - \frac{c}{m}v(t)\right).$$

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In algorithmic form we have

$$v_{n+1} = v_n + h\left(g - \frac{c}{m}v_n\right), \quad n = 0, 1, 2, \ldots,$$

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See MATLAB example `SkydiveDemo.m`

Improved Mathematical Model

The dependence of the drag force due to air resistance is actually proportional to the square of the velocity, so $F_d = -\tilde{c}v^2$. Here $\tilde{c}$ is now a different *drag coefficient* (measured in kg/m).

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This leads to the second and improved model we will use:

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- This ODE is **nonlinear** first-order (but still separable). Its analytical solution is (since $\int \frac{\mathrm{d}x}{a^2-x^2} = \frac{1}{a}\tanh^{-1}(\frac{x}{a})$ or $\frac{1}{2a}\ln\left|\frac{x+a}{x-a}\right|$, depending on which table/program you consult)

$$v(t) = \sqrt{\frac{gm}{\tilde{c}}}\tanh\left(\sqrt{\frac{g\tilde{c}}{m}}t\right) = \sqrt{\frac{gm}{\tilde{c}}}\frac{e^{2\sqrt{\frac{g\tilde{c}}{m}}t} - 1}{e^{2\sqrt{\frac{g\tilde{c}}{m}}t} + 1}. \tag{4}$$

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The terminal velocity is again obtained for $t \to \infty$, so $v_T = \sqrt{\frac{gm}{\tilde{c}}}$.

Improved Mathematical Model (cont.)

- A corresponding numerical solution via Euler's method is given in algorithmic form as

$$v_{n+1} = v_n + h\left(g - \frac{\tilde{c}}{m}(v_n)^2\right), \quad n = 0, 1, 2, \ldots,$$

where h is the stepsize, and $v_n = v(t_n)$ with $v_0 = 0$ as before.

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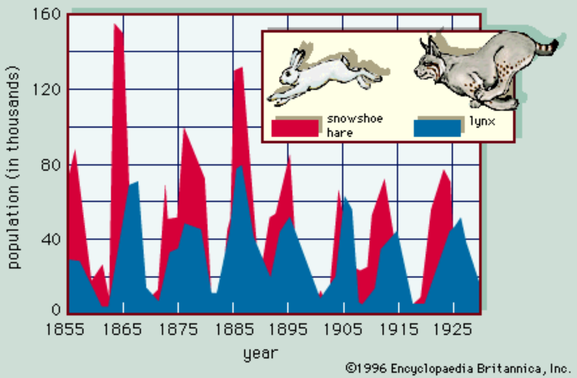
Remark

Note how simple the change in Euler's method is (just square the v-term in `Skydive.m`), and compare this to the extra effort that is needed to solve the nonlinear ODE analytically.

Physical Problem

According to records of the Hudson Bay Company, snowshoe hares and Canadian lynx populations have fluctuated as in the figure below

(see also [Marty '95, Zhang et al. '07] according to which this situation is **not** a predator-prey problem)



Mathematical Model

We treat lynx as predators and hares as prey and model their dependence by a Lotka-Volterra system

$$\begin{aligned} \frac{\mathrm{d}H(t)}{\mathrm{d}t} &= aH(t) - bH(t)L(t) \\ \frac{\mathrm{d}L(t)}{\mathrm{d}t} &= -cL(t) + dH(t)L(t) \end{aligned} \tag{5}$$

Here t denotes time, H population of hares, L population of lynx,

- $a = 0.5$ denotes birth rate of hares
- $b = 0.02$ denotes death rate of hares (depends on interaction with lynx “how good are lynx at killing hares”)
- $c = 0.4$ denotes death rate of lynx
- $d = 0.004$ denotes birth rate of lynx (depends on interaction with hares “how well do hares feed lynx”)

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Again, the simplest numerical method for first-order IVPs is Euler's method. Here

$$\frac{dH(t)}{dt} = aH(t) - bH(t)L(t) \quad \to \quad H_{n+1} = H_n + h\left(aH_n - bH_nL_n\right)$$
$$\frac{dL(t)}{dt} = -cL(t) + dH(t)L(t) \quad \to \quad L_{n+1} = L_n + h\left(-cL_n + dH_nL_n\right)$$

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This is now a *system of ODEs*, but the MATLAB code is the same (see `LynxHareDemo.m`)

Projectile Motion

This example is discussed at

http://blog.wolfram.com/2010/09/27/do-computers-dumb-down-math-education/

Load `matheducation.nb` into Mathematica and play with it!

The TED talk mentioned in the document is here:

http://www.ted.com/talks/lang/eng/conrad_wolfram_teaching_kids_real_math_with_computers.html

From YouTube

Modeling Summary

There are many other kinds of mathematical modeling situations such as

- *data fitting* (e.g., find the best approximation – from a certain linear/nonlinear function class – to given measurement data)
- *parameter estimation* (e.g., find the best parameters for one of the models used earlier – drag coefficient, birth/death rate, etc.)
- *statistical/probabilistic modeling* (e.g., non-deterministic models in finance or weather prediction)
- *discrete modeling* (e.g., determining the best location of a fire department or hospital)
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An entertaining overview of the field of mathematical modeling is provided by Charlie's activities on the TV show *NUMB3RS*.

Modeling Summary (cont.)

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For example, the skydiving model could be further improved by including a gravitational "constant" g that depends on the altitude x according to Newton's inverse square law of gravitational attraction

$$g(x) = g(0)\frac{R^2}{(R+x)^2},$$

where $R \approx 6.37 \times 10^6$(m) denotes the earth's radius, and $g(0) = 9.81(\text{m}/\text{s}^2)$ denotes the values of the gravitational constant at the earth's surface (see Chapter 7).

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The central idea is to match a given function locally by some (low-degree) polynomial, and then evaluate this polynomial instead.

Example

Match $f(x) = \sqrt{x}$ at $x_0 = 1$ by a quadratic polynomial, i.e., find constants a_0, a_1, a_2 such that

$$p_2(x) = a_0 + a_1 x + a_2 x^2 \approx f(x) \tag{6}$$

for values of x near $x_0 = 1$.

Return

Solution

We will determine the coefficients a_0, a_1, a_2 by matching derivatives of f at $x_0 = 1$, i.e., we will enforce (3 conditions for 3 coefficients)

$$\begin{aligned} p_2(1) &= f(1) = 1 \\ p_2'(1) &= f'(1) = \frac{1}{2} \\ p_2''(1) &= f''(1) = -\frac{1}{4} \end{aligned}$$

since we know $f'(x) = \frac{1}{2\sqrt{x}}$, $f''(x) = -\frac{1}{4x^{3/2}}$.

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In fact, in many cases we will not actually know the functions f, f', f'', etc., but only their values at the specified point.
Note that this is not the most efficient way to obtain the Taylor approximation (but it illustrates where it comes from).

Since our assumption (6) implies

$$\begin{aligned} p_2'(x) &= a_1 + 2a_2 x, \\ p_2''(x) &= 2a_2 \end{aligned}$$

we obtain a system of three linear equations in the three unknowns a_0, a_1 and a_2:

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Solving this triangular system we get $a_2 = -\frac{1}{8}$, $a_1 = \frac{3}{4}$, and $a_0 = \frac{3}{8}$ so that

$$p_2(x) = \frac{3}{8} + \frac{3}{4}x - \frac{1}{8}x^2.$$

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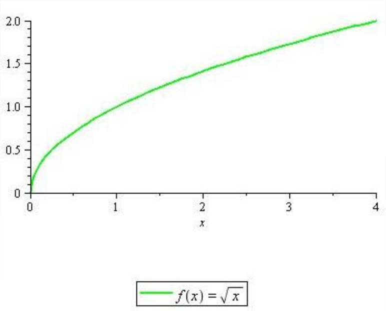

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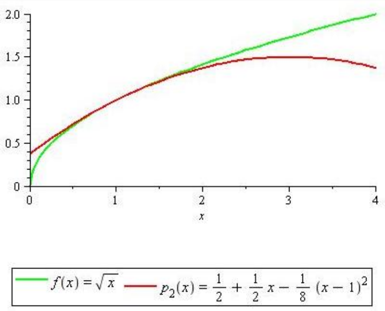

Taylor Polynomials

In general, we can use Taylor's formula to obtain an n-th degree polynomial which matches the first n derivatives of f at some number x_0:

$$f(x) \approx p_n(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)}{2}(x - x_0)^2 + \frac{f'''(x_0)}{6}(x - x_0)^3 + \ldots + \frac{f^{(n)}(x_0)}{n!}(x - x_0)^n$$

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Taylor Polynomials

In general, we can use Taylor's formula to obtain an n-th degree polynomial which matches the first n derivatives of f at some number x_0:

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The polynomial in (7) is called the n-th degree Taylor polynomial for f at x_0.

Example

Let $f(x) = e^x$ and find $p_n(x)$ for $x_0 = 0$.

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Since $f^{(k)}(x) = e^x$, $k = 0, 1, 2, \ldots, n$, we get

$$p_n(x) = \sum_{k=0}^{n} \frac{f^{(k)}(x_0)}{k!}(x - x_0)^k$$

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Theorem (Taylor's Theorem)

Assume f is $n+1$ times continuously differentiable on an interval I containing the point x_0. Then there exists a number ξ between x and x_0 such that

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The problem is that ξ is somewhere between x and x_0, but we don't know exactly where. Therefore we may obtain estimates for the error by examining certain "worst cases" of $E_{n+1}(x)$.

How to use Taylor's theorem?

Example

Let $f(x) = e^x$ and $x_0 = 0$. How accurate is $p_n(\frac{1}{2})$? More precisely, how large should n be so that the error $E_{n+1}(\frac{1}{2}) = \sqrt{e} - p_n(\frac{1}{2}) < 10^{-4}$?

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From Taylor's theorem we have

$$E_{n+1}(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x - x_0)^{n+1}$$

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We also know $f^{(n+1)}(x) = e^x$ for all x. Thus

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Solution (cont.)

We concluded above that $0 \le \xi \le \frac{1}{2}$, so we get (since the exponential function is increasing)

$$\frac{1}{2^{n+1}(n+1)!} \le E_{n+1}(\frac{1}{2}) = \frac{e^{\xi}}{2^{n+1}(n+1)!} \le \frac{e^{1/2}}{2^{n+1}(n+1)!}.$$

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The whole point of the exercise is to approximate the value of $\sqrt{e} = e^{1/2}$, so we need to use a *known* upper bound above.
Since we know that $2 < e < 3$, we can safely estimate

$$\frac{e^{1/2}}{2^{n+1}(n+1)!} < \frac{2}{2^{n+1}(n+1)!} = \frac{1}{2^{n}(n+1)!}$$

Solution (cont.)

Therefore, to ensure $E_{n+1}(\frac{1}{2}) < 10^{-4}$ we want to pick n such that

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This implies $n = 5$ (since $2^4 5! = 1920$ and $2^5 6! = 23040$).

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Note that the remainder depends on the point x of evaluation, and that in many cases the Taylor series will converge only for certain values of x near the point x_0 (within a ball/interval whose radius is called the radius of convergence). See the Maple worksheet `Taylor.mw`.

Alternate formulation of Taylor's theorem

For our purposes it will often be better to use Taylor's theorem in the following form:

Theorem

Assume f is $n+1$ times continuously differentiable on an interval I containing both x_0 and x_0+h for some (small) number h. Then there exists a number ξ somewhere between x_0 and x_0+h such that

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Note that we get this formulation from the previous one by replacing x by x_0+h so that $x - x_0 = h$.

In this new representation we can say

$$E_{n+1}(x_0) = \mathcal{O}(h^{n+1}), \quad \text{as } h \to 0,$$

which means $|E_{n+1}(x_0)| \leq C|h|^{n+1}$ for some constant C.

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Remark

From the alternate form of Taylor's theorem we can get the important estimates

$$f(x+h) = f(x) + \mathcal{O}(h) \tag{8}$$

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Estimate (9) implies

$$f'(x) = \frac{f(x+h) - f(x)}{h} + \mathcal{O}(h),$$

which plays a crucial role in our understanding of many numerical methods (e.g., Euler's method).

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Consider $\sum_{k=1}^{\infty}(-1)^k a_k$ *with* $a_k \geq 0$. *If the sequence* $\{a_k\}$ *is decreasing and* $\lim_{k\to\infty} a_k = 0$, *then the series converges.*

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Consider $\sum_{k=1}^{\infty}(-1)^k a_k$ *with* $a_k \geq 0$. *If the sequence* $\{a_k\}$ *is decreasing and* $\lim_{k\to\infty} a_k = 0$, *then the series converges. Moreover,*

$$E_{n+1} = \left| \underbrace{\sum_{k=1}^{\infty}(-1)^k a_k}_{=S} - \underbrace{\sum_{k=1}^{n}(-1)^k a_k}_{=S_n} \right| \leq a_{n+1},$$

i.e., the truncation error is bounded by the next (unused) term.

Outline

Most computer programming languages (such as C/C++/C#, Java, Fortran, or MATLAB) use floating-point arithmetic. Even though we usually don't have to worry much about this in everyday computing, it is good to have a basic understanding of floating-point numbers for those rare occasions when something unexpected happens.

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Most technical computing environments (including MATLAB) use the IEEE standard for floating-point arithmetic. In particular, MATLAB uses the IEEE double-precision format[1] which uses a word length of 64 bits to represent a number (see also the details in Chapter 1.7 of [NCM]).

[1] and since MATLAB 7 also single-precision

Normalized Floating-Point Numbers

Numbers are represented as

$$x = \pm(1 + f) \cdot 2^e,$$

where $0 \le f < 1$ is the fraction or mantissa, and the exponent $-1022 \le e \le 1023$ is an integer.

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- Finite f implies finite precision (i.e., discrete spacing of floating point numbers),
- finite e implies finite range (there is a minimum and maximum representable number).

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	binary	decimal
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Exceptions: Numbers larger than `realmax` will cause *overflow*, while those smaller than `realmin` will lead to *underflow*. The number zero is also treated as an exception.

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Note the “hole around zero”.

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`floatgui` with `t` $= 1$, `emin` $= -2$, `emax` $= 1$

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&= \frac{1}{2^4}\left(1+\frac{1}{2}+\frac{0}{2^2}+\frac{0}{2^3}+\frac{1}{2^4}+\frac{1}{2^5}+\frac{0}{2^6}+\frac{0}{2^7}+\frac{1}{2^8}+\ldots\right) \\
&= \frac{1}{16}\left(1+\frac{9}{16}+\frac{9}{16^2}+\frac{9}{16^3}+\frac{9}{16^4}+\ldots\right)
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A (perhaps surprising) weakness of the binary (or hexadecimal) computer representation of numbers is the representation of the decimal number $1/10$.

In fact we have,

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See "disasters due to bad numerical computing".

Example

Solve the following linear system with MATLAB

$$\begin{aligned} 17x_1 + 5x_2 &= 22 \\ 1.7x_1 + 0.5x_2 &= 2.2. \end{aligned}$$

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The system

$$\begin{aligned} x_1 + 2x_2 &= 2 \\ 2x_1 + 4x_2 &= 4 \end{aligned}$$

causes no such problems (see also `RoundoffDemo.m`).

Example

Evaluate $f(x) = \sqrt{x^2 + 1} - 1$ in MATLAB for $x = 10^{-n}$, $n = 0, 1, \ldots, 5$ using both double-precision and single-precision.

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Solution

The "exact" answers (obtained in Maple with much higher precision) are

x	$\sqrt{x^2+1}$	$f(x)$
1	$\sqrt{2} = 1.4142135623730950488$	0.4142135623730950488
0.1	$\sqrt{1.01} = 1.0049875621120890270$	0.0049875621120890270
0.01	$\sqrt{1.0001} = 1.0000499987500624961$	0.0000499987500624961
0.001	$\sqrt{1.000001} = 1.0000004999998750001$	0.0000004999998750001
0.0001	$\sqrt{1.00000001} = 1.0000000049999999875$	0.0000000049999999875
0.00001	$\sqrt{1.0000000001} = 1.0000000000500000000$	0.0000000000500000000

Use `LossOfSignificanceDemo.m`.

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\begin{aligned}
f(x) &= \sqrt{x^2+1} - 1 \\
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\end{aligned}
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Continue `LossOfSignificanceDemo.m` (can even improve double-precision this way).

Outline

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A *Very Elementary MATLAB Tutorial* is available directly from The MathWorks.

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- In addition to its interactive mode, MATLAB is also one of the easiest programming languages for solving mathematical problems.
- MATLAB's basic capabilities can be extended by calling functions defined in additional *toolboxes*.

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- Other MATLAB windows:
    - Command History window
    - Current Directory window
    - Workspace window (provides information about all the variables in use)

Other important things

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- In addition to the windows-based interface with all its bells and whistles MATLAB also has a command-line interface that can be invoked by using additional switches such as `matlab -nodesktop`.

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- Basic use of the editor is straightforward.
- Many advanced features are also available (such as adding breakpoints to your code for debugging purposes).

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- Go to the Command window. Make sure the folder your Command window is looking at is the same one you saved your program in!
- Run the program by entering its name (without the `.m` extension) at the command prompt.
- If your code contained an error, MATLAB will interrupt execution of the program and provide you with an error message. You can click on the error message, and will be taken to the corresponding place in the code in the Editor.

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