Numerical methods for Physics and Astrophysics: Lab exercises

P. Ajith*
International Centre for Theoretical Sciences, Tata Institute of Fundamental Research, Bangalore 560012, India.
(Dated: April 8, 2014)

I. LAB 1

A. Finite differencing, convergence, error estimates

We derived the following finite-differencing approximants for the derivative of a function $f(x)$:

$$\textit{Forward differencing}: \quad f'(x) \simeq \frac{f(x+h)-f(x)}{h} + O(h) \tag{1.1}$$

$$\textit{Backward differencing}: \quad f'(x) \simeq \frac{f(x)-f(x-h)}{h} + O(h) \tag{1.2}$$

$$\textit{Central differencing}: \quad f'(x) \simeq \frac{f(x+h)-f(x-h)}{2h} + O(h^2) \tag{1.3}$$

Problems:

1. Write a Python function to compute derivatives using these three finite differencing methods. Compute the derivative of the function $f(x) = e^x \sin(x)$ over the range $x = [0, 2\pi]$. Plot the numerically computed derivative $f'_{(h)}(x)$ for three different values of h.
2. Plot the error $\Delta f'_{(h)}(x) := |f'_{(h)}(x) - f'(x)|$ for three different values of h, and estimate the order of convergence of each finite-difference approximation.
3. Reduce the step size h successively. At what value of h does the round off error dominate the error budget?
4. Derive a central differencing approximant for the second derivative $f''(x)$ using the Taylor expansions of $f(x+h)$ and $f(x-h)$.

B. Richardson extrapolation

We have seen that, if the order of the error in the numerical estimate of a function $f(x)$ is known, Richardson extrapolation provides a powerful way of improving the accuracy of the estimate. If we have two numerical estimates $f_h(x)$ and $f_{h/2}(x)$ each having an error of $O\,h^k$, a better estimate is given by

$$f(x) \simeq \frac{2^k\, f_{h/2}(x) - f_h(x)}{2^k - 1} + O(h^l), \tag{1.4}$$

where l is the next-to-leading-order error term (for e.g., $l = k + 2$ for central differencing, while $l = k + 1$ for forward/backward differencing).

Problems:

1. Gravitational-waves (GWs) have two independent polarization states – called "plus" and "cross" states. GW signals from the coalescence of black-hole binaries, in the simplest case, are circularly polarized:

$$h_+(t) = A(t)\, \cos\varphi(t), \quad h_\times(t) = A(t)\, \sin\varphi(t). \tag{1.5}$$

*Electronic address: ajith@icts.res.in

Download the data file [1] containing $h_+(t)$ and $h_\times(t)$. (This is the reduced form of the data produced by a numerical-relativity simulation of black-hole binaries performed by the Caltech-Cornell-CITA collaboration and is publicly available at [2]). Compute the phase evolution $\varphi(t)$, the frequency evolution $\omega(t) := d\varphi(t)/dt$ and the rate of change of frequency $\dot{\omega}(t) := d\omega(t)/dt$ using second-order central difference approximation.

2. Estimate the order of convergence of the numerical computation of $\omega(t)$ and $\dot{\omega}(t)$.
3. Perform an extrapolation of $\omega(t)$ and $\dot{\omega}(t)$ to the next order using estimates of two different time-resolutions.
4. Derive an explicit expression for $f'(x)$ with error $O(h^4)$ using Richardson extrapolation. This is the fourth-order finite differencing approximant for the derivative, which we will use later.

II. LAB 2

A. Ordinary differential equations: Calculation of gravitational waves from inspiralling compact binaries

Problems:

The time evolution of the orbital phase $\varphi(t)$ of a binary of black holes evolving under the gravitational radiation reaction can be computed, in the post-Newtonian approximation, by solving the following coupled ODEs:

$$\frac{dv}{dt} = -\frac{\mathcal{F}(v)}{dE(v)/dv}, \qquad \frac{d\varphi}{dt} = \frac{v^3}{m}, \tag{2.1}$$

where $E(v)$ is the binding energy of the orbit, $\mathcal{F}(v)$ is the energy flux of radiated gravitational waves, $m := m_1 + m_2$ is the total mass of the binary, $v = (m\omega)^{1/3}$, ω being the orbital frequency. (Here we use geometric units, in which $G = c = 1$. This means that in all the expressions m has to be replaced by Gm/c^3.)

The binding energy and gravitational-wave flux are given as post-Newtonian expansions in terms of the small parameter v

$$E(v) = -\frac{1}{2}\mu v^2 \left[1 + O(v^2)\right], \quad \mathcal{F}(v) = \frac{32}{5}\left(\frac{\mu}{m}\right)^2 v^{10}\left[1 + O(v^2)\right], \tag{2.2}$$

where $\mu := m_1 m_2/m$ is the reduced mass of the system.

1. Compute v as a function of t by solving the first equation in Eq. (2.1) using Scipy's `odeint` routine. Assume the following parameters $m_1 = m_2 = 5M_\odot$, $v_0 = 0.3$, $\varphi_0 = 0$. Plot $v(t)$.
2. Solve the coupled system in Eq. (2.1) to compute v and φ. Compute and plot the two gravitational-wave polarizations:

$$h_+(t) = 4\frac{\mu}{m}v^2\,\cos\varphi(t), \quad h_\times(t) = 4\frac{\mu}{m}v^2\,\sin\varphi(t). \tag{2.3}$$

3. Repeat the same calculation using the adaptive Runge-Kutta method by Dormand & Prince using Scipy's `integrate.ode` module (choose method = "dopri5"). This method is very similar to the Runge-Kutta-Fehlberg method that we learned in the class.

III. LAB 3

A. Ordinary differential equations: Structure of a relativistic, spherically symmetric star

The interior structure of a relativistic, spherically symmetric star is described by a metric that has the line element

$$ds^2 = -e^{2\Phi(r)}\,c^2dt^2 + \left(1 - \frac{2Gm(r)}{rc^2}\right)^{-1} dr^2 + r^2\,d\Omega^2, \tag{3.1}$$

where $m(r)$ is called the *mass function* (which encapsulates the gravitational mass inside the radius r), $e^{2\Phi(r)}$ is the *lapse function* (which relates the proper time with the coordinate time). Outside the "surface" of the star (in vacuum), the spacetime is described by the Schwarzschild metric; the lapse function becomes

$$\Phi(r) = \frac{1}{2}\ln\left(1 - \frac{2Gm_\star}{rc^2}\right) \tag{3.2}$$

where $m_\star$ is the total (gravitational) mass of the star. The structure can be computed by solving the following set of ordinary differential equations, derived by Tolman, Oppenheimer and Volkoff (TOV).

$$\frac{dm(r)}{dr} = 4\pi r^2 \rho(r), \tag{3.3}$$

$$\frac{dP(r)}{dr} = -\frac{G(\rho + P(r)/c^2)}{r^2}\left[m(r) + \frac{4\pi r^3 P(r)}{c^2}\right]\left[1 - \frac{2Gm(r)}{c^2 r}\right]^{-1}, \tag{3.4}$$

$$\frac{d\Phi(r)}{dr} = \frac{Gm(r) + 4\pi G r^3 P(r)/c^2}{c^2 r[r - 2Gm(r)/c^2]}. \tag{3.5}$$

The TOV equations have to be supplemented by an *equation of state* $P = P(\rho)$, that relates the pressure P to the energy density ρ. We assume the equating of state to be of polytropic form

$$P(r) = K\,\rho(r)^\gamma. \tag{3.6}$$

We also need to specify initial conditions for the variables m, P, Φ. The following conditions can be used

$$m(r=0) = 0, \quad P(r=0) = P_c = P(\rho_c), \quad \Phi(r_\star) = \frac{1}{2}\ln\left(1 - \frac{2Gm_\star}{r_\star c^2}\right) \tag{3.7}$$

Problems:

1. Compute the structure, i.e., $m(r)$ and $P(r)$, of a neutron star with central density $\rho_c = 5\times10^{17}$ kg/m^3 by solving Eqs. (3.3) and (3.4). Assume a polytropic equation of state with $\gamma = 5/3$ and $K = 5380.3$ (SI units). What is the mass $m_\star$ and radius $r_\star$ of the neutron star? (Useful tip: You will need to start the integration at $r = \Delta r$, where Δr is a small number. You can assume $m(r = \Delta r) := 4/3\,\pi\rho_c(\Delta r)^3$).
2. Compute the lapse function $e^{2\Phi(r)}$ by solving Eq.(3.5) starting from $r = r_\star$ to $r = 0$. On top of that, plot the lapse function for a Schwarzschild black hole (see Eq.3.2) from $r = r_s$ to $r = 2r_\star$, where $r_s \equiv 2Gm_\star/c^2$ is the Schwarzschild radius of the star. This exterior solution should match the interior solution at $r = r_\star$.

IV. LAB 4

A. Non-linear ordinary differential equations showing chaotic behavior: Lorenz equations

The Lorenz equations were originally developed as a simplified mathematical model for atmospheric convection by Edward Lorenz. This was the first set of equations where deterministic chaos was observed. The equations are given by

$$\frac{dx(t)}{dt} = \sigma[y(t) - x(t)], \quad \frac{dy(t)}{dt} = x(t)[\rho - z(t)] - y(t), \quad \frac{dz(t)}{dt} = x(t)y(t) - \beta z(t), \tag{4.1}$$

where ρ, σ and β are parameters of the system.

1. Problems:

1. Solve the Lorenz system for $\rho = 28, \sigma = 10$ and $\beta = 8/3$ with the following initial conditions $x(t=0) = y(t=0) = z(t=0) = 1$. Plot $x(t)$, $y(t)$ and $z(t)$ for $t = 0...100$. Is the solution deterministic or stochastic?
2. Repeat the calculation with same parameters except for a tiny change in the initial condition for x: i.e., $x(t=0) = 1 + 10^{-9}$. Plot $x(t=0) = y(t=0) = z(t=0) = 1$ on top of the earlier estimate. Explain the result.
3. Make a 3D plot of x, y, z. You should see the famous butterfly shaped structure now!
4. Optional exercise: Make an animation of the above [1].

[1] You can either use the matplotlib animation package or convert a number of PNG files to a gif animation using ImageMagick.

B. Stochastic ordinary differential equations: Langevin equation

The random motion of a particle in a fluid due to collisions with the molecules of the fluid, called the Brownian motion, is described by the Langevin equation:

$$m\frac{d^2\mathbf{x}}{dt^2} = -\lambda\frac{d\mathbf{x}}{dt} + \boldsymbol{\eta}(t), \tag{4.2}$$

where m is the mass of the particle, $\mathbf{x}$ its position vector, λ a damping coefficient, and $\boldsymbol{\eta}(t)$ (called the *noise term*) describes the stochastic processes affecting the system.

1. Problems:

1. Using the Euler-Maruyama method, compute the $1-d$ Brownian motion trajectories generated by the Langevin equation $dx/dt = \eta(t)$, where $\eta(t)$ is Gaussian noise with zero mean and unit variance. Plot $x(t)$ for $t \in [0, 100]$ assuming $x(t=0) = 0$. Is the solution deterministic or stochastic?
2. Generalize the code so that it can deal with arbitrary number of particles. Plot $x(t)$ for 1000 particles on a single plot. Compute the average displacement $\bar{x}(t)$ of the particles (from $x(t=0)$) as a function of t and plot it against t. What is the relation between $\bar{x}(t)$ and t?
3. Using the `hist` function, plot the probability distribution $P(x)$ of $x(t)$ at $t = 10, 50, 100$.

V. LAB 5

A. Two-point boundary value problems: The shooting method

Solve the TOV equations described in Sec. III A as a two-point boundary value problem using the Shooting method. Use the Newton-Raphson method for root finding. The boundary conditions are given in Eq. (3.7).

VI. PARTIAL DIFFERENTIAL EQUATIONS

A few explicit first order numerical methods for solving the advection equation $\frac{\partial u}{\partial t} = -v\frac{\partial u}{\partial x}$ are given below:

$$\text{Forward time centered space(FTCS)}: \quad u_j^{n+1} = \frac{-v\Delta t}{2\Delta x}\left[u_{j+1}^n - u_{j-1}^n\right] + u_j^n \tag{6.1}$$

$$\text{Upwind method (for } v > 0): \quad u_j^{n+1} = \frac{-v\Delta t}{\Delta x}\left[u_j^n - u_{j-1}^n\right] + u_j^n \tag{6.2}$$

$$\text{Upwind method (for } v < 0): \quad u_j^{n+1} = \frac{-v\Delta t}{\Delta x}\left[u_{j+1}^n - u_j^n\right] + u_j^n \tag{6.3}$$

1. Problems:

1. Solve the advection equation with $v = 1$ and initial condition $u(t=0, x) := \exp[-(x-x_0)^2]$ (Gaussian pulse) where $x \in [0, 25]$ and $x_0 = 5$ using the FTCS scheme. Is the evolution stable?
2. Repeat the calculation with upwind methods using Courant factor $\lambda := |v\Delta t|/\Delta x = 1/2, 1, 2$. Which of the evolutions are stable?
3. Plot the order of convergence of $u(x,t)$ as a function of x at $t = 10$ (use $\lambda = 1$).

VII. FOURIER AND SPECTRAL METHODS

A. Fast Fourier transform (FFT)

1. Problems:

1. Hercules X-1 is a high-mass X-ray binary (HMXB) system having a magnetized spinning neutron star which happens to be an X-ray pulsar. Here [3] you are given the data of an RXTE [4] observation after cleaning and pre-processing. The file contains two columns, (i) time (in seconds) and (ii) count-rate of X-ray photons (i.e., number of photons detected per unit time). Plot the count-rate as function of time. This is called lightcurve in X-ray astronomy. Compute the FFT of the given time-series and plot its absolute value against the frequency. Are you able to find any periodic signal(s)? The lowest frequency signal corresponds to the spin frequency of the neutron star. What is the spin period of this pulsar? Can you identify other periodic signals and how they are related to the lowest frequency signal? [2]

B. Power spectrum estimation using FFT

1. Problems:

1. A sample data set from the LIGO gravitational-wave observatory can be downloaded from here [5]. This contains 256 seconds of LIGO data from 2005, sampled at a rate of 4096 Hz. Compute the power spectral density of the data using Welch's modified periodogram method.

C. Time-frequency signal detection methods

1. Problems

1. 4U 1636–536 is a low-mass X-ray binary (LMXB) system consisting of a rapidly spinning weakly magnetized neutron star which does not exhibit any coherent X-ray pulsation like Hercules X-1. However, X-ray radiation from this source shows signals of high frequency (500–1000 Hz) quasi-periodic oscillations (QPOs). Here [6] you are given another data of RXTE observation. This contains the arrival times of photons. Identify the frequency span of this QPO using a time-frequency spectrogram or a PSD. Note: Firstly, you need to sample the data with a fixed sampling rate, say 4096 Hz.

D. Comouting correlations using FFT: Matched filtering

In the case a known signal $h(t)$ buried in stationary Gaussian, white noise, the optimal technique for signal extraction is the *matched filtering*, which involves cross-correlating the data with a *template* of the signal. The correlation function between two time series $x(t)$ and $\hat{h}(t)$ (both assumed to be real-valued) for a time shift τ is defined as:

$$R(\tau) = \int_{-\infty}^{\infty} x(t)\, \hat{h}(t+\tau)\, dt. \tag{7.1}$$

Above, $\hat{h(t)} := h(t)/||h||$, where the norm $||h||$ of the template is defined by

$$||h||^2 = \int_0^{t_c} |h(t)|^2/\sigma^2\, dt,$$

where σ^2 is the variance of the noise. The optimal signal-to-noise ratio (SNR) is obtained when the template exactly matches with the signal. i.e., $\mathrm{SNR}_{\mathrm{opt}} = ||h||$. If the SNR is greater than a predetermined threshold (which corresponds to an acceptably small false alarm probability), a detection can be claimed.

---

[2] This problem and data are graciously provided by Dr. Arunava Mukherjee (IUCAA).

1. Problems

1. You are given a time-series data set $d(t)$ here [7]. This contains a simulated gravitational-wave signal from a black hole binary buried in zero-mean, Gaussian white noise $n(t)$ with standard deviation $\sigma = 10^{-21}$. i.e.,

$$d(t) = n(t) + m\, h_+(t)/D_L, \tag{7.2}$$

where $h_+(t)$ is given by Eq. (2.3), $m = m_1 + m_2$ is the total mass of the binary, and D_L is the (unknown) luminosity distance to the binary. Detect the location of the signal in the data by maximizing the correlation of the waveform templates computed in Eq. (2.3) with the data.:

$$R_{\max} = \max{}_{m,\mu,\tau}\, R(\tau), \tag{7.3}$$

where $R(\tau)$ is given by Eq. (7.1). We have the prior information that the parameters of the signal are in the following range: $5 < m/M_\odot < 15$, $0.2 < \mu/m < 0.25$. Estimate the parameters m, μ of the signal (parameters that maximize the correlation).

[1] URL http://home.icts.res.in/~ajith/Downloads/nr_data.gz.
[2] URL http://www.black-holes.org/waveforms/.
[3] URL http://home.icts.res.in/~ajith/Downloads/extracted_lightcurve_HerX-1.dat.gz.
[4] RXTE is an X-ray timing satellite, URL https://heasarc.gsfc.nasa.gov/docs/xte/rxte.html.
[5] Download the file L1-STRAIN_4096Hz-815045078-256.txt.gz from, URL http://www.ligo.org/science/GRB051103/index.php.
[6] URL http://home.icts.res.in/~ajith/Downloads/4U1636-536_LC-extract.dat.gz.
[7] URL home.icts.res.in/~ajith/Downloads/mock_gw_data.dat.gz.