Lecture 1 Numerical methods: principles, algorithms and applications: an introduction

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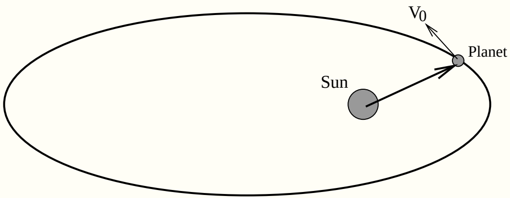
Outline

1. Solar system (two-body problem)

Schematics of two body problem



1. Solar system (two-body problem)

- Governing equations: Hamiltonian system

$$\begin{cases} \dfrac{d\boldsymbol{x}}{dt} & = & \boldsymbol{v}, \\ \dfrac{d(m\boldsymbol{v})}{dt} & = & -\nabla V(\boldsymbol{x}). \end{cases}$$

  Simply take $V(\boldsymbol{x}) = -\frac{GmM}{r}$. Define Hamiltonian

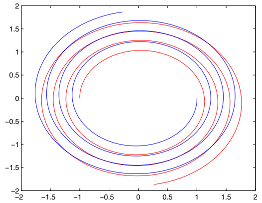
$$H = \frac{1}{2}m\boldsymbol{v}^2 + V(\boldsymbol{x})$$

  then $\frac{dH}{dt} = 0$.

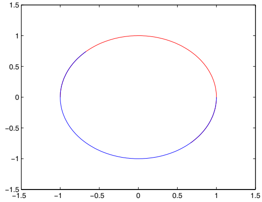
- Numerical solution of ODEs

1. Solar system (two-body problem)

- Long time numerical integration $(T \gg 1)$
  1. Bad scheme (Forward Euler)

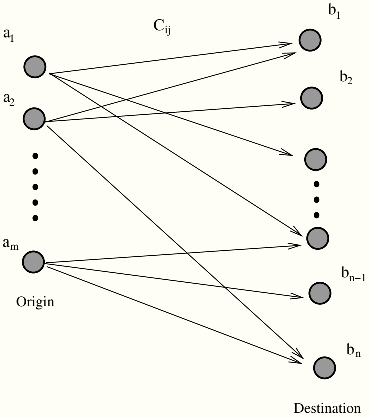


  2. Good scheme (Symplectic scheme)



2. Transportation problem

Schematics of transportation problem



2. Transportation problem

- Formulation:

$$\min s = \sum_{i=1}^{m}\sum_{j=1}^{n} c_{ij}x_{ij}$$

subject to the condition

$$\sum_{i=1}^{m} x_{ij} = b_j,\ \ j = 1, \ldots, n$$

$$\sum_{j=1}^{n} x_{ij} = a_i,\ \ i = 1, \ldots, m$$

$$x_{ij} \geq 0,\ \ i = 1, \ldots, m;\ \ j = 1, \ldots, n.$$

where a_i is the supply of the i-th origin, b_j is the demand of the j-th destinations, x_{ij} is the amount of the shipment from source i to destination j and c_{ij} is the unit transportation cost from i to j.

- Optimization problem (Simplex method)

3. Image processing

- Image restoring

$$\inf_{u\in\mathcal{L}} E(u) = \frac{1}{2}\int_\Omega |u_0 - Ru|^2 dx + \lambda \int_\Omega \phi(|\nabla u|)dx$$

Here Ω is the domain, u_0 is the degraded image, R is the blurring operator which is known *a priori*, ϕ is a particularly chosen function. u will be the recovered image.

- Nonlinear optimization problem or nonlinear PDE problem

3. Image processing

- Total variation denoising

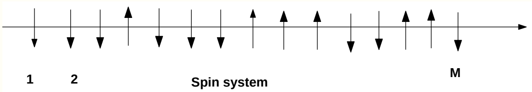
$$\phi(|\nabla u|) = |\nabla u|$$

A blurred image with 80 lost packets

Deblurring and error concealment by TV inpainting

4. Stochastic simulations

Ising model for mean field ferromagnet modeling



- Ising model in statistical physics
  Define the Hamiltonian

$$H(\sigma) = -J \sum_{<ij>} \sigma_i \sigma_j,$$

where $\sigma_i = \pm 1$, $< ij >$ means to take sum w.r.t all neighboring spins $|i - j| = 1$. The internal energy per site

$$U_M = \frac{1}{M} \sum_{\sigma} H(\sigma) \frac{\exp\{-\beta H(\sigma)\}}{Z_M} = \frac{1}{M} \langle H(\sigma) \rangle = -\frac{1}{M} \frac{\partial \ln Z_M}{\partial \beta},$$

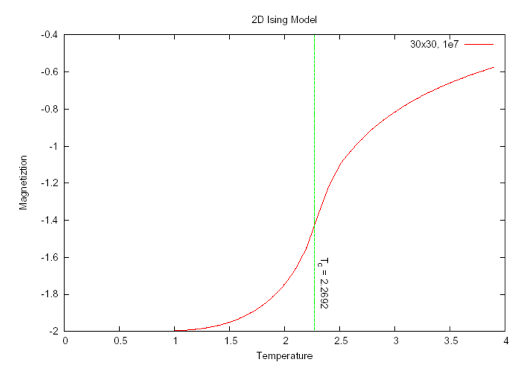
where

$$Z_M = \sum_{\sigma} \exp\{-\beta H(\sigma)\}$$

is the partition function and $\beta = (k_B T)^{-1}$.

4. Stochastic simulations

Finding the critical temperature T_c for 2D Ising model (Metropolis algorithm)



4. Stochastic simulations

- Biological network

  Suppose there are N_s species of molecules $S_i,\ i = 1, \ldots, N_s$, and M_R reaction channels $R_j,\ j = 1, \ldots, M_R$. x_i is the number of molecules of species S_i. Then the state of the system is given by

  $$\boldsymbol{x} = (x_1, x_2, \ldots, x_{N_s}).$$

  Each reaction R_j is characterized by a rate function $a_j(x)$ and a vector ν_j that describes the change of state due to reaction (after the $j-th$ reaction, $\boldsymbol{x} \rightarrow \boldsymbol{x} + \nu_j$). In shorthand denote

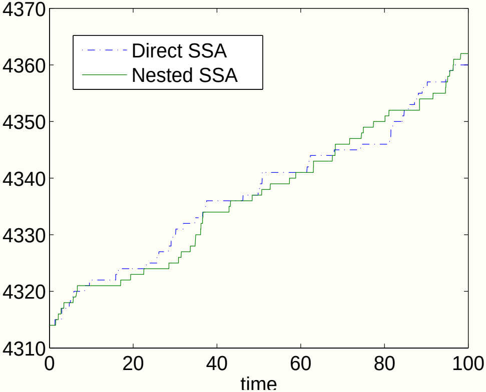
  $$R_j = (a_j, \nu_j)$$

  How to simulate this biological process?

4. Stochastic simulations

Stochastic simulation (Kinetic Monte Carlo)

(Number of molecules vs Time)



Extracted from a paper on stochastically simulating the number of one kind of molecules in a chemical reaction.

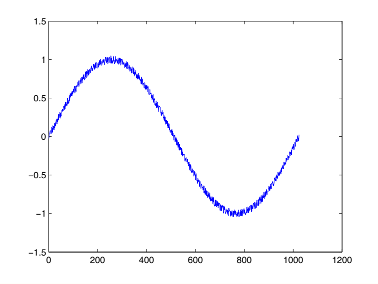
5. Signal processing

- Filtering

  Given a discrete time signal $\{u_j\}_{j=0}^{N-1}$, analyze the high frequency and low frequency part. Discrete Fourier Transform

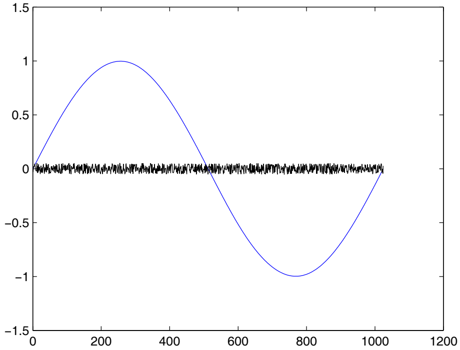
$$\hat{u}_k = \sum_{j=0}^{N-1} u_j e^{-jk\frac{2\pi i}{N}}, \qquad k = 0, 1, \ldots, N-1.$$

- Basic technique: FFT
- A polluted signal



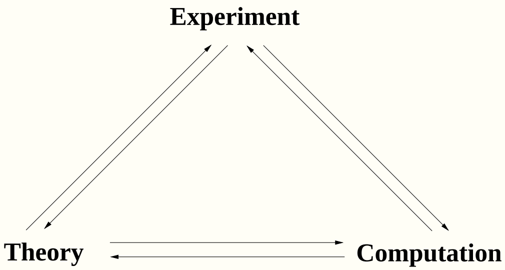
5. Signal processing

- High pass and low pass filter (signal and noise)



Three approaches in scientific research

Schematics for the relation of theory, computation and experiment



Top 10 algorithms in 20th century
— from "Computing in Science and Engineering"

1. Metropolis algorithm
2. Simplex method
3. Krylov subspace iteration methods
4. Matrix decomposition approach
5. Fortran Compiler
6. QR algorithm
7. Quicksort algorithm
8. Fast Fourier Transform (FFT)
9. Integer relation detector
10. Fast multipole method

The algorithm 1,2,4,6,8 will be taught in this course.

Three different eras of computing

Numerical analysis $\longrightarrow$ Scientific computing $\longrightarrow$ Computational science

Outline

Qin Jiushao algorithm (Horner's algorithm)

- Compute the value of polynomial

$$p(x) = a_n x^n + a_{n-1} x^{n-1} + \cdots + a_0$$

naively. The computational efforts will be

$$\frac{(n+1)(n+2)}{2} \text{ multiplications and } n \text{ additions}$$

- Nested multiplication

$$p(x) = ((a_n x + a_{n-1}) \cdot x + a_{n-2}) \cdots) x + a_0$$

The computational efforts will be

$$n \text{ multiplications and } n \text{ additions}$$

Solving linear system

Solving the linear system $\boldsymbol{Ax} = \boldsymbol{b}$.

- Cramer's rule
  From Cramer's rule, if $\det(\boldsymbol{A}) \neq 0$ it is solvable and the solution can be explicitly represented as
  $$x_i = \frac{\det(\boldsymbol{A}_i)}{\det(\boldsymbol{A})}$$
  and $\boldsymbol{A}_i$ is the matrix with i-th column replaced by $\boldsymbol{b}$.
- Working load for computing N-determinant with definition:
  $$(N-1) \cdot N! \text{ multiplications and } N! - 1 \text{ additions.}$$
  It is an astronomy number! When $N = 20$, $N! \sim 2 \times 10^{18}$. If the computer power is 10Gflops/s, we need 200 years at least, which is impossible.

Computational efficiency

Theoretically solving a problem is NOT equivalent that it could be solved with computer because of the computational efficiency! In general, an $O(n^4)$ algorithm is unacceptable!

Floating point arithmetic

- Binary floating point system

$$\mathcal{F} = \{\pm 0.d_1 d_2 \dots d_t \times 2^m\} \cup \{0\}$$

where $d_1 = 1$, $d_j = 0$ or $1 (j > 1)$. t is called precision, $L \leq m \leq U$.
For any $x \in \mathbb{R}$, denote $fl(x)$ the floating point representation in computer.
We have relative error

$$\left| \frac{fl(x) - x}{x} \right| \leq 2^{-t} := \epsilon_{mach}$$

- The floating point system has

$$\text{Underflow limit} \quad UFL = 2^L \times 0.1$$

$$\text{Overflow limit} \quad OFL = 2^U \times 0.11 \cdots 1$$

infinity Inf and not a number Nan.

Some issues for floating point arithmetic

- Cancellation

$$0.3256734 - 0.3256721 = 0.0000013$$

Difference between two approximately equal reals cause loss of significants!

$$\sin(x+\epsilon) - \sin(x) = 2\cos(x+\frac{\epsilon}{2})\sin\frac{\epsilon}{2}$$

The right hand side is more suitable for computing than the left side hand.

- Summation

$$1 + \sum_{i=1}^{n} \frac{1}{n} = 2$$

  - The first order

$$1 + \frac{1}{n} + \cdots + \frac{1}{n} = 1 \text{ in computer}$$

  - The second order

$$\begin{aligned} & (\frac{1}{n} + \frac{1}{n}) + \cdots + (\frac{1}{n} + \frac{1}{n}) + 1 \\ = \quad & (\frac{2}{n} + \frac{2}{n}) + \cdots + (\frac{2}{n} + \frac{2}{n}) + 1 \\ = \quad & \cdots\cdots + 1 = 2 \end{aligned}$$

Outline

Course plan

- 3 hours powerpoint teaching per week;
- 2 hours (or more) computer work per week (50 points);
- Homework 10 points;
- Final exam 40 points;
- Notes to be downloaded from

  http://dsec.pku.edu.cn/~tieli

  with Account and Password: lnm2005.

References

1. A. Quarteroni and F. Saleri, *Scientific computing with MATLAB*, Berlin and New York, Springer Verlag, 2003.
2. D. Kahaner, C. Moler and S. Nash, *Numerical methods and software*, Prentice Hall, 1989.
3. E. Süli and D.F. Mayers, *An introduction to numerical analysis*, Cambridge and New York, Cambridge University Press, 2003.
4. S.D. Conti and C. de Boor, *Elementary numerical analysis: an algorithmic approach*, New York, McGraw-Hill, 1980.
5. G. Dahlquist and A. Bjork, *Numerical methods*, Prentice Hall, 1989.
6. G.H. Golub and C.F. Van Loan, *Matrix computation*, Johns Hopkins University Press, 1996.

Homework assignment 1

Familiarize software MATLAB about the basic definition of variables, arrays, function definition, subroutine definition, basic linear algebra operations and graphical operations.