UNIVERSITY OF TEXAS ARLINGTON

PHYS 5319-001: Math Methods in Physics III

Differentiation & ODE

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Differentiation

For a function *f(x)*, the derivative is defined as

$$\frac{df}{dx} \equiv \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

Problem for numeric solution: subtractive cancellation

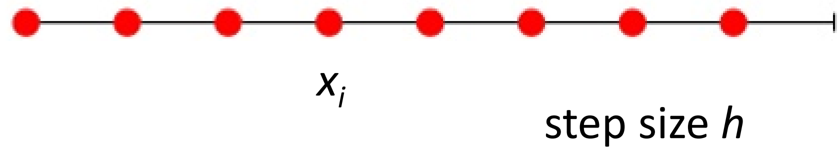
number precision: e.g. xx.xxxxxxxxxxxxx????

If *f(x+h)* only differs *f(x)* at the 9th decimal, $\Rightarrow$ only 6 digits left!

When the step size $h \to 0$ $\Rightarrow$ the difference will reach the machine precision ϵ_m!

Also, too small *h* will increase the number of grid.

-Forward Difference



Taylor expansion

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \cdots$$

So, the computed expression

$$f_c'(x) \approx \frac{f(x+h) - f(x)}{h}$$

$$\approx f'(x) + O(h)$$

Only need the forward step info

e.g. $f(x) = a + bx^2$ Exact: $f'(x) = 2bx$

$$f_c'(x) \approx \frac{f(x+h) - f(x)}{h} = 2bx + bh$$

Only good when h<<2x

-Central Difference

$$f_c'(x) \approx \frac{f\left(x+\frac{h}{2}\right) - f(x-\frac{h}{2})}{h}$$

$$\equiv D_c f(x,h)$$

Stepping forward by h/2 and backward by h/2

From Taylor expansion of $f\left(x \pm \frac{h}{2}\right)$:

$$f_c'(x) \approx f'(x) + \frac{1}{3!}\left(\frac{h}{2}\right)^2 f^{(3)}(x) + \cdots$$

$O(h^2)$

All the odd terms of *h* cancelled!

e.g. $f(x) = a + bx^2$

$$f_c'(x) \approx 2bx$$

-Extrapolated Difference

To manipulate O(h^2) vanish since we know the analytic form of errors

$instead\ of\ D_c f(x,h), we\ introduce$

$$f_c'(x) \approx f'(x) + \frac{1}{3!}\left(\frac{h}{2}\right)^2 f^{(3)}(x)$$

$$D_c f(x,\frac{h}{2}) \equiv \frac{f\left(x+\frac{h}{4}\right) - f(x-\frac{h}{4})}{h/2} \approx f'(x) + \frac{1}{3!}\left(\frac{h}{4}\right)^2 f^{(3)}(x) + \cdots$$

Mixing $D_c f(x,h)$ & $D_c f(x,h/2)$ to vanish $O(h^2)$:

$$f_c'(x) \approx \frac{4D_c\left(x,\frac{h}{2}\right) - D_c(x,h)}{3}$$

$$\approx f'(x) + \frac{1}{3}\left\{4\frac{1}{5!}\left(\frac{h}{4}\right)^4 f^{(5)}(x) - \frac{1}{5!}\left(\frac{h}{2}\right)^4 f^{(5)}(x)\right\}$$

$$-\frac{h^4}{120 \times 4 \times 16} f^{(5)}(x)$$

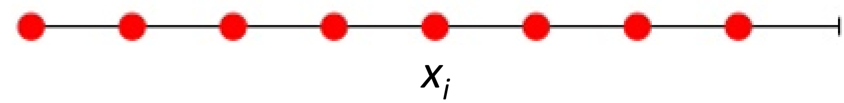
$$O(h^4)$$

A better way to compute $f_c'(x) \approx \dfrac{4D_c\left(x, \frac{h}{2}\right) - D_c(x,h)}{3}$

$$\Rightarrow \quad f_c'(x) = \frac{1}{3h}\left\{8\left[f\left(x+\frac{h}{4}\right) - f\left(x-\frac{h}{4}\right)\right] - \left[f\left(x+\frac{h}{2}\right) - f(x-\frac{h}{2})\right]\right\}$$

Why? Avoid a large number +/- a small number. Numbers in the same order of magnitude subtract each other first.

step size here: h/4



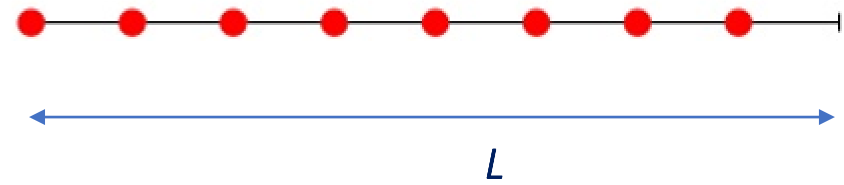
Cost: *Not only the nearest neighbor points, but also the 2nd n.n. points info is needed.*

Question: more neighboring points, more accurate?

Fourier Transform

For a periodic (in *L*) function *f(x)*

$f_i, i = 1,2, \ldots N$



FT

$$g(k) = \frac{1}{L}\int_0^L f(x)e^{ikx}dx$$

$$= \sum_{j=1}^{N} f_j e^{ikx_i}$$

FT^{-1}

$$f(x) = \sum_{l=1}^{N} g_l e^{-ik_l x}$$

Since *f(x+L)=f(x)* $\Rightarrow e^{ikL}$=1,

$$kL = 2\pi n, n = 0,1,2, \ldots, N-1$$

We have N discrete k-points:

$$k = \frac{2\pi n}{L}, n = 0,1,2, \ldots, N-1$$

$g_l \equiv g(k_l)$, represented in Fourier space

Now, $\frac{d}{dx}$ on $f(x)$:

$$f'(x) = \sum_{l=1}^{N}(-ik_l)g_l e^{-ik_l x} = \sum_l G_l\, e^{-ik_l x}$$

Need info from *N* points!

-second derivatives

$$f''(x) \equiv \frac{d^2 f}{dx^2} \equiv \frac{d}{dx}\left(\frac{df}{dx}\right)$$

Central-Difference

$$f''(x) \approx \frac{f'\left(x + \frac{h}{2}\right) - f'(x - \frac{h}{2})}{h}$$

apply Forward-Difference to the numerators:

$$f''(x) \approx \frac{[f(x+h) - f(x)] - [f(x) - f(x-h)]}{2h^2}$$

But for FT case, just a multiplication of $(-ik_l)$ again

$$f''(x) = \sum_{l=1}^{N} (-ik_l)^2 g_l e^{-ik_l x}$$

Differential Equations

A real physics problem often involves differential equation(s).
Could be a partial differential equation (PDE),
Or an ordinary differential equation (ODE).

Analytically, a PDE $\Rightarrow$ ODEs by separation of variables *e.g. Hydrogen atom*

Numerically, you may directly solve some. e.g. Poisson equation:

$$\nabla^2\varphi(\vec{r}) = -\rho(\vec{r})/4\pi\varepsilon_0$$

In Fourier space (transform needed) $$-k^2\varphi(\vec{k}) = -\rho(\vec{k})/4\pi\varepsilon_0$$

$$\Rightarrow \quad \varphi(\vec{k}) = \rho(\vec{k})/(4\pi\varepsilon_0 k^2)$$

Then an FT^{-1} back to the real space, $\boldsymbol{\varphi(\vec{r})}$.

But in most cases, we still need to dealing with ODEs

-Types of ODE

order$\Rightarrow$ degree of derivatives

e.g. 1st-order: $$\frac{dy}{dt} = f(t, y)$$

More generally, 2nd-order: $$\frac{d^2y}{dt^2} = f(t, \frac{dy}{dt}, y)$$

"Linear" vs. "nonlinear"

Linear $\Rightarrow$ law of linear superposition

Nonlinear $\Rightarrow$ contains higher power of *y(t)*. A linear super position not working.

Standard form:

$$\frac{d\vec{y}}{dt} = \vec{f}(t, \vec{y})$$

Or a set of coupled 1st order ODEs:

$$\frac{dy_i(x)}{dx} = f_i(x, y_1, y_2, \dots, y_N)$$

-Numerical solution: (integration):

1. Start from the known initial value;
2. Use the derivative function to advance one step
3. Repeat till to the end

ODEs with initial values

- Starting with 1st order ODE

$$\frac{d}{dt}x(t) = f(x,t)$$

with initial condition $x(0) = x_0$.

- The Taylor series expansion of x around t gives

$$x(t+\Delta t) = x(t) + \frac{dx(t)}{dt}\Delta t + \frac{1}{2!}\frac{d^2x(t)}{dt^2}(\Delta t)^2 + \ldots \qquad (1)$$

Assume a reasonably smooth function $x(t)$ and a small interval Δt, we can propagate $x(t)$ to $x(t+\Delta t)$ to any accuracy desired, as long as we know the derivatives of $x(t)$.

- However, often the (higher order) derivatives for a general t is not known, and we want a propagation for a time interval $\gg \Delta t$.

- The problem then becomes: how to estimate the derivatives of an unknown function and the suitable repetitions of propagation by Δt.

- Several numerical methods here:
  - Euler method
  - Runge-Kutta approximation
  - Euler-Cromer method
  - Verlet method
  - …

Numerical solutions for 1st order ODE

- When Δt is small, it is a good approximation by simply ignoring the second and higher orders of Δt in Eq. (1) as

$$x(t+\Delta t) \approx x(t) + \frac{dx}{dt}\Delta t = x(t) + f(x(t),t)\Delta t \qquad (2)$$

- This is the First-order Approximation – Euler method.

- Obtaining $x(t+\Delta t)$ from $x(t)$ with Eq. (2), we can estimate $x(t+2\Delta t)$ from $x(t+\Delta t)$ as

$$x(t+\Delta t+\Delta t) = x(t+\Delta t) + f(\mathrm{x}(t+\Delta t), t+\Delta t)\Delta t$$

- Iteratively, we can obtain $x(t+N\Delta t)$. $(N\Delta t \rightarrow the\ interested)$

- *e.g.* for radioactive decay

$$\frac{dN(t)}{dt} = -\lambda N(t)$$

- Applying the Euler method, we can estimate the number of active nuclei $N(t + \Delta t)$ at $\mathrm{t} + \Delta t$ as

$$N(t + \Delta t) \approx N(t) + \frac{dN(t)}{dt}\Delta t = N(t) - \lambda N(t)\Delta t$$

- And $N(t + 2\Delta t)$ at $\mathrm{t} + 2\Delta t$ as

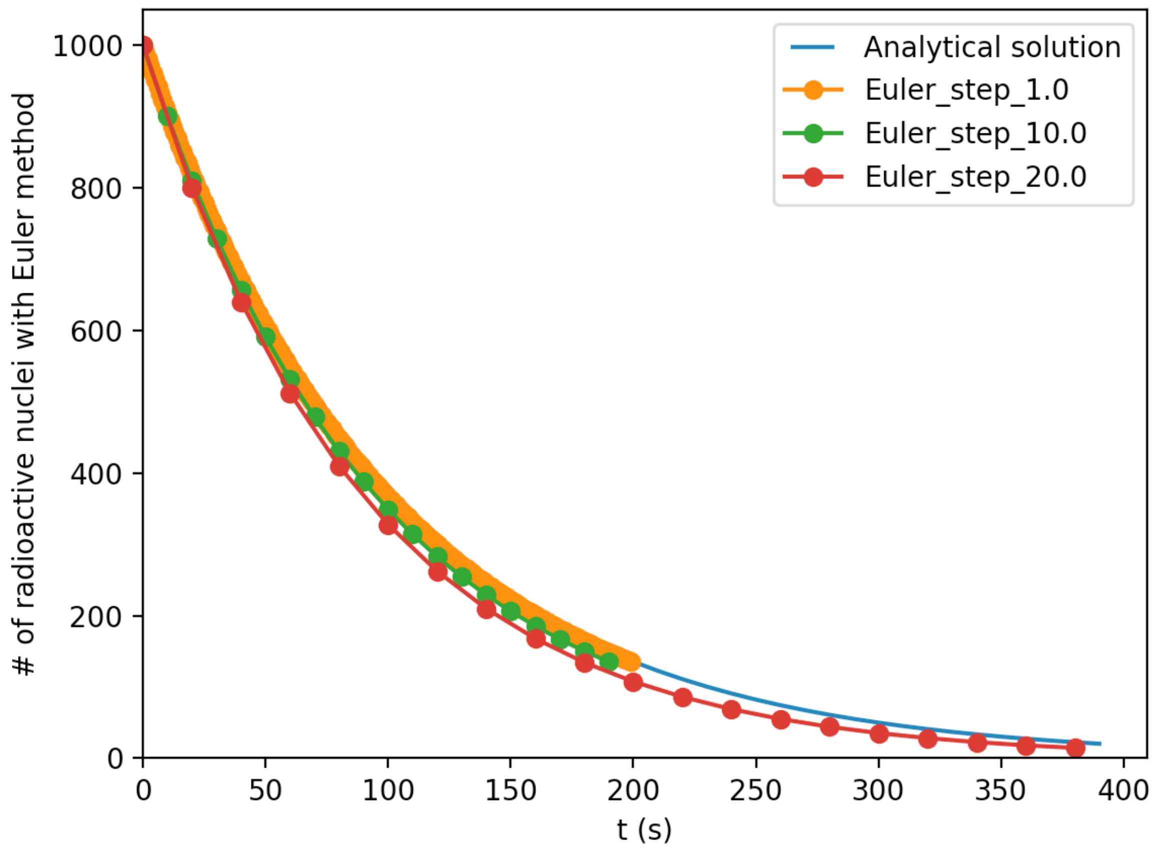
$$N(t + 2\Delta t) \approx N(t + \Delta t) + \frac{dN(t)}{dt}\Delta t = N(t + \Delta t) - \lambda N(t + \Delta t)\Delta t$$

- …
- And $N(t + i\Delta t)$ at $\mathrm{t} + \mathrm{i}\Delta t$ as

$$N(t + i\Delta t) \approx N(t + (i-1)\Delta t) - \frac{dN(t)}{dt}\Delta t = N(t + (i-1)\Delta t) - \lambda N(t + (i-1)\Delta t)\Delta t$$

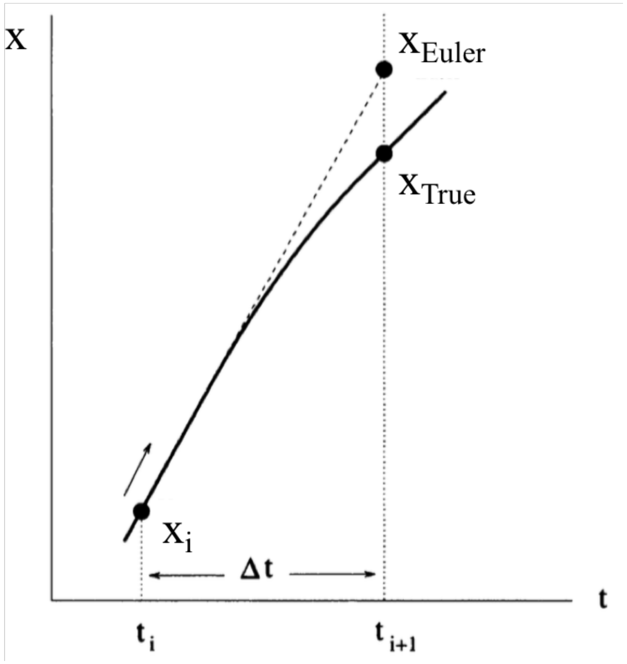
Apply Euler approximation to a specific decay example: $\frac{dN(t)}{dt} = -\lambda N(t)$ with $\lambda = 0.01, N_0 = 1000 \; when \; t_0 = 0.$

- The Euler approximation was found inaccurate compared to the analytical solution;
- The inaccuracy level is time step size affected.
- The computational time is also associated to the time step size.



- How to interpret Euler approximation geometrically?

$$x(t+\Delta t) \approx x(t) + \frac{dx}{dt}\Delta t = x(t) + f(x(t),t)\Delta t$$



Graphically, the Euler method corresponds to the linear extrapolation up to $(t + \Delta t)$ by using a line tangent to $x(t)$ at t.

A larger interval Δt, would cause a larger discrepancy between x_{true} and x_{Euler}.

How to systematically improve it?

2^{nd} order ODE:

e.g. Newton's 2^{nd} law

$$\frac{d^2x}{dt^2} = F(x,t)/m$$ with $x(0)$& $v(0)$ given.

In molecular dynamics: $m_k \ddot{\vec{x}}_k(t) = F_k(\vec{x}(t)) = -\nabla_{\vec{x}_k} V(\vec{x}(t))$

Split it into two coupled 1^{st} order ODE:

$$\frac{dx}{dt} = v(t)$$

$$\frac{dv}{dt} = F(x,t)$$

Assuming m=1 here

Euler method:

$$x(t+\Delta t) \approx x(t) + v(t)\Delta t$$

$$v(t+\Delta t) \approx v(t) + F(x(t),t)\Delta t$$

Error $O(\Delta t^2)$

Verlet method

$$x(t+\Delta t) = 2x(t) - x(t-\Delta t) + [\frac{F(x(t))}{m}]\Delta t^2$$

Error $O(\Delta t^4)$