Computation II — integration, ODEs

1 Integration vs. Solving ODEs

The evaluation of

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

is equivalent to solving

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

for $y(b)$.

$\Rightarrow$ ODE solvers can be used for numerical integration.

- Warranted for functions with multiple length scales.

2 Trapezoid and Simpson's rules

Trapezoid Rule: (straight line fits)

Deriving Trapezoid rule

Taylor series of I about x_1:

$$\begin{aligned} I(x_2) &= I(x_1 + \Delta x) \\ &= I(x_1) + \Delta x f(x_1) + \frac{(\Delta x)^2}{2} f'(x_1) + \frac{(\Delta x)^3}{3!} f''(x_1) + O(\Delta x)^4. \end{aligned}$$

Replace f' with forward difference expression:

$$f'(x_1) = \frac{f(x_1 + \Delta x) - f(x_1)}{\Delta x} - \frac{\Delta x}{2} f''(x_1) + O(\Delta x)^2.$$

Substituting and collecting terms:

$$I(x_2) = I(x_1) + \frac{\Delta x}{2}[f(x_2) + f(x_1)] - \frac{(\Delta x)^3}{12} f''(x_1) + O(\Delta x)^4.$$

or:

$$\int_{x_1}^{x_2} f(x)dx = h[\frac{1}{2}f_1 + \frac{1}{2}f_2] + O(h^3 f'').$$

Extended Trapezoid Rule:

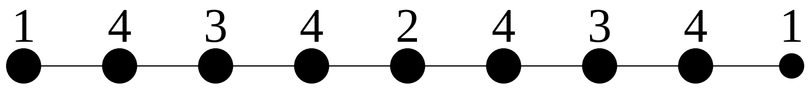
$$\int_{x_1}^{x_N} f(x)dx = h[\frac{1}{2}f_1 + f_2 + \cdots + f_{N-1} + \frac{1}{2}f_N] + O(f''/N^2).$$

Simpson Rule: (parabola fits)

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

Note how a symmetry increases the error to h^5.
Extended Simpson Rule:

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



Note how previous work can be used as the number of intervals doubles.
Also look at the combination:

$$S = \frac{4}{3}S_{2N} - \frac{1}{3}S_N.$$

where the S_N are trapezoid sums over N intervals. S is just Simpson's rule.

3 Richardson extrapolation

- Perform the integration to various values of h.
- Extrapolate to $h = 0$.

Note: for trapezoid, use polynomial in h^2.

4 Improper integrals

- Infinite limit

  Make a change of variable:

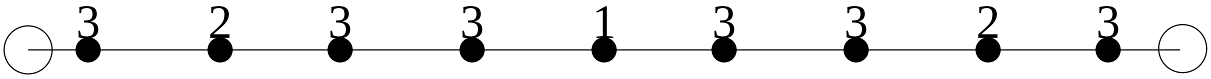
$$\int_a^b f(x)dx = \int_{1/b}^{1/a} \frac{1}{t^2} f\left(\frac{1}{t}\right) dt.$$

- Integrable singularities

  Use an open-ended formula:

$$\int_{x_1}^{x_N} f(x)dx = h[f_{3/2} + f_{5/2} + \cdots + f_{N-1/2}] + O(f''/N^2).$$

  We now step TRIPLE to use previous evaluations:



5 Gaussian Quadrature

Choose both abscissas and weights:

$$I \approx w_1 f(x_1) + w_2 f(x_2) + w_3 f(x_3) + \cdots$$

- More degrees of freedom allows higher order with same number of function evaluations.

- Choose weights to match the class of integrand.

  That is, make it exact for

$$\int_a^b W(x) f(x) dx$$

  where $f(x)$ is a polynomial of a given degree.

- *Warning:* High order does not mean high accuracy.

Consider polynomial whose roots are the chosen absissas:

$$g(x) = (x - x_1)(x - x_2)(x - x_3)$$

if our formula is to be exact for $g(x)$ times polynomials of degree < 3, then

$$\int_a^b W(x)g(x)x^n dx = 0$$

for all $n < 3$.
That is, $g(x)$ is orthonormal to all polynomials of degree < 3.
Therefore $g(x)$ can be easily constructed by Gramm-Schmitt orthogonalization.
The weights can be gotten by making it exact for $f(x) = 1, x, x^2$:

$$\begin{aligned}
b - a &= w_1 + w_2 + w_3 \\
\frac{1}{2}(b^2 - a^2) &= w_1 x_1 + w_2 x_2 + w_3 x_3 \\
\frac{1}{3}(b^3 - a^3) &= w_1 x_1^2 + w_2 x_2^2 + w_3 x_3^2
\end{aligned}$$

This is a linear set of equations in w_i.

6 Multidimensional integrals

Difficulties:

- Many function evaluations are needed: N_1^D.
- Complicated boundaries

Strategies:

- Reduce dimensionality of problem
- Simple boundary and smooth: Recursively use 1-D integrators.

- Complicated boundary, smooth & low accuracy: Monte Carlo integration

7 Summary

- Gauss quadrature for smooth well know functions that need to be evaluated many times at high accuracy.
- Romberg for general purpose smooth function.
- Trapezoid or Simpson for ill-behaved functions: oscillating or large high-order derivatives.

8 Runge-Kutta

The workhorse.
Fourth order:

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

Going to higher order is generally not justified.
Error can be estimated by half-stepping. This gives an overhead of 1.375.
Use $\Delta \sim h^5$ to adjust stepsize.

9 Bulirsch-Stoer

For high-order, accurate integrations:

- Richardson extrapolation

  Allows high order with few function evalutions.

- Rational function extrapolation

  Allows large extrapolations without worries about poles.

- Use method with even error function: modified midpoint method,

$$
\begin{aligned}
z_1 &= y_n + \frac{h}{2} f'(x_n, y_n) \\
z_2 &= z_1 + h f'(x_{n+1/2}, z_1) \\
y_{n+1} &= \frac{1}{2}[z_2 + z_1 + \frac{h}{2} f'(x_{n+1}, z_2)]
\end{aligned}
$$

Allows function approximation in h^2.

Extrapolator can give error estimate.

Adjust stepsize to keep number of extrapolations resonable.

10 Predictor-Corrector

- Extrapolate from past function values, *e.g.*

$$y_{n+1} = y_n + h\left[\frac{3}{2} f'(x_n, y_n) - \frac{1}{2} f'(x_{n-1}, y_{n-1})\right].$$

- Correct using derivative at new point, *e.g.*

$$y_{n+1} = y_n + h\left[\frac{1}{2} f'(x_{n+1}, y_{n+1}) + \frac{1}{2} f'(x_n, y_n)\right].$$

Note the similarity to the trapezoid rule.

The corrector can also give a truncation error estimate.

11 Stiff Equations

Consider

$$y'' = 100y.$$

The solution is

$$y = Ae^{-10x} + Be^{10x}$$

Any numerical introduction of the growing solution will dominate the decaying solution.

Now consider

$$y' = -cy.$$

The forward Euler scheme gives a solution

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

This is unstable for $h > 2/c$.

The backward Euler gives

$$y_{n+1} = y_n + hy'_{n+1} = \frac{y_n}{1 + ch},$$

which is stable.

From this we get a "semi-implicit" method:

$$y_{n+1} = y_n + h\left[f'(x_{n+1}, y_n) + \left.\frac{\partial f'}{\partial y}\right|_{y_n}(y_{n+1} - y_n)\right].$$

This must be solved for y_{n+1}.

12 Boundary value problems

- Shooting

  This involves root-finding: use multi-dimensional Newton-Raphson.

- Internal critical points

  These can be solved using a variation of the shooting method.

- Relaxation methods

  Replace ODEs with FDEs on a mesh. *e.g.*

$$y_k - y_{k-1} - (x_k - x_{k-1}) f' \left(\frac{1}{2}(x_k + x_{k-1}), \frac{1}{2}(y_k + y_{k-1}) \right) = 0$$

  A solution is found by expanding these in a Taylor series in Δy_k. This gives a set of linear equations in Δy.

13 Summary

- Ratty function, quick and dirty integration: Runge-Kutta
- Smooth function, accuracy needed: Bulirsch-Stoer
- Smooth, well-known function, maximum accuracy with minimum function evaluations: Predictor-corrector.

14 Symplectic integrators

The equations of motion for many physical systems can be derived from a Hamiltonian formalism:

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \quad ; \quad \dot{p}_i = -\frac{\partial H}{\partial q_i}.$$

These equations of motion define a symplectic transformation implying:

1. The sum of the areas projected by an arbitrary closed loop in the $2N$ dimensional phase space is preserved.
2. Most of the features of the dynamics will be preserved under a small perturbation. (KAM theorem)

A numerical integration can be thought of as a transformation

$$(\mathbf{q}_0, \mathbf{p}_0) \rightarrow (\mathbf{q}_\tau, \mathbf{p}_\tau),$$

and this transformation is repeated.
A symplectic transformation will evolve the system under a surrogate Hamiltonian:

$$H_N = H + H_{err},$$

where H_{err} reflects the truncation error.
Therefore the numerical integration will

- preserve global invariants similar to those conserved in the original Hamiltonian,
- preserve the topological structure of phase space.

Constructing symplectic integrators

A transformation can be shown to be symplectic if it can be derived from a generating function, or if it is a product of symplectic transformations.
Consider a Hamiltonian of the form

$$H = H_T + H_V$$

where H_T and H_V are both integrable (as is the case when $H_T = \frac{1}{2}\mathbf{p}^2$ and $H_V = V(\mathbf{q})$).
Hamilton's equations can be written

$$\dot{\mathbf{z}} = \{\mathbf{z}, H_T + H_V\}$$

where $\mathbf{z}$ is $(\mathbf{q}, \mathbf{p})$ and $\{\,,\,\}$ are Poisson brackets. Introducing the operators

$$T \equiv \{\,, H_T\} \quad \text{and} \quad V \equiv \{\,, H_V\},$$

the formal solution of the above is

$$\mathbf{z}(\tau) = \exp[\tau(T + V)]\mathbf{z}(0).$$

We can calculate $\exp(\tau T)$ and $\exp(\tau V)$, so we just need to approximate $\exp[\tau(T + V)]$ in terms of these. This is done via the BCH identity:

$$\exp A \exp B = \exp\left(A + B + \frac{1}{2}[A, B] + \frac{1}{12}[A - B, [A, B]] + \langle\text{more terms}\rangle\right).$$

Consider

$$\exp(\tau T)\exp(\tau V) = \exp[\tau(T + V) + \langle\text{error}\rangle].$$

So $\exp(\tau T)\exp(\tau V)$ evolves the system under the Hamiltonian

$$H_N = H_T + H_V + H_{err}.$$

and we have a simple symplectic integrator.