Imperial College London

Computational Physics: Numerical Integration

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Lecture 13

Outcomes

By the end of this lecture, you should be able to:

- Compute definite integrals numerically using the trapezoidal rule
- Also compute them using Simpson's Rule
- Implement modified methods to deal with various improper integrals
- Implement Runge-Kutta initial-value problem methods to compute definite integrals
- Explain their relationship to the Newton-Coates formulae

Numerical Integration

The Problem, v1

We need to solve

$$I = \int_a^b f(x)\mathrm{d}x$$

The Problem, v2

This is equivalent to solving the initial-value problem

$$\frac{\mathrm{d}y}{\mathrm{d}x} = f(x); \qquad y(a) = 0$$

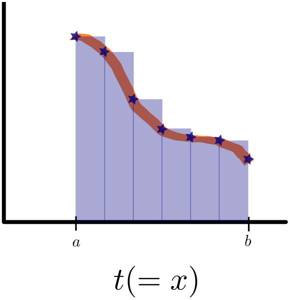
at $x = b$, i.e. $I \equiv y(b)$

We need to do this efficiently; i.e., without calling the function $f(x)$ too many times.

Numerical Integration

Computing Directly

- "Quadrature" $\equiv$ numerical integration via direct sampling of integrand (i.e. v1)
- Effectively adding the areas of rectangles with different heights and widths
- An example of a *Riemann Sum*
- Could use something a little more involved than simple rectangles



Numerical Integration

Two main issues:

- Sampling
  - Are there enough rectangular pieces to estimate I accurately?
    $\rightarrow$ This is a question of the **magnitude** of the step-size h
  - Are they distributed efficiently?
    $\rightarrow$ This is a question of the **variation** of h with x
- Interpolation
  - Do the tops of the individual pieces look like $f(x)$, especially if we are going beyond simple rectangles?
    $\rightarrow$ A question of interpolating function

Both affect accuracy, not independently
(i.e. one perfect $\Rightarrow$ other irrelevant)
Initially, we will focus on

- equal-width rectangles $\Rightarrow$ h constant for all x
- choices of interpolating functions

Variable step size later (solving integrals by ODE)

Numerical Integration

Possible Problems

Further issues arise when

- a or $b \to \infty$
- $f(a)$ or $f(b) = \frac{0}{0}$ but I is still convergent (e.g. $\mathrm{sinc}(x) \equiv \sin(x)/x$)
- there is an integrable singularity at some $a \leq x \leq b$

These are referred to as **improper integrals**. We will also see how to handle these cases later today

Rules and Integrators

Simplest quadrature building blocks are N-point rules

- **Closed rules** estimate

$$\int_{x_0}^{x_N} f(x)\,\mathrm{d}x$$

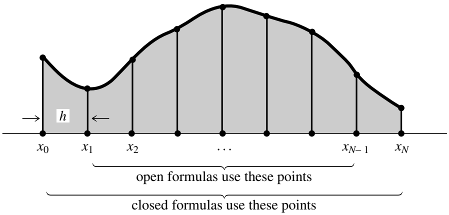
  using $f(x_0 \ldots x_N)$ (including the end-point values)

- **Open rules** estimate

$$\int_{x_0}^{x_N} f(x)\,\mathrm{d}x$$

  using, for example, $f(x_1 \ldots x_{N-1})$ (without using the end-point values)

- Analogous to N-point interpolation methods



Will typically use $N = 2, 3$ and build up integrations over more points using these, to produce *extended* rules

Rules and Integrators

- also a **midpoint rule** based on $f(x_{i+\frac{1}{2}},\ x_{i+\frac{3}{2}},\ \text{etc})$
- n-point rules can be patched together to give **extended rules**
- just like doing $n-1$ degree interpolation over an extended abscissa
- extended rules can be closed or open at each end

- n-point rules for fixed h are Newton-Coates Rules
- **Gaussian quadrature** makes use of n-point rules for $h = h(x)$
- **Importance sampling** chooses h to focus on where $f(x)$ is largest ($\rightarrow$ Part II)

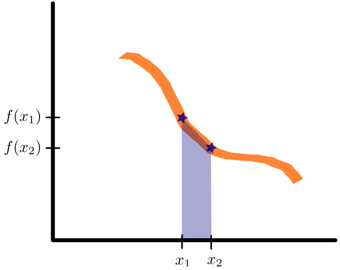
Closed Newton–Coates Rules

The Trapezoidal Rule

Trapezoidal Rule

$$\int_{x_i}^{x_{i+1}} f(x)\,\mathrm{d}x = h\left[\frac{1}{2}f(x_i) + \frac{1}{2}f(x_{i+1})\right] + O\left(h^3\frac{\mathrm{d}^2 f}{\mathrm{d}x^2}\right)$$

- 2-point $\Rightarrow$ degree 1 polynomial
- $\Rightarrow$ connect-the-dots, linear interpolation style



Closed Newton–Coates Rules

Simpson's Rule

Simpson's Rule according to Numerical Recipes

$$\int_{x_i}^{x_{i+2}} f(x)\,\mathrm{d}x = h\left[\frac{1}{3}f(x_i) + \frac{4}{3}f(x_{i+1}) + \frac{1}{3}f(x_{i+2})\right] + O\left(h^5\frac{\mathrm{d}^4 f}{\mathrm{d}x^4}\right)$$

- Three-point $\Rightarrow$ degree-2 polynomial (yes, quadratic interpolation again)
  - take the second-order Lagrange polynomial that passes the three points
  - integrate to obtain the coefficients above

Rules and Integrators

Other Rules

- There are also higher-order Newton-Coates rules...
  - with names such as Boole's, Milne's etc.
  - but we will not look at these here as they do not add much
  - therefore for the course you don't have to know about those names either

Numerical Integration

Extended Trapezoidal Rule

Extended Trapezoidal Rule

$$\int_{x_0}^{x_{n-1}} f(x)\,\mathrm{d}x = h\left[\frac{1}{2}f(x_0) + f(x_1) + f(x_2) + \ldots + f(x_{n-2}) + \frac{1}{2}f(x_{n-1})\right]$$

- Just end-to-end patching together of trapezoidal rules over all 2-point intervals
- Just like linear interpolation over a uniform grid of abscissae

Numerical Integration

Extended Simpson's Rule

Extended Simpson's Rule

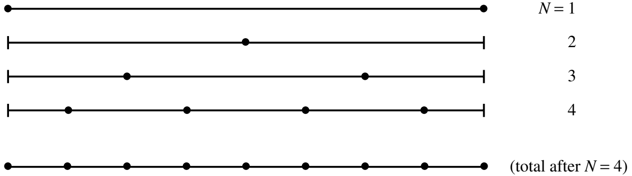
$$\int_{x_0}^{x_{n-1}} f(x)\,\mathrm{d}x = h\left[\frac{1}{3}f(x_0) + \frac{4}{3}f(x_1) + \frac{2}{3}f(x_2) + \frac{4}{3}f(x_3)\ldots\right.$$
$$\left.\ldots + \frac{4}{3}f(x_{n-4}) + \frac{2}{3}f(x_{n-3}) + \frac{4}{3}f(x_{n-2}) + \frac{1}{3}f(x_{n-1})\right] \quad (1)$$

- Non-overlapping three-point Simpson's Rules patched together
- Like quadratic interpolation over a uniform grid of abscissae

Numerical Integration

Implementation of Extended Trapezoidal Rule

1. Evaluate $f(a)$ and $f(b)$
2. Use these as a first estimate $I_1 = h_1 \frac{1}{2}\left[f(a) + f(b)\right]$
3. Evaluate the midpoint $f(\frac{a+b}{2})$
4. Use this to update your estimate $I_2 = h_2\left[\frac{1}{2}f(a) + f(\frac{a+b}{2}) + \frac{1}{2}f(b)\right]$
5. See if $\left|\frac{I_2 - I_1}{I_1}\right| < \epsilon_{\text{required}}$
6. If not, keep filling in intermediate points and making more trapezoids until it is.



Numerical Integration

Implementation of Extended Simpson's Rule

As with the implementation of Extended Trapezoidal Rule, except

- Use $f(\frac{a+b}{2})$ in the first step, and start with three-point Simpson's rule
- There is an error cancellation between successive iterations of the trapezoidal rule T_i and T_{i+1} such that

$$S_i = \frac{4}{3}T_{i+1} - \frac{1}{3}T_i$$

- $\Rightarrow$ implementation can be easily piggybacked on code for extended trapezoidal rule
- (as usual, see Numerical Recipes for details)

Numerical Integration

Romberg Integration

- This ‘cancellation’ is no coincidence
- Exists for higher order Newton-Coates rules too
- $\Rightarrow$ with correct weights, successive extended trapezoidal rule evaluations can be used to obtain arbitrarily high-order estimates
- Successive iterations can also be extrapolated down to $h = 0$
- This iterative algorithm is called **Romberg Integration**
- See Numerical Recipes for (minimal) details

Numerical Integration

Improper Integrals

When should one consider one's integral improper?

1. Its limit exists but cannot be evaluated at a or b
   example: $\mathrm{sinc}(0)$
2. Its upper or lower limit is $\pm\infty$
3. It has an integrable singularity somewhere you know
   example: $x^{-\gamma}$ at $x = 0$, where $1 > \gamma \geq 0$
4. It has an integrable singularity somewhere you don't know

Improper Integrals

Non-Evaluable Points

1. When evaluation at a or b is not allowed
   - Use the **midpoint rule** around a or b

$$\int_{x_0}^{x_1} f(x)\,\mathrm{d}x = h\left[f\left(\frac{x_0+x_1}{2}\right)\right]$$

   - Stitch it up to your preferred extended closed (or open) rule to make a compound extended rule

Improper Integrals

Range Boundaries at Infinity

2. When $a = -\infty$ or $b = \infty$
   - Transform the asymptotic part of the integral via $x \to \frac{1}{t}$

$$\Rightarrow \int_a^b f(x)\,\mathrm{d}x = \int_{1/b}^{1/a} \frac{1}{t^2} f\left(\frac{1}{t}\right)\,\mathrm{d}t$$

   - Then use an open rule on the transformed integral
   - Works for *1 limit only*, only when a, b *have same signs*
   - Where both are infinite or opposite signs, split it

Improper Integrals

Singularities

3. When an integrable singularity exists at a known $x = x_{\text{sing}}$
   - Split the integral at $x = x_{\text{sing}}$, so that you have two integrals each with an integrable singularity at *one* limit
   - Transform the nasty bit of the integral via

$$x \to \alpha, \quad \text{with } \alpha = t^{\frac{1}{1-\gamma}} + x_{\text{sing}} \quad \text{for lower limit } x_{\text{sing}} \tag{2}$$

$$\alpha = x_{\text{sing}} - t^{\frac{1}{1-\gamma}} \quad \text{for upper limit } x_{\text{sing}} \tag{3}$$

giving (with either $a' = x_{\text{sing}}$ or $b' = x_{\text{sing}}$)

$$\int_{a'}^{b'} f(x)\,\mathrm{d}x = \frac{1}{1-\gamma} \int_0^{(b'-a')^{1-\gamma}} t^{\frac{\gamma}{1-\gamma}} f(\alpha)\,\mathrm{d}t$$

(Choose some $0 \leq \gamma < 1$ of your choice—but best matched to γ in $f(x) \to (x - x_{\text{sing}})^{-\gamma}$ if this is how your function behaves as $x \to x_{\text{sing}}$)

   - Use an open rule on the transformed integral

Improper Integrals

Singularities

4. When an integrable singularity exists at an unknown x
   - Think hard—do you have to be able to do this?
   - Try using a variable step size method to find and 'inch over' the singularity, i.e.
     - ODE techniques
     - Gaussian quadrature
     - or even MC integration with the PDF somehow peaked around (unknown!) problem x

Numerical Integration

Using ODE Solvers

Doing a definite integral is equivalent to solving the initial-value problem (IVP)

$$\frac{\mathrm{d}y}{\mathrm{d}x} = f(x); \qquad y(a) = 0$$

for $x = b$, i.e. $I \equiv y(b)$

We see this by

$$\begin{aligned} I \equiv \int_a^b f(x)\,\mathrm{d}x &= \int_a^b \frac{\mathrm{d}y}{\mathrm{d}x}\,\mathrm{d}x \\ &= \int_{y(a)}^{y(b)} \mathrm{d}y \\ &= y(b) - y(a) \end{aligned}$$

Choice of y(a) is arbitrary as we only care about its derivative
$\rightarrow$ choose $y(a) = C \Rightarrow I = y(b) - C$. Just choose $C = 0$.
$\Rightarrow I = y(b)$

Numerical Integration

Using ODE Solvers

So, we need to 'evolve' $y(x)$ from $x = a$ to $x = b$.

We know $y(a)$ and $\frac{\mathrm{d}y}{\mathrm{d}x}(x)$, but not $y(b)$.

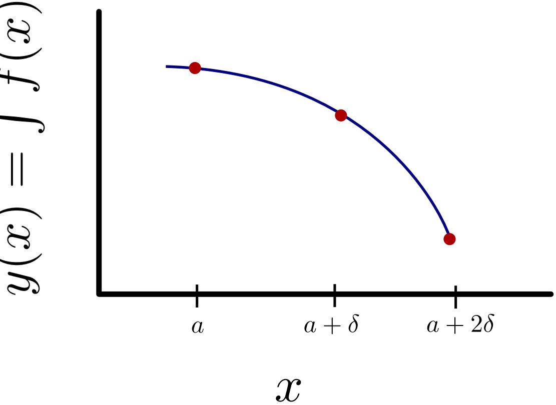
Basic (read: naive) strategy:

1. Start with y(a) = 0.
2. Calculate $\frac{\mathrm{d}y}{\mathrm{d}x}|_{x=a} = f(a)$
3. Take a (small) step to $x = a + \delta$
4. y becomes $y(a + \delta) = y(a) + \delta\frac{\mathrm{d}y}{\mathrm{d}x}|_{x=a}$
5. Evaluate $\frac{\mathrm{d}y}{\mathrm{d}x}|_{x=a+\delta}$
6. Step on, using $y(a + 2\delta) = y(a + \delta) + \delta\frac{\mathrm{d}y}{\mathrm{d}x}|_{x=a+\delta}$
7. Keep on rolling until $a + n\delta = b$

Integration Using ODE Solvers

Euler's Method

This is Euler's Method



Integration Using ODE Solvers

Euler's Method

In practice, we need to refine this strategy

- More stable stepping scheme (e.g. Runge Kutta)
- Error checking
  - How do we know if the derivative has actually stayed roughly constant over δ?
- Adaptive step-size
  - Need to adjust δ so evolution is slower (i.e. δ smaller) where $\frac{dy}{dx}(x)$ changes more rapidly

Integration Using ODE Solvers

RK4

Q.

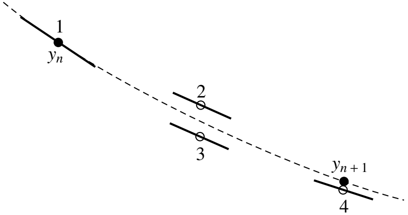
So how about using RK4 for doing definite integrals?

Initial-Value Problems

Fourth-Order Runge-Kutta Method

- This is a method that is widely in use, not just an illustrative example
- Weighted average of 4 different intermediate points
  - $\rightarrow$ weighting is such that h^3 and h^4 errors cancel
  - $\rightarrow$ error of order h^5, in just four evaluations of f

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



Integration Using ODE Solvers

RK4

Q.

So how about using RK4 for doing definite integrals?

A.

Not a good idea.

Integration Using ODE Solvers

RK4

Normal RK4 step:

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

Integration Using ODE Solvers

RK4

Q.

So how about using RK4 for doing definite integrals?

A.

Not a good idea.

- f does not depend on y
- $\Rightarrow k_2 = k_3$
- $\Rightarrow$ more efficient would be to just evaluate one of them.

Integration Using ODE Solvers

RK4

Normal RK4 step:

$$k_1 = hf(x_n, y_n)$$

$$k_2 = hf(x_n + \frac{h}{2}, y_n + \frac{k_1}{2})$$

$$k_3 = hf(x_n + \frac{h}{2}, y_n + \frac{k_2}{2})$$

$$k_4 = hf(x_n + h, y_n + k_3)$$

$$y_{n+1} = y_n + \frac{1}{6}k_1 + \frac{1}{3}k_2 + \frac{1}{3}k_3 + \frac{1}{6}k_4$$

reduces to:

$$k_1 = hf(x_n, y_n)$$

$$k_2 = hf(x_n + \frac{h}{2})$$

$$k_3 = hf(x_n + h)$$

$$y_{n+1} = y_n + \frac{1}{6}k_1 + \frac{2}{3}k_2 + \frac{1}{6}k_3$$

But wait!—that reminds one of...

Integration Using ODE Solvers

RK4

...Simpson's Rule!

Exactly Simpson's Rule with $h \to \frac{h}{2}$

$$\int_{x_n}^{x_{n+1}} f(x)\,\mathrm{d}x = \frac{h}{2}\left[\frac{1}{3}f(x_n) + \frac{4}{3}f(x_{n+\frac{1}{2}}) + \frac{1}{3}f(x_{n+1})\right] + O(h^5)$$

Not so surprising when we think about error cancellations in RK4 and the fact that

$$y(x_{n+1}) = y(x_n) + \int_{x_n}^{x_{n+1}} \frac{\mathrm{d}y}{\mathrm{d}x}(x)\,\mathrm{d}x = y(x_n) + \int_{x_n}^{x_{n+1}} f(x)\,\mathrm{d}x$$

$\Rightarrow$ RK4 is just Simpson's Rule generalised to an $f(x)$ that also depends on $y(x) \equiv \int f(x)\,\mathrm{d}x$

...same is actually more than likely also true of RK2 and the Trapezoidal Rule...

Summary

There are a number of decent options for doing numerical integration:

- Trapezoidal Rule
- Simpson's Rule – reliable workhorse for smooth functions
- Romberg Integration
- Collapsed RK45 – best when function is highly variable
- Monte Carlo Integration – best for many-dimensional integrals

- Thank you for submitting your Assignment!
- Marking is underway
- Feedback survey for YU, PS and the demonstrators at tomorrow’s Practical Session
- Let us know which Project you are thinking of doing
    - rough numbers are fine
    - over to menti.com