Basis for Numerical Analysis and Mathematical Modeling

Selis Önel, PhD

Mathematical Modeling and Numerical Analysis

Mathematical model→ uses mathematical language to describe a system

Application fields:

- Natural sciences and engineering disciplines
  - Physics, biology, earth science, meteorology, electrical engineering, chemical engineering, mechanical engineering, …
- Social sciences
  - Economics, psychology, sociology, political science, …

Mathematical Modeling and Numerical Analysis

- Eykhoff"s definition of Mathematical model (1974) →

'A representation of the essential aspects of an existing system (or a system to be constructed) which presents knowledge of that system in usable form'.

- Mathematical models can take many forms: (including but not limited to)
  - dynamical systems,
  - statistical models,
  - differential equations,
  - game theoretic models.

These models and other types can overlap

a given model can involve a variety of abstract structures

Ref: www.sciencedaily.com/articles/m/mathematical_model.htm

Reading Suggestion

- Read the following article
- Does it give you an idea about what mathematical modeling is

http://pages.cpsc.ucalgary.ca/~gaines/reports/PSYCH/IJISG91/index.html

Modeling Practical Reasoning

Brian R Gaines

Knowledge Science Institute,

University of Calgary

Calgary, Alberta, Canada T2N 1N4

gaines@cpsc.ucalgary.ca

Mathematical Modeling and Numerical Analysis

Basic groups of variables:

1. decision variables,
2. input variables,
3. state variables,
4. exogenous variables (fundamental in path analysis and structural equation modeling; in causal modeling these are the variables with no causal links (arrows) leading to them from other variables in the model)
5. random variables,
6. output variables

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Random Variable

- is a variable that takes different real values as a result of the outcomes of a random event or experiment
- is a real valued function defined over the elements of a sample space

There can be more than one random variable associated with an experiment.

Ex: if a coin is tossed ten times, one random variable associated with this experiment could be the number times the head shows up, a second random variable could be the number times the tail shows up and a third random variable could be the difference between number of times the head shows up and the number of times the tail shows up.

http://www.statistics.com/resources/glossary/r/randvar.php

Mathematical Modeling and Numerical Analysis

- Mathematical modelling problems are often classified into black box or white box models, according to how much a priori information is available of the system
- Black-box model is a system of which there is no a priori information available
- White-box (glass box or clear box) model is a system where all necessary information is available
- Practically all systems are somewhere between the black-box and white-box models, so this concept only works as an intuitive guide for approach
- It is preferable to use as much a priori information as possible to make the model more accurate

Ref: www.sciencedaily.com/articles/m/mathematical_model.htm

Computer Simulation

- Useful part of mathematical modelling of many natural systems in
  - physics, chemistry and biology,
  - human systems in economics, psychology, and social science
  - the process of engineering new technology
- Used to gain insight into the operation of these systems
- Mathematical model
  - Attempts to find analytical solutions to problems
  - Is a set of equations that has physical meaning
  - Uses a set of parameters and initial conditions
  - Enables the prediction of the behavior of the system
- Computer simulations build on, and are a useful adjunct to purely mathematical models in science, technology and entertainment.

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Mathematical Modeling and Numerical Analysis

Diagnosis of a physical problem:

- Define the physical problem
- Formulate it mathematically
- Solve the mathematical formulae
  - Analytical methods (Exact solution)
  - Numerical methods (Approximate solution)
- Interpret the results

Error in Numerical Analysis

An approximation error can occur because:

- Measurement of data is not precise (due to the instruments), or
- Approximations are used instead of the real data (e.g., 3.14 instead of π)

Absolute error is:

$$\epsilon = |b - a|$$

If **a≠0**, the **relative error** is:

$$\eta = \frac{|b-a|}{|a|},$$

Percent error is:

$$\delta = \frac{|b-a|}{|a|} \times 100\%.$$

Approximation Errors

- Round-off errors: Due to use of numbers with limited significant figures to represent exact numbers.

  ex: *e*, π, $\sqrt{7}$ (no fixed number of significant figures)

  ex: Computer base-2 representation cannot precisely represent certain exact base-10 numbers.

- Truncation errors: Due to use of approximations to represent exact mathematical procedures

Round-off Errors

Double-precision uses 16 digits

```
>> format long e
>> pi
ans =
   3.141592653589793e+000
>> sqrt(7)
ans =
   2.645751311064591e+000
```

Floating-point Representation: Used for fractional quantities in computers. Mantissa holds only a finite number of significant figures

$m \cdot b^x \rightarrow$ m: mantissa (significand)

b: base of number system

x: exponent

Numbers

Base 10	Base 2			
	2^3	2^2	2^1	2^0
1	0	0	0	1
2	0	0	1	0
3	0	0	1	1
4	0	1	0	0
5	0	1	0	1
6	0	1	1	0
7	0	1	1	1
8	1	0	0	0
9	1	0	0	1
10	1	0	1	0

Reference: Gilat, Subramaniam: *Numerical Methods with Matlab*

Numbers

10^4	10^3	10^2	10^1	10^0		10^{-1}	10^{-2}	10^{-3}	10^{-4}
↓	↓	↓	↓	↓		↓	↓	↓	↓
6	0	7	2	4	.	3	1	2	5

$$6\times10^4+0\times10^3+7\times10^2+2\times10^1+4\times10^0+3\times10^{-1}+1\times10^{-2}+2\times10^{-3}+5\times10^{-4}=60{,}724.3125$$

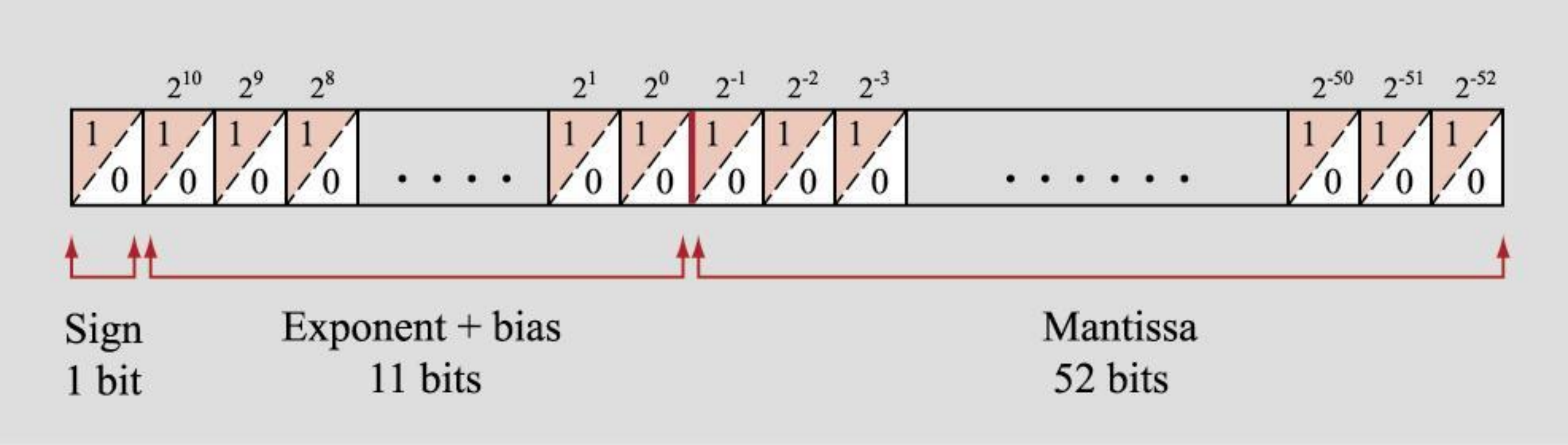
2^4	2^3	2^2	2^1	2^0		2^{-1}	2^{-2}	2^{-3}
↓	↓	↓	↓	↓		↓	↓	↓
1	0	0	1	1	.	1	0	1

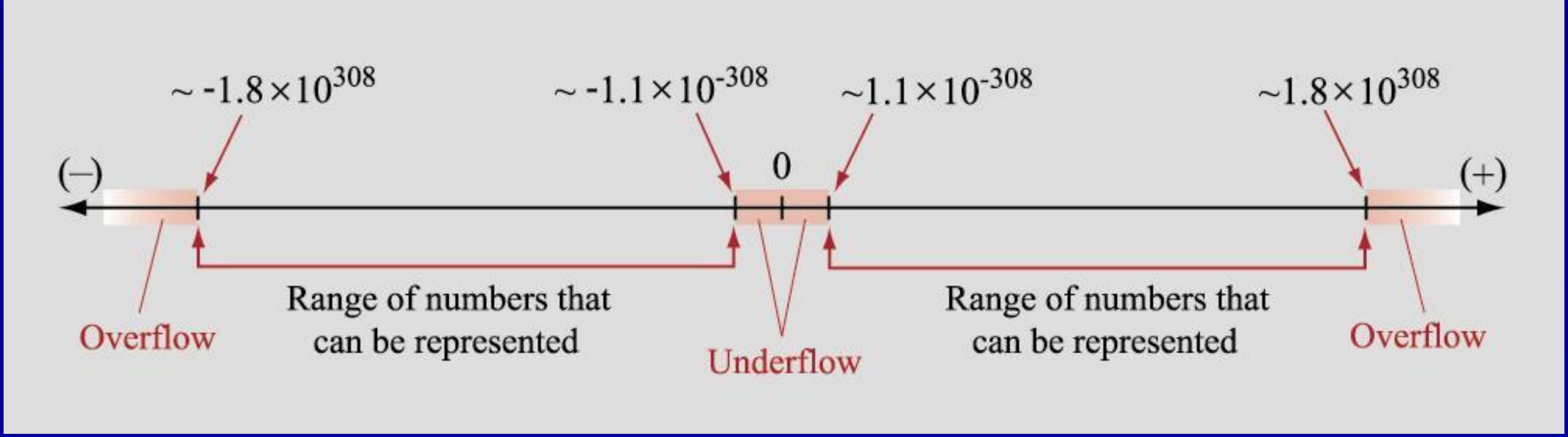
$$1\times2^4+0\times2^3+0\times2^2+1\times2^1+1\times2^0+1\times2^{-1}+0\times2^{-2}+1\times2^{-3}$$

$$1\times16+0\times8+0\times4+1\times2+1\times1+1\times0.5+0\times0.25+1\times0.125 = 19.625$$

Reference: Gilat, Subramaniam: *Numerical Methods with Matlab*

Numbers





Reference: Gilat, Subramaniam: *Numerical Methods with Matlab*

Truncation Errors

Truncation error

(or *discretization error)* :

- Due to use of approximations to represent exact mathematical procedures
- Due to using finite number of steps in computation
- Present even with infinite-precision arithmetic, because it is caused by truncation of the infinite Taylor series to form the algorithm

Derivative of velocity of a car

$$\frac{dv}{dt} \cong \frac{\Delta v}{\Delta t} = \frac{v(t_{i+1}) - v(t_i)}{t_{i+1} - t_i}$$

Truncation Errors and Taylor Series

Why is Taylor series important in the study of Numerical Methods?

- Provides ways to predict a function value at one point in terms of the function value and its derivatives at another point
- States that any smooth function can be approximated as a polynomial

Reference: S. C. Chapra and R. P. Canale, Numerical Methods for Engineers, 3rd Ed., WCB/McGraw-Hill, 1998, p.79

Truncation Errors and Taylor Series

- A Taylor series of a real (or complex) function *f(x)* is infinitely differentiable in a neighborhood of a real (or complex) number *a,* i.e. it is the power series:

$$f(a)+\frac{f'(a)}{1!}(x-a)+\frac{f''(a)}{2!}(x-a)^2+\frac{f^{(3)}(a)}{3!}(x-a)^3+\cdots,$$

or

$$\sum_{n=0}^{\infty}\frac{f^{(n)}(a)}{n!}(x-a)^n,$$

- *f*(*x*) is usually equal to its Taylor series evaluated at *x* for all *x* sufficiently close to *a*
- If *a* = 0 → Maclaurin series

Why Use Approximating Functions?

- Replace f(x) (ex: transcendental functions ln x, sin x, erf x, …) with g(x) (ex: a power series) which can handle arithmetic operations

Errors

- Once an error is generated, it will generally propagate through the calculation.

  ex: operation + on a calculator (or a computer) is inexact. It follows that a calculation of the type a+b+c+d+e is even more inexact.