LECTURE 1: Numerical Methods: Integration and ODE&PDEs

Numerical Integration (also called Quadrature)

$$I = \int_a^b f(x)dx$$

Special case of differential equation

$$\frac{dy}{dx} = f(x), \;\; y(a) = 0$$

LECTURE 1: Numerical Methods: Integration and ODE&PDEs

- ODE: higher order differential equations can always be rewritten as a series of 1st order:

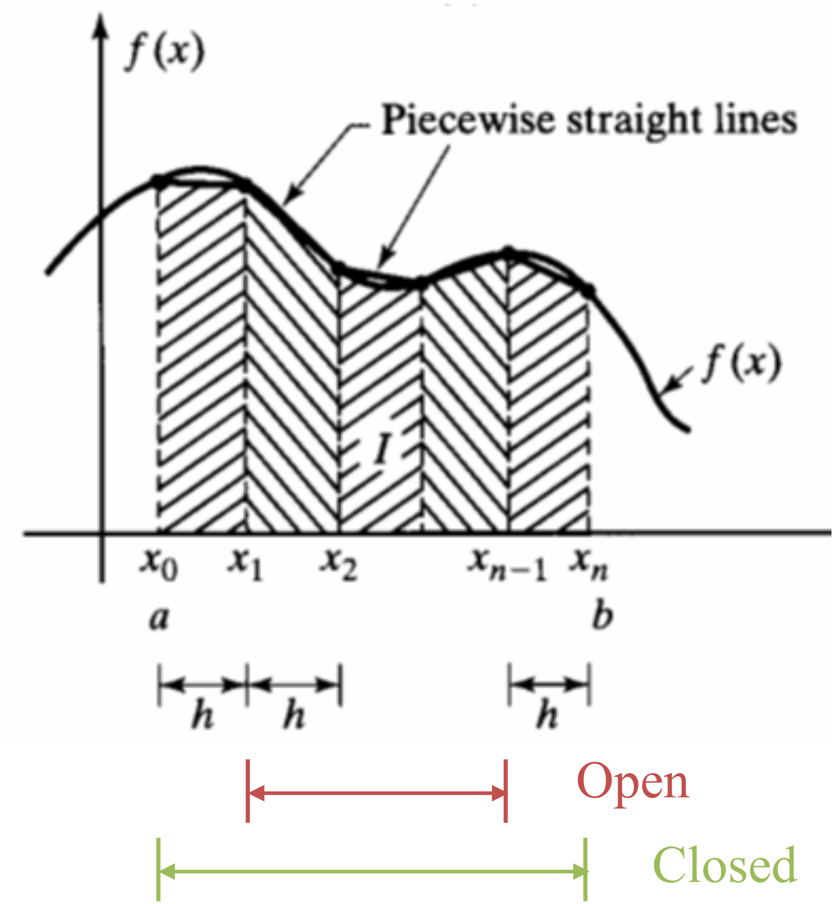
$$\frac{d^2y}{dx^2} + q(x)\frac{dy}{dx} = r(x)$$

$$\frac{dy}{dx} = z(x)$$

$$\frac{dz}{dx} = r(x) - q(x)z(x)$$

- We also need to specify boundary conditions. Typical case is initial value problem: we specify at initial time. For example, specify initial position and velocity of a particle and then use Newton's law to solve for its time evolution

Simple Trapezoidal Rule



$$x_i = x_0 + ih$$
$$f(x_i) = f_i$$

$$\int_{x_1}^{x_2} f(x)dx =$$
$$\frac{h}{2}(f_1 + f_2) + \mathcal{O}(h^3 f'')$$

- Exact for linear $f(x)$

Image credit: *http://www.unistudyguides.com/wiki/Numerical_Integration*

Simpson's Rule

$$\int_{x_1}^{x_3} f(x)dx = h(\frac{1}{3}f_1 + \frac{4}{3}f_2 + \frac{1}{3}f_3) + \mathcal{O}(h^5 f'''')$$

- Exact for $f(x) = \alpha x + \beta x^2 + \gamma x^3$
- Open if we cannot compute $f(x_0)$ or $f(x_{N+1})$

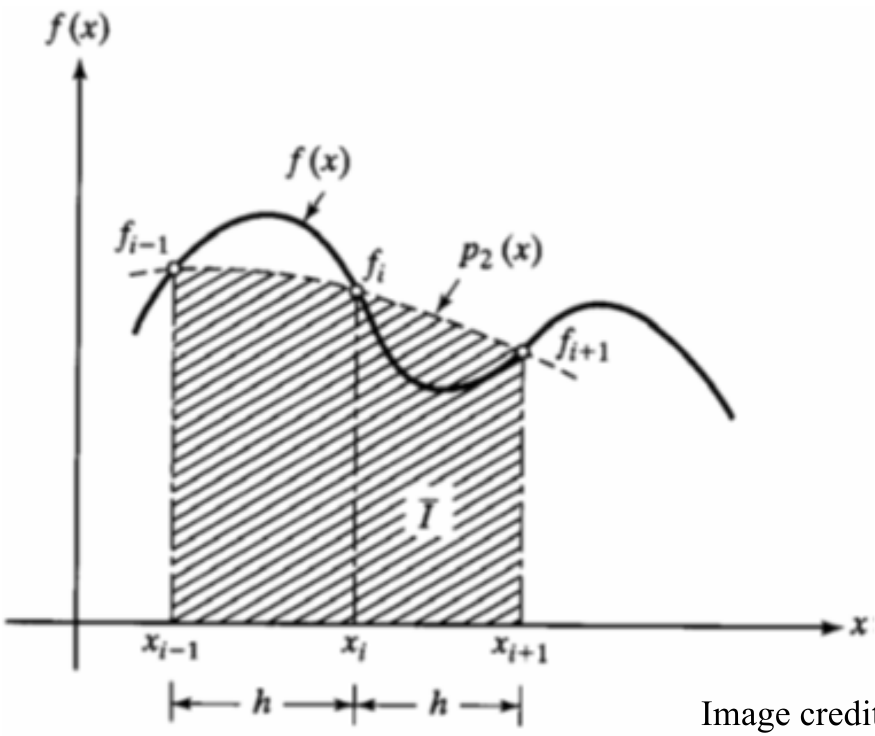


Image credit: *http://www.unistudyguides.com/wiki/Numerical_Integration*

Extended Formula

Trapezoid:

$$\int_{x_1}^{x_N} f(x)dx = h\left[\frac{1}{2}f_1 + f_2 + f_3 + \cdots + f_{N-1} + \frac{1}{2}f_N\right] + O\left(\frac{(b-a)^3 f''}{N^2}\right)$$

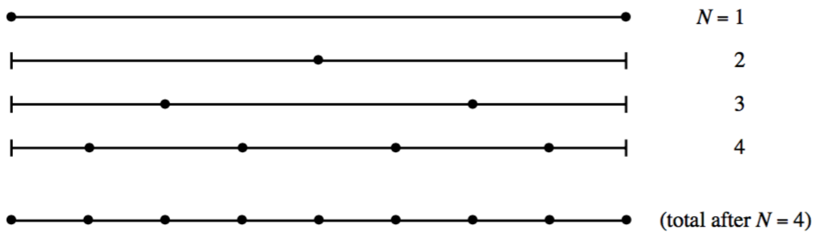
Simpson:

$$\int_{x_1}^{x_N} f(x)dx = h\left[\frac{1}{3}f_1 + \frac{4}{3}f_2 + \frac{2}{3}f_3 + \frac{4}{3}f_4 + \cdots + \frac{2}{3}f_{N-2} + \frac{4}{3}f_{N-1} + \frac{1}{3}f_N\right] + O\left(\frac{1}{N^4}\right)$$

Open Extended Trapezoid:

$$\int_{x_1}^{x_N} f(x)dx = h\left[\frac{3}{2}f_2 + f_3 + f_4 + \cdots + f_{N-2} + \frac{3}{2}f_{N-1}\right] + O\left(\frac{1}{N^2}\right)$$

- How do we achieve a given accuracy?
- We cannot guess *N* ahead of time, so we need to vary it.



- If we double $N \rightarrow 2N$, we can reuse function evaluations.

- Error Estimate: Difference between two subsequent steps
- Also need to put a limit to the number of steps:

$$N_{\text{max}} = 2^{\text{JMAX}-1}, \;\; \text{JMAX} = 20$$

$\rightarrow$ QTRAP of NR or QSIMP + TRAPZD

- Final refinement: Extended trapezoidal error is even in $1/N$:

$$\int_{x_1}^{x_N} f(x)dx = h\left[\frac{1}{2}f_1 + f_2 + f_3 + \cdots + f_{N-1} + \frac{1}{2}f_N\right]$$
$$- \frac{B_2 h^2}{2!}(f'_N - f'_1) - \cdots - \frac{B_{2k} h^{2k}}{(2k)!}(f_N^{(2k-1)} - f_1^{(2k-1)}) - \cdots$$

- Apply to N and $2N$: $I = \frac{4}{3} I_{2N} - \frac{1}{3} I_N$ cancels out leading error.

$$I_{\rm true} = I_N + E_t$$

$$E_t(N) = \frac{C}{N^2} = I_{\rm true} - I_N \qquad E_t(2N) = \frac{C}{4N^2} = I_{\rm true} - I_{2N}$$

$$I_{\rm true} = I_{2N} - \frac{I_{2N} - I_N}{3} = \frac{4}{3} I_{2N} - \frac{1}{3} I_N$$

→ We get Simpson's Rule

Romberg Integration

- Use N, $2N$, $4N$, … to cancel out higher orders $O(N^{-2k})$ using polynomial extrapolation

Romberg Integration

→ Romberg is the best routine for uniform interval sampling

Doubling N from I_1 to I_2,

$$I_1 + ch_1^2 = I_2 + ch_2^2,$$

$$I_2 - I_1 = ch_1^2 - ch_2^2 = 3ch_2^2,$$

$$\epsilon_2 = ch_2^2 = \tfrac{1}{3}(I_2 - I_1).$$

$$R_{i,1} = I_i\,,$$

$$R_{i,2} = I_i + \tfrac{1}{3}(I_i - I_{i-1}) = R_{i,1} + \tfrac{1}{3}(R_{i,1} - R_{i-1,1}).$$

$$\begin{array}{lllllll}
I_1 \equiv R_{1,1} & & & & & & \\
& \searrow & & & & & \\
I_2 \equiv R_{2,1} & \rightarrow & R_{2,2} & & & & \\
& \searrow & & \searrow & & & \\
I_3 \equiv R_{3,1} & \rightarrow & R_{3,2} & \rightarrow & R_{3,3} & & \\
& \searrow & & \searrow & & \searrow & \\
I_4 \equiv R_{4,1} & \rightarrow & R_{4,2} & \rightarrow & R_{4,3} & \rightarrow & R_{4,4} \\
& \searrow & & \searrow & & \searrow & & \searrow
\end{array}$$

Improper Integrals

- Cannot be evaluated   Ex) $\left.\frac{\sin(x)}{x}\right|_{x=0}$

Use open formula: Extended Midpoint Rule

- Infinite boundaryc   Ex) $\int_{-\infty}^{\infty} f(x)dx$

- Integrable singularity   Ex) $\int_0^{x_0} x^{-\frac{1}{2}} dx$

Change of variables

$$\int_a^b f(x)dx = \int_{1/b}^{1/a} \frac{1}{t^2} \cdot f(1/t)dt$$

$ab > 0$

$b \to \infty, a > 0$

$a \to -\infty, b < 0$

Examples: Change of variables

- Integrable singularity

If the integrand diverges as $(x-a)^{-\gamma}$,
$0 \le \gamma < 1$, near $x = a$,

$$\int_a^b f(x)dx = \frac{1}{1-\gamma}\int_0^{(b-a)^{1-\gamma}} t^{\frac{\gamma}{1-\gamma}} f(t^{\frac{1}{1-\gamma}} + a)dt \qquad (b > a)$$

- Exponential fall-off

$$t = e^{-x} \qquad \text{or} \qquad x = -\log t$$

$$\int_{x=a}^{x=\infty} f(x)dx = \int_{t=0}^{t=e^{-a}} f(-\log t)\frac{dt}{t}$$

Gaussian Quadratures

- Move beyond equally spaced points
- Choose abscissas and weights, achieving twice the order of accuracy
- Higher order $\neq$ Higher accuracy!
- We can choose to be high accuracy for polynomial times a function *W(x)*

$$\int_a^b W(x) f(x) dx \approx \sum_{j=1}^{N} w_j f(x_j)$$

Weights & Abscissas tabulated for several cases

Read about orthogonal polynomials
construction of weights & abscissas in NR

- Commonly used cases:

Rescale for other intervals

Gauss-Legendre:

$$W(x) = 1 \qquad -1 < x < 1$$

Gauss-Chebyshev:

$$W(x) = (1 - x^2)^{-1/2} \qquad -1 < x < 1$$

Gauss-Laguerre:

$$W(x) = x^\alpha e^{-x} \qquad 0 < x < \infty$$

Gauss-Hermite:

$$W(x) = e^{-x^2} \qquad -\infty < x < \infty$$

Gauss-Jacobi:

$$W(x) = (1 - x)^\alpha (1 + x)^\beta \qquad -1 < x < 1$$

Multidimensional Integrals

are HARD!

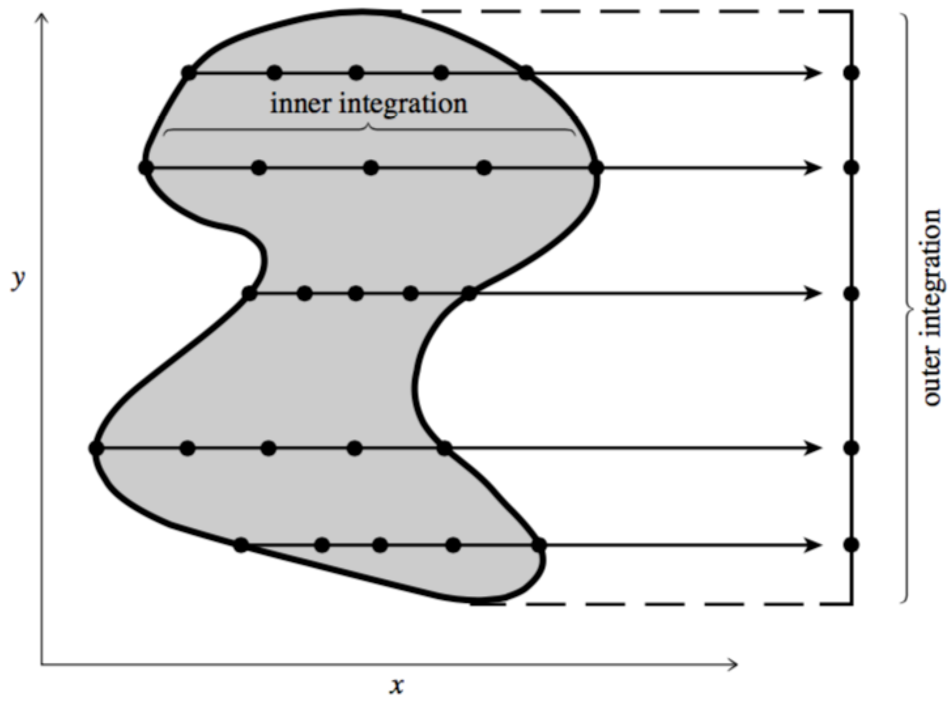
- Number of points scales as N^M, where M: # of dimensions
- Boundary can be complicated

Can dimension be reduced?

$$\int_0^x dt_n \int_0^{t_n} dt_{n-1} \cdots \int_0^{t_3} dt_2 \int_0^{t_2} f(t_1) dt_1$$
$$= \frac{1}{(n-1)!} \int_0^x (x-t)^{n-1} f(t) dt$$

If complicated boundary, low res, not strongly peaked integrand
→ Monte Carlo Integration (to be discussed later)

If boundary is simple and function is smooth
→ Repeated 1-D integrals



$$I = \int\int dx dy f(x,y)$$

$$H(x) = \int_{y_1}^{y_2} f(x,y)dy$$

$$I = \int_{x_1}^{x_2} H(x)dx$$

Best to use Gaussian Quadratures for high precision

Image credit: Press et al., *Numerical Recipes,* 3rd ed. (pg. 198)

Summary

- Workhorse for 1-D integrals is:
  Romberg: simple, nested error estimate

- Input: EPS (Error), Max # of iterations

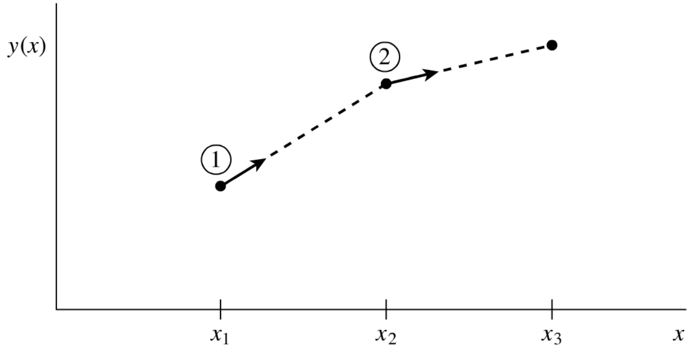
- If evaluations expensive, use Gaussian Quadratures

- If many dimensions, use 1-D repeated integrals,
  with Gauss Q. preferred

- Complicated boundary + many dim integrals
  → Use Monte Carlo

Euler Method, 2nd Order Midpoint …

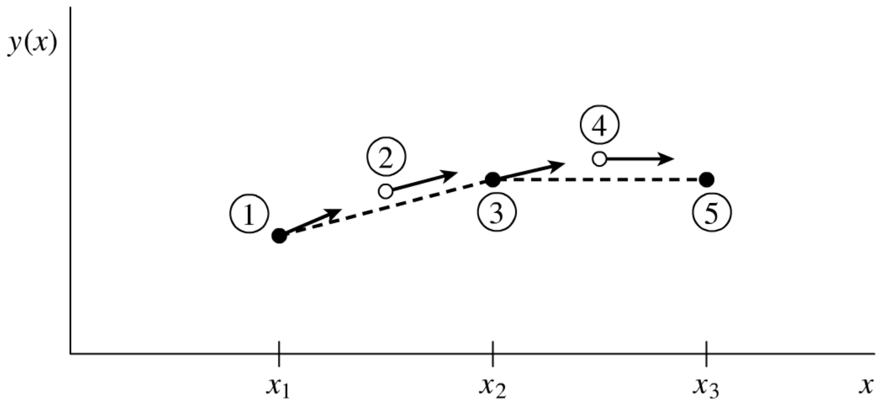
- We start with the simplest method, 1st order (explicit) Euler:
  dy/dx = f(x,y), dx = h



- $$y_{n+1} = y_n + hf(x_n, y_n)$$

- 2nd order extension (midpoint, or 2nd order Runge-Kutta)

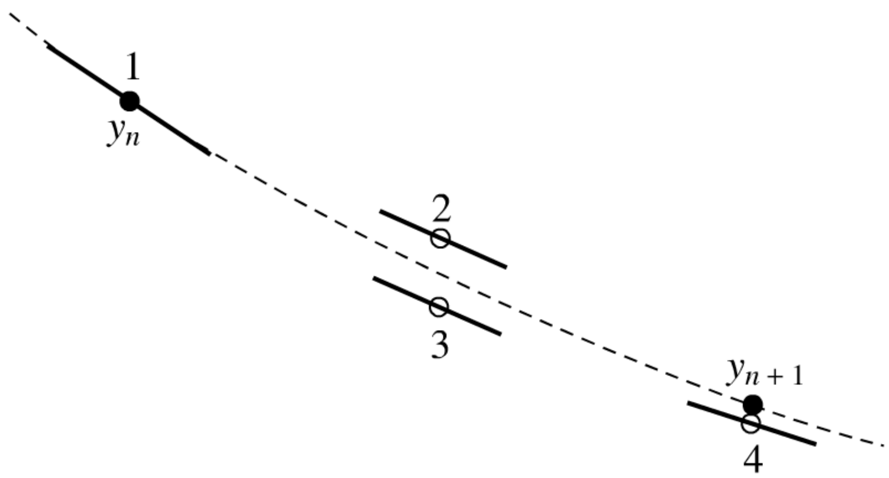
$$k_1 = hf(x_n, y_n)$$
$$k_2 = hf\left(x_n + \tfrac{1}{2}h, y_n + \tfrac{1}{2}k_1\right)$$
$$y_{n+1} = y_n + k_2 + O(h^3)$$



4^{th} Order Runge-Kutta

- Historically often the method of choice

$$
\begin{aligned}
k_1 &= hf(x_n, y_n) \\
k_2 &= hf(x_n + \tfrac{1}{2}h, y_n + \tfrac{1}{2}k_1) \\
k_3 &= hf(x_n + \tfrac{1}{2}h, y_n + \tfrac{1}{2}k_2) \\
k_4 &= hf(x_n + h, y_n + k_3) \\
y_{n+1} &= y_n + \tfrac{1}{6}k_1 + \tfrac{1}{3}k_2 + \tfrac{1}{3}k_3 + \tfrac{1}{6}k_4 + O(h^5)
\end{aligned}
$$



4^{th} Order Runge-Kutta

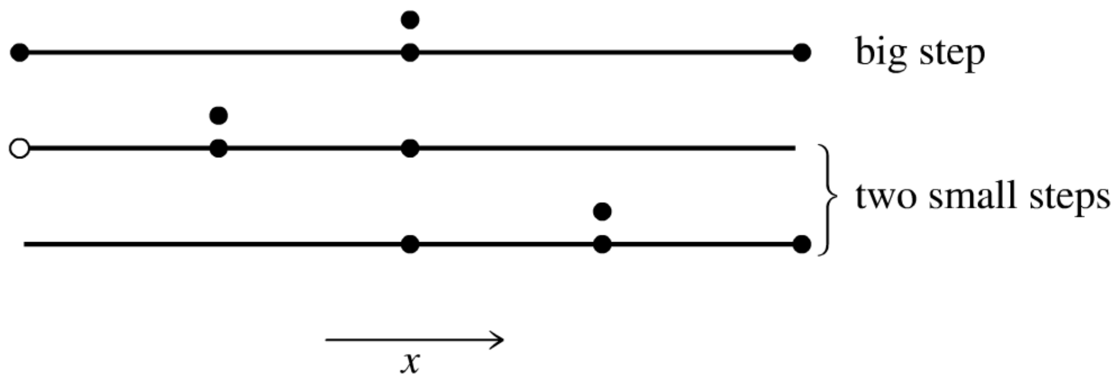
- Add adaptive stepsize control, doubling the step.
- Richardson extrapolation adds one more order

$$y(x+2h) = y_1 + (2h)^5\phi + O(h^6) + \ldots$$

$$y(x+2h) = y_2 + 2(h^5)\phi + O(h^6) + \ldots$$

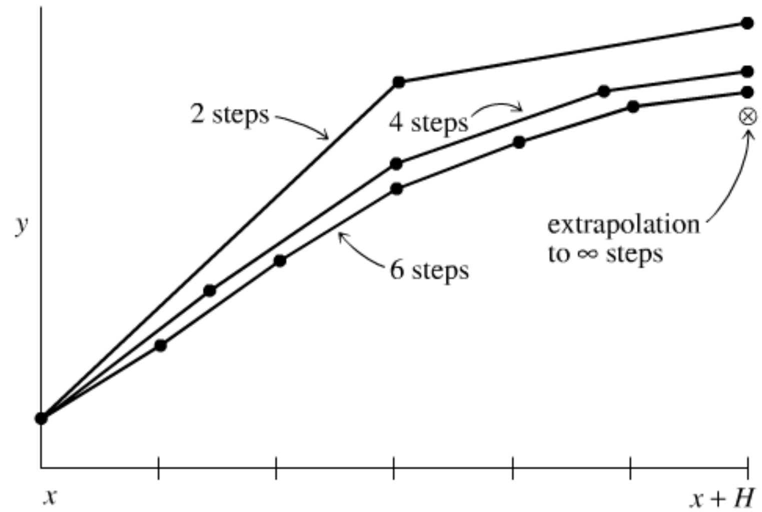
$$y(x+2h) = y_2 + \frac{\Delta}{15} + O(h^6)$$

$$\Delta \equiv y_2 - y_1$$



Bulirsch-Stoer method: “infinite” order extrapolation

- Uses Richardson’s extrapolation again (we also used it for Romberg integration): we estimate the error as a function of interval size h, then we try to extrapolate it to h=0
- As in Romberg we need to have the error to be in terms of h^2 instead of h
- Can use polynomial or rational function extrapolation: we discussed both for interpolations

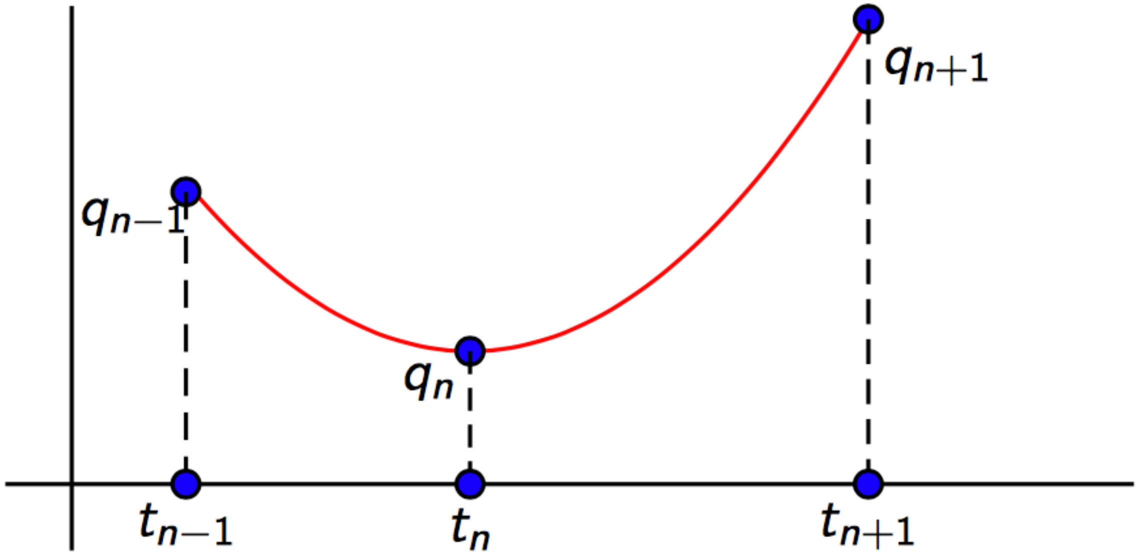


2^{nd} Order Conservative Equations

$$\ddot{q} = f(q)$$

- Stormer-Verlet with two step formulation: we are interpolating parabola through 3 points
- Gains a factor of 2

$$q_{n+1} - 2q_n + q_{n-1} = h^2 f(q_n)$$



One Step Formulation: Leap-frog

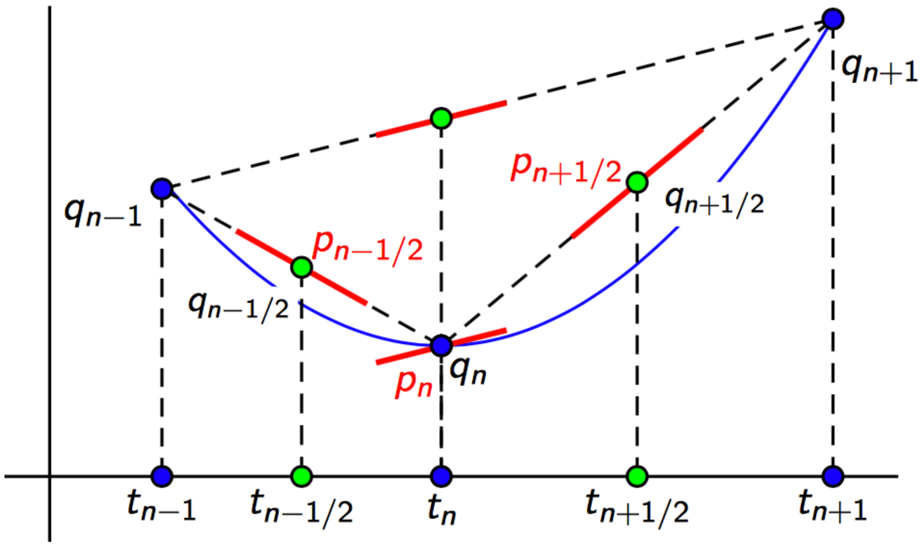
- We introduce momentum $p = \dot{q}, \quad \ddot{q} = f(q)$

$$\dot{q} = p, \qquad \dot{p} = f(q)$$

$$p_{n+1/2} = p_n + \frac{h}{2} f(q_n)$$

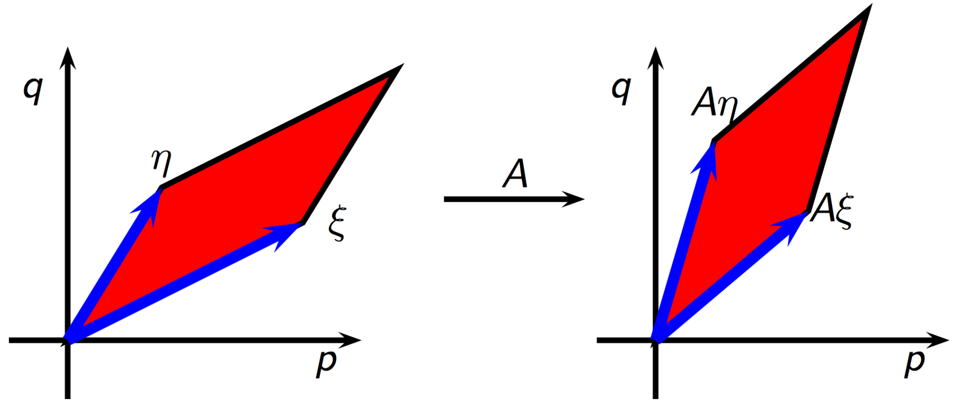
$$q_{n+1} = q_n + h p_{n+1/2}$$

$$p_{n+1} = p_{n+1/2} + \frac{h}{2} f(q_{n+1})$$



Generalization: Symplectic Integrators

- Symplectic integrators preserve phase space (p,q) volume: p,q must be canonical variables
- Symplectic transformation preserves phase space area (p,q) (Lioville's theorem)



- Hamiltonian is not conserved, but a related quantity is and one does not accumulate amplitude error, only phase error
- Useful if one needs to integrate a system for a long time (e.g. planet orbits etc)

Leapfrog is Symplectic

Hamiltonian problem $\dot{p} = -H_q(p, q)$, $\dot{q} = H_p(p, q)$

Theorem. The Störmer-Verlet method

$$
\begin{aligned}
p_{n+1/2} &= p_n - \frac{h}{2} H_q(p_{n+1/2}, q_n) \\
q_{n+1} &= q_n + \frac{h}{2}\Big(H_p(p_{n+1/2}, q_n) + H_p(p_{n+1/2}, q_{n+1})\Big) \\
p_{n+1} &= p_{n+1/2} - \frac{h}{2} H_q(p_{n+1/2}, q_{n+1})
\end{aligned}
$$

is symplectic.

Euler can be made symplectic

applied to $\dot{p} = -H_q$, $\dot{q} = H_p$:

$$\begin{aligned} p_{n+1} &= p_n - hH_q(p_{n+1}, q_n) \\ q_{n+1} &= q_n + hH_p(p_{n+1}, q_n) \end{aligned} \qquad \text{(SE1)}$$

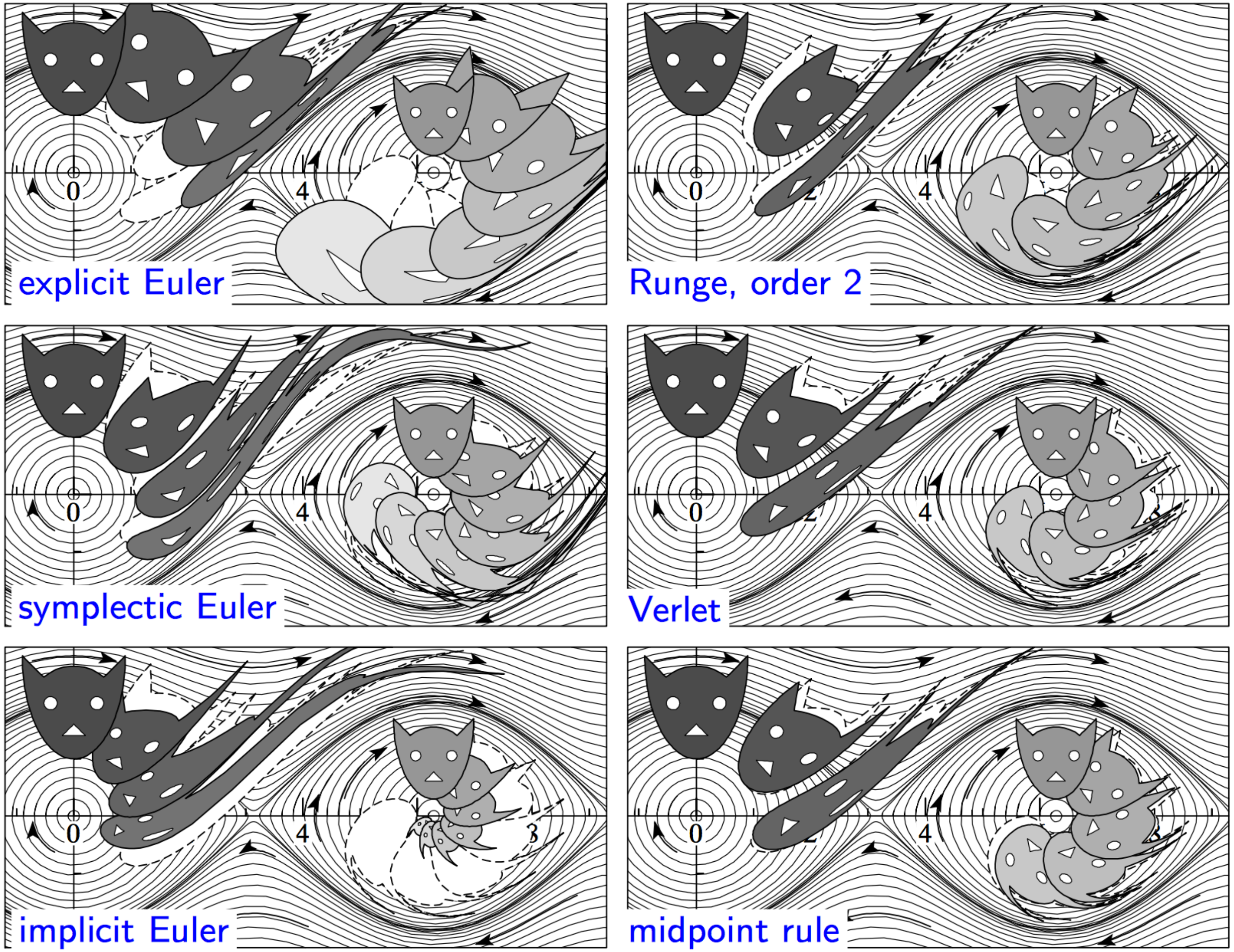
or

$$\begin{aligned} q_{n+1} &= q_n + hH_p(p_n, q_{n+1}) \\ p_{n+1} &= p_n - hH_q(p_n, q_{n+1}) \end{aligned} \qquad \text{(SE2)}$$

Theorem. (de Vogelaere, 1956)
The symplectic Euler method is symplectic.

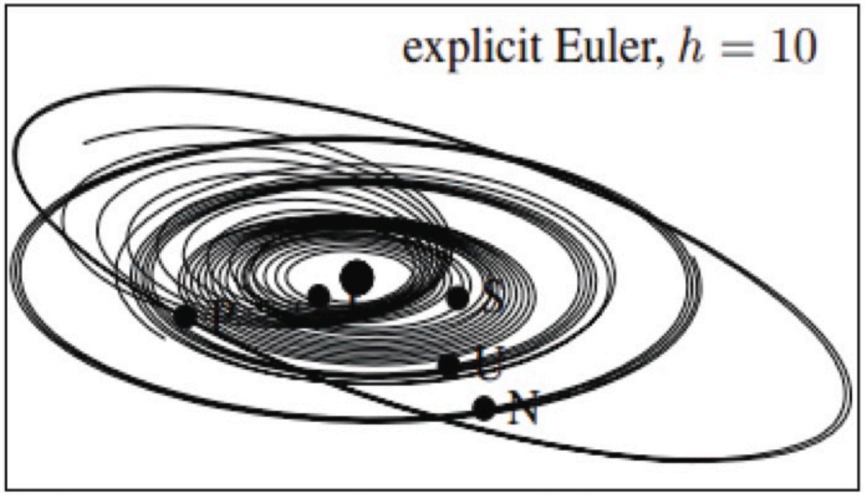
Theorem. The implicit midpoint rule is symplectic.

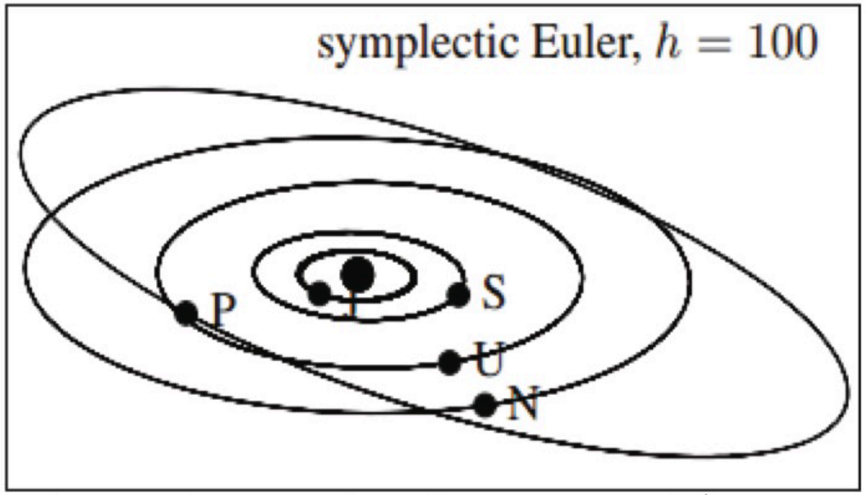
Phase Space Flow



Example: Planetary Orbit Integration

- Explicit Euler's orbits decay. This is not cured by higher order (Runge-Kutta, B-S…)
- Symplectic integrators preserve the orbit amplitude (but not the phases, not shown)





Stiff Equations

- Explicit (forward) Euler:

$$y' = -cy$$

$$y_{n+1} = y_n + hy'_n = (1 - ch)y_n$$

- Unstable if $h > 2/c$, since y goes to infinity
- Example:

$$u' = 998u + 1998v \qquad u(0) = 1 \qquad v(0) = 0$$

$$v' = -999u - 1999v$$

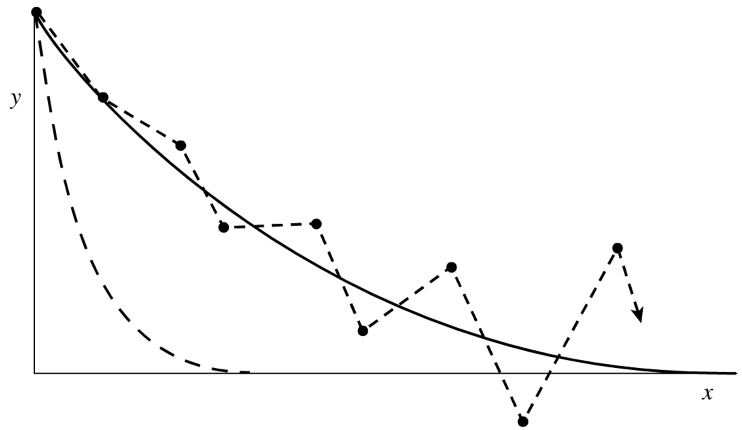
$$u = 2e^{-x} - e^{-1000x}$$

$$u = 2y - z \qquad v = -y + z \qquad v = -e^{-x} + e^{-1000x}$$

- But the system is unstable if h > 1/1000
- Solution: implicit (backward Euler)

$$y_{n+1} = y_n + hy'_{n+1}$$

$$y_{n+1} = \frac{y_n}{1 + ch}$$



General Appraoch

- If we are solving a linear system: $\mathbf{y}' = -\mathbf{C} \cdot \mathbf{y}$

$$\mathbf{T}^{-1} \cdot \mathbf{C} \cdot \mathbf{T} = \mathrm{diag}(\lambda_0 \ldots \lambda_{N-1}) \qquad \mathbf{z}' = -\mathrm{diag}(\lambda_0 \ldots \lambda_{N-1}) \cdot \mathbf{z}$$

$$\mathbf{z} = \mathrm{diag}(e^{-\lambda_0 x} \ldots e^{-\lambda_{N-1} x}) \cdot \mathbf{z}_0$$

- Exact solution: $\mathbf{y} = \mathbf{T} \cdot \mathrm{diag}(e^{-\lambda_0 x} \ldots e^{-\lambda_{N-1} x}) \cdot \mathbf{T}^{-1} \cdot \mathbf{y}_0$

- Explicit scheme: $\mathbf{y}_0 = \sum_{i=0}^{N-1} \alpha_i \boldsymbol{\xi}_i \qquad \mathbf{y}_n = \sum_{i=0}^{N-1} \alpha_i (1 - h\lambda_i)^n \boldsymbol{\xi}_i$

- Stability condition: $|1 - h\lambda_i| < 1 \qquad i = 0, \ldots, N-1 \qquad h < \frac{2}{\lambda_{\max}}$

- Implicit scheme: $\mathbf{y}_{n+1} = (\mathbf{1} + \mathbf{C}h)^{-1} \cdot \mathbf{y}_n$

- Always stable: $|1 + h\lambda_i|^{-1} < 1 \qquad i = 0, \ldots, N-1$

Stiff Nonlinear Equations

- In general, implicit scheme hard to solve

$$\mathbf{y}' = \mathbf{f}(\mathbf{y})$$

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\mathbf{f}(\mathbf{y}_{n+1})$$

- Linearize f :
- (Newton's method)

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\left[\mathbf{f}(\mathbf{y}_n) + \left.\frac{\partial \mathbf{f}}{\partial \mathbf{y}}\right|_{\mathbf{y}_n} \cdot (\mathbf{y}_{n+1} - \mathbf{y}_n)\right]$$

- Invert Jacobian: $\mathbf{y}_{n+1} = \mathbf{y}_n + h\left[\mathbf{1} - h\frac{\partial \mathbf{f}}{\partial \mathbf{y}}\right]^{-1} \cdot \mathbf{f}(\mathbf{y}_n)$

- This is semi-implicit Euler method
- There are also stiff versions of higher order ODE

Partial Differential Equations

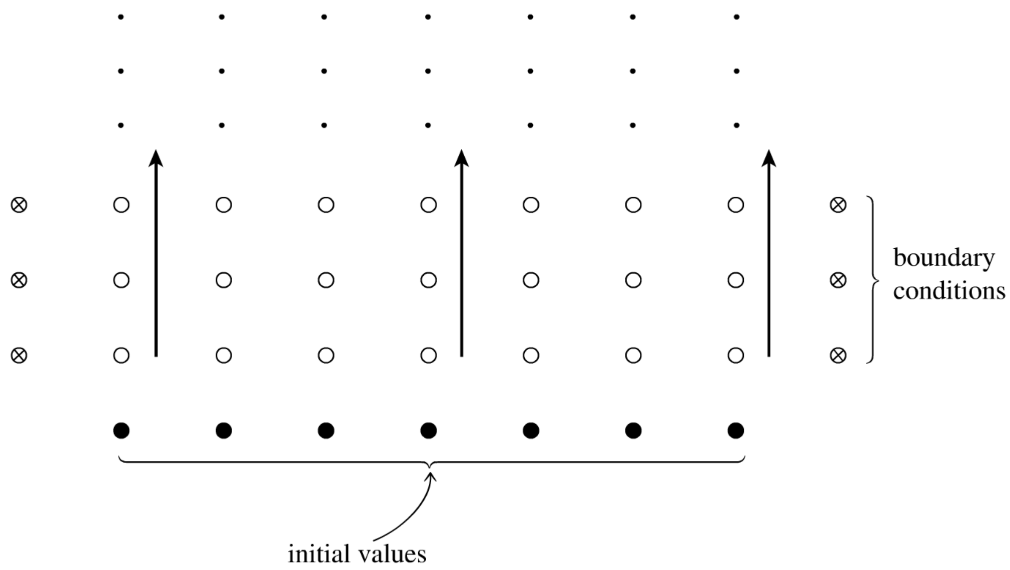
- This is a vast subject, and we will only mention its existence
- Hyperbolic, e.g. wave equation: $$\frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2}$$
- Parabolic, e.g. diffusion equation: $$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(D \frac{\partial u}{\partial x}\right)$$
- Both of these are initial value (Cauchy) problems
- Boundary value problem: elliptic, Elliptic, e.g. Poisson equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \rho(x, y)$$

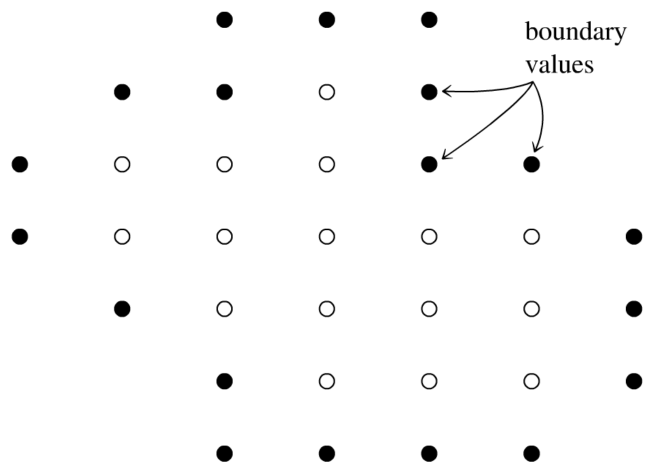
- If source ρ=0 this is Laplace equation

Finite Difference Method

- Discretize on a grid…



(a)



Summary

- ODEs and PDEs are central to numerical analysis in physical sciences, engineering…
- ODEs have a relatively stable methods
- PDEs have a vast array of approaches: relaxation, finite differences, finite elements, spectral methods, matrix methods, multi-grid, Monte Carlo, variational…

Literature

Numerical Integration:

- *Numerical Recipes*, Press et al., Chapter 4
  (http://apps.nrbook.com/c/index.html)
- *Computational Physics*, Mark Newman, Chapter 5
  (http://www-personal.umich.edu/~mejn/cp/chapters/int.pdf)

ODE&PDEs

- *Numerical Recipes*, Press et al., Chapter 17-20