Computational Astrophysics I: Introduction and basic concepts

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Numerical Integration and Differentiation

Numerical Integration I

(see also Landau et al. 2007)

Computing integrals

Often integrals have to be evaluated numerically. Examples:

- measured $dN(t)/dt$, the rate of some events, e.g., photons per unit time interval. Task: Determine the number of photons in the first second:

$$N(1) = \int_0^1 \frac{dN(t)}{dt} dt \tag{1}$$

- radiative rates in the statistical equations for non-LTE population numbers (stellar atmospheres, photoionized nebulae)

$$R_{\ell u} = \int \frac{4\pi}{h\nu} \sigma_{\ell u}(\nu) J_\nu d\nu \quad \text{where (in 1d): } J_\nu = \frac{1}{2} \int_{-1}^{1} I_\nu \, d(\cos\theta) \tag{2}$$

Also, *analytical* integration sometimes difficult or impossible (e.g., elliptic integrals), but numerically straightforward. So, Riemann definition

$$\int_a^b f(x)dx = \lim_{h \to 0} \left[h \sum_{i=1}^{(b-a)/h} f(x_i) \right] \tag{3}$$

summing up areas of boxes of height $f(x)$ and width $h \rightarrow$ numerical quadrature

$$\int_a^b f(x)\color{blue}{dx} \approx \sum_{i=1}^{N} f(x_i)\color{blue}{w_i} \tag{4}$$

$\rightarrow$ problem: find appropriate sampling $f_i \equiv f(x_i)$, with *weights* w_i
generally: result improves with N

some hints

- remove singularities before integration
- sometimes splitting of interval is helpful, e.g.,

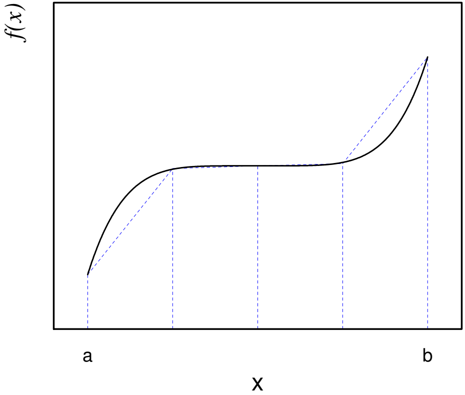
$$\int_{-1}^{1} f(|x|)dx = \int_{-1}^{0} f(-x)dx + \int_{0}^{1} f(x)dx \tag{5}$$

- or transformation/substitution

$$\int_{0}^{1} x^{1/3} dx = \int_{y(0)=0^{1/3}}^{y(1)=1^{1/3}} y\,3y^2 dy \qquad \left(y(x) = x^{1/3} \rightarrow\ dx = 3x^{2/3} dy = 3y^2 dy\right) \tag{6}$$

The Trapezoid rule

- uses values $f(x)$ at *evenly* spaced x_i $(i = 1, \ldots, N)$ with step size h on *integration region* $[a, b]$, including endpoints



- hence, $N - 1$ *intervals* of length h:

$$h = \frac{b-a}{N-1} \qquad x_i = a + (i-1)h \quad (7)$$

- so construct trapezoid on interval i of width $h \rightarrow f(x)$ approximated by straight line between $(a + i \cdot h, f_i)$ and $(a + (i+1) \cdot h, f_{i+1})$

Trapezoid rule II

with average height $(f_i + f_{i+1})/2$:

$$\int_{x_i}^{x_i+h} f(x)dx \simeq \frac{h(f_i + f_{i+1})}{2} = \frac{1}{2}hf_i + \frac{1}{2}hf_{i+1} \tag{8}$$

i.e. Eq. (4): $\int_a^b f(x)dx \approx \sum_{i=1}^N f(x_i)w_i$ for $N = 2$ and $w_i = \frac{1}{2}h$

- hence for full integration region $[a, b]$

$$\int_a^b f(x)dx \approx \frac{h}{2}f_1 + hf_2 + hf_3 + \ldots + hf_{N-1} + \frac{h}{2}f_N \tag{9}$$

i.e. $w_i = \{h/2, h, \ldots, h, h/2\}$

Simpson's rule

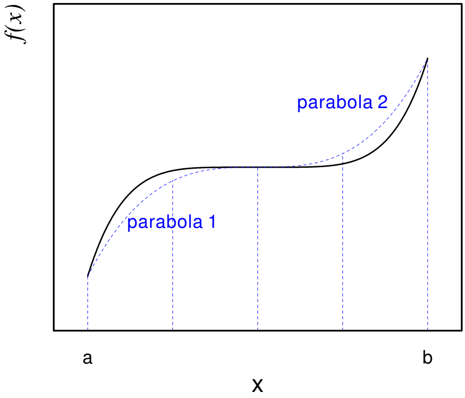
- similar to Trapezoid rule, but with *odd* number of points N
- for each interval: $f(x)$ approximated by parabola

$$f(x) = \alpha x^2 + \beta x + \gamma \tag{10}$$

hence area for each interval:

$$\int_{x_i}^{x_i+h} (\alpha x^2 + \beta x + \gamma) dx \tag{11}$$

$\rightarrow$ like integrating the corresponding Taylor series up to *quadratic* term



- need to determine α, β, γ for $f(x)$, so consider interval $[-1, 1]$

$$\int_{-1}^{1} (\alpha x^2 + \beta x + \gamma) dx = \frac{1}{3}\alpha x^3 + \frac{1}{2}\beta x^2 + \gamma x \Big|_{-1}^{+1} = \frac{2\alpha}{3} + 2\gamma \tag{12}$$

and $f(-1) = \alpha - \beta + \gamma$, $f(0) = \gamma$, $f(1) = \alpha + \beta + \gamma$, therefore:

$$\Rightarrow \alpha = \frac{f(1) + f(-1)}{2} - f(0), \quad \beta = \frac{f(1) - f(-1)}{2}, \quad \gamma = f(0) \tag{13}$$

so insert Eqn. (13) into Eq. (12)

$$\int_{-1}^{1} (\alpha x^2 + \beta x + \gamma) dx = \frac{2\alpha}{3} + 2\gamma = \frac{f(-1)}{3} + \frac{4f(0)}{3} + \frac{f(1)}{3} \tag{14}$$

Simpson's rule III

- or more general: use two neighboring intervals to evaluate $f(x)$ at three points for the parabola fit

$$\int_{x_i-h}^{x_i+h} f(x)dx = \int_{x_i-h}^{x_i} f(x)dx + \int_{x_i}^{x_i+h} f(x)dx \tag{15}$$

$$\simeq \frac{h}{3}f_{i-1} + \frac{4h}{3}f_i + \frac{h}{3}f_{i+1} \tag{16}$$

$\rightarrow$ pairs of intervals (hence: odd N)

- so for total integration region $[a, b]$

$$\int_a^b f(x)dx \approx \frac{h}{3}f_1 + \frac{4h}{3}f_2 + \frac{2h}{3}f_3 + \frac{4h}{3}f_4 + \ldots \frac{2h}{3}f_{N-2} + \frac{4h}{3}f_{N-1} + \frac{h}{3}f_N \tag{17}$$

with $w_i = \left\{\frac{h}{3}, \frac{4h}{3}, \frac{2h}{3}, \frac{4h}{3}, \ldots, \frac{4h}{3}, \frac{h}{3}\right\}$ $\rightarrow$ check: $\sum_{i=1}^{N} w_i \stackrel{!}{=} (N-1)h$

Integration error I

$\rightarrow$ numerical integration : use algorithm with least number of integration points for accurate answer
estimate error from Taylor expansion at midpoint of interval, e.g., for trapezoid rule $hf^{(2)}\frac{h^2}{12}$, $\times$ number of subintervals $N = [b-a]/h$:

$$E_\mathrm{trap} = \mathcal{O}\left(\frac{[b-a]^3}{12\,N^2}\right) f^{(2)}, \qquad E_\mathrm{Simps} = \mathcal{O}\left(\frac{[b-a]^5}{180\,N^4}\right) f^{(4)} \tag{18}$$

$$\epsilon_\mathrm{trap,\,Simps} \simeq \frac{E_\mathrm{trap,\,Simps}}{f} \tag{19}$$

Note that for Simpson's rule 3rd derivate cancels and $E \propto 1/N^4$
$\rightarrow$ Simpson's rule should converge faster

check: find N for minimum total error (usually for $\epsilon_{\text{ro}} \approx \epsilon_{\text{appr}}$):

$$\epsilon_{\text{tot}} = \epsilon_{\text{ro}} + \epsilon_{\text{approx}} \approx \sqrt{N}\epsilon_{\text{m}} + \epsilon_{\text{trap, Simps}} \tag{20}$$

$$\rightarrow \epsilon_{\text{ro}} \overset{!}{=} \epsilon_{\text{trap, Simps}} = \frac{E_{\text{trap, Simps}}}{f} \tag{21}$$

Assuming some scale:

$$\frac{f^{(n)}}{f} \approx 1 \qquad b - a = 1 \qquad \Rightarrow \quad h = \frac{1}{N} \tag{22}$$

Integration error III

For double precision ($\epsilon_\mathrm{m} \approx 10^{-15}$) and **trapezoid rule:**

$$\sqrt{N}\epsilon_\mathrm{m} \approx \frac{f^{(2)}(b-a)^3}{fN^2} = \frac{1}{N^2} \tag{23}$$

$$\Rightarrow N \approx \frac{1}{(\epsilon_\mathrm{m})^{2/5}} = \left(\frac{1}{10^{-15}}\right)^{2/5} = 10^6 \tag{24}$$

$$\Rightarrow \epsilon_\mathrm{ro} \approx \sqrt{N}\epsilon_\mathrm{m} = 10^{-12} \tag{25}$$

For double precision ($\epsilon_\mathrm{m} \approx 10^{-15}$) and **Simpson's rule:**

$$\sqrt{N}\epsilon_\mathrm{m} \approx \frac{f^{(4)}(b-a)^5}{fN^4} = \frac{1}{N^4} \tag{26}$$

$$\Rightarrow N \approx \frac{1}{(\epsilon_\mathrm{m})^{2/9}} = \left(\frac{1}{10^{-15}}\right)^{2/9} = 2154 \tag{27}$$

$$\Rightarrow \epsilon_\mathrm{ro} \approx \sqrt{N}\epsilon_\mathrm{m} = 5 \times 10^{-14} \tag{28}$$

Integration error IV

We conclude:

- Simpson's rule is better
- Simpson's rule gives errors close to ϵ_{m} (in general for higher order integration algorithms, e.g., RK4)
- best numerical approximation not for $N \to \infty$, but small $N \leq 1000$
- however, as $\epsilon_{\mathrm{Simps}} \sim f^{(4)} \to$ only for sufficiently smooth functions, i.e., for narrow peak-like functions trapezoidal rule might be more efficient

So far: improvement by smart choice of weights w_i, but still equally spaced points x_i (= const. h) for integral evaluation (cf. Eq. (4)),
now: additional freedom of choosing x_i so that *order is twice* that of previous integration formulae (so-called Newton-Cotes formulae, see → interpolation) for *same number of nodes N*
→ compute $N \times f(x_i)$.
→ choose w_i and x_i such that integral is *exact* for
orthogonal polynomials × specific weight function $W(x)$

$$\int_a^b g(x)dx = \int_a^b W(x)f(x)dx \approx \int_a^b W(x)p_n(x)dx = \sum_{i=1}^{N} f(x_i)\, w_i \tag{29}$$

Note that the integration of the orthogonal polynomials is on $[-1;+1]$, hence a transformation of the variables is usually necessary, e.g., for $W(x) \equiv 1$:

$$\int_a^b f(x)dx \approx \frac{b-a}{2} \sum_{i=1}^{N} f\left(\frac{b-a}{2}x_i + \frac{a+b}{2}\right) w_i \tag{30}$$

Example: Gauß-Chebyshev quadrature

The weight function is $W(x) = \frac{1}{\sqrt{1-x^2}}$, i.e, with $f(x) = g(x)\sqrt{1-x^2}$

$$\int_{-1}^{+1} g(x)dx = \int_{-1}^{+1} \frac{f(x)}{\sqrt{1-x^2}}dx \approx \int_a^b \frac{T_n(x)}{\sqrt{1-x^2}}dx = \sum_{i=1}^{N} w_i f(x_i) = \sum_{i=1}^{N} w_i g(x_i)\sqrt{1-x_i^2} \tag{31}$$

with analytic(!) $w_i = \frac{\pi}{N}$, and $x_i = \cos\left(\frac{2i-1}{2N}\pi\right)$ are the zeros of the associated Chebyshev polynomials of 1st kind $T_n(x)$, with $T_{n+1}(x) = 2xT_n(x) - T_{n-1}$, $T_0(x) = 1$, $T_1(x) = x$ and

$$\int_{-1}^{+1} T_n(x)\, w(x)\, T_m(x)dx = \delta_{nm} \tag{32}$$

And for the Chebyshev polynomials of 2nd kind $U_n(x)$ analogously: $W(x) = \sqrt{1-x^2}$, $w_i = \frac{\pi}{N+1}\sin^2\left(\frac{i}{N+1}\pi\right)$, $x_i = \cos\left(\frac{i}{N+1}\pi\right)$

Gaussian quadrature III

Gauß-Chebyshev quadrature in C++ for some $f(x)$ on $[a;b]$

```
double gaussc (double const &a, double const &b, int const &N) {
   ...
 for ( i = 0 ; i < N ; ++i ) {
   x[i] = cos ( ((2. * (i+1) - 1.) * M_PI ) / (double(N) *2.) )  ;
   w[i] = M_PI / double(N) * (b-a) / 2. ; // transform weights [-1;1]->[a;b]
 }
 sum = 0. ;
 for (i = 0 ; i < N ; ++i) { // transform x in f(x), but not in sqrt()
   sum += f( x[i]*(b-a)/2. + (a+b)/2. ) * w[i] * sqrt(1.-x[i]*x[i]) ;
 }
 return sum  ;
}
```

$\rightarrow$ note that this is maybe not optimum for some function $f(x)$, but should be rather used for functions of the form $f(x)/\sqrt{1-x^2}$

Gaussian quadrature IV

Most often: $W(x) \equiv 1 \rightarrow$ Gauß-Legendre quadrature with Legendre Polynomials $P_n(x)$, which are the solutions to Legendre's differential equation (a special case of the Sturm-Liouville differential equation) $\rightarrow$ Laplace equation in 3D for spherical coordinates $\rightarrow$ QM

$$\frac{d}{dx}\left[(1-x^2)\frac{dP_n(x)}{dx}\right] + n(n+1)P_n(x) = 0 \tag{33}$$

$$\rightarrow \; P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}\left(x^2-1\right)^n \qquad \text{(Rodrigues' formula)} \tag{34}$$

so, $P_0(x) = 1$, $P_1(x) = x$, $P_2(x) = \frac{1}{2}(3x^2-1)$, ...
Then, the n weights (for the n points of the interval)

$$w_i = \frac{2}{(1-x_i^2)[P_n'(x_i)]^2} \tag{35}$$

where x_i are the n zeros of $P_n(x)$

Table: Exact values for Gauß-Legendre integration for $n = 2, 3$

n	P_n	P'_n	x_i	w_i
2	$\frac{1}{2}(3x^2 - 1)$	$3x$	$\pm\frac{1}{\sqrt{3}}$	$1, 1$
3	$\frac{1}{2}(5x^3 - 3x)$	$\frac{1}{2}(15x^2 - 3)$	$0, \pm\sqrt{\frac{3}{5}}$	$\frac{8}{9}, \frac{5}{9}, \frac{5}{9}$

Alternatively, the n zeros of $P_n(x)$ can be computed, e.g., via Newton's method ($x_{k+1} = x_k - P(x_k)/P'(x_k)$), one may use the start approximation ($i = 1, \ldots, n$):

$$x_i \approx \cos\left(\frac{4i - 1}{4n + 2}\pi\right) \tag{36}$$

Then the values of $P_n(x)$ and $P'_n(x)$ for Newton's method can be obtained via recursion:

$$nP_n(x) = (2n-1)xP_{n-1}(x) - (n-1)P_{n-2}(x) \tag{37}$$

$$\rightarrow\ P_n(x) = [(2n-1)xP_{n-1}(x) - (n-1)P_{n-2}(x)]/n \tag{38}$$

$$(x^2 - 1)P'_n(x) = nxP_n(x) - nP_{n-1}(x) \tag{39}$$

$$\rightarrow\ P'_n(x) = (nxP_n(x) - nP_{n-1}(x))/(x^2 - 1) \tag{40}$$

Gaussian quadrature VI

Finally, the transformation from $t \in [-1; +1] \to x \in [a; b]$ can be done via the midpoint $\frac{a+b}{2}$

$$x_i = t_i \frac{b-a}{2} + \frac{a+b}{2} \tag{41}$$

$$w_{i,x} = w_{i,t} \frac{b-a}{2} \tag{42}$$

Alternatively, other mappings are possible, allowing for integration of improper integrals with the Gauß-Legendre quadrature

interval	midpoint	$x_i(t_i)$	$w_{i,x}$
$[0;\infty]$	a	$a\dfrac{1+t_i}{1-t_i}$	$\dfrac{2a}{(1-t_i)^2}w_{i,t}$
$[-\infty;+\infty]$	scale a	$a\dfrac{t_i}{1-t_i^2}$	$\dfrac{a(1+t_i^2)}{(1-t_i)^2}w_{i,t}$
$[b;+\infty]$	$a+2b$	$\dfrac{a+2b+at_i}{1-t_i}$	$\dfrac{2(b+a)}{(1-t_i)^2}w_{i,t}$
$[0;b]$	$ab/(b+a)$	$\dfrac{ab(1+t_i)}{b+a-(b-a)t_i}$	$\dfrac{2ab^2}{(b+a-(b-a)t_i)^2}w_{i,t}$

Gaussian quadrature VIII

Moreover, there exist other orthogonal polynomials useful for Gauß quadrature

interval	polynomials	$W(x)$
$[-1;1]$	Legendre	1
$[-1;1]$	Chebyshev 1st kind	$\frac{1}{\sqrt{1-x^2}}$
$[-1;1]$	Chebyshev 2nd kind	$\sqrt{1-x^2}$
$(-1;1)$	Jacobi	$(1-t)^\alpha(1+x)^\beta, \quad \alpha,\beta > -1$
$[0;+\infty)$	Laguerre	e^{-x}
$[0;+\infty)$	Generalized Laguerre	$x^\alpha e^{-x}, \quad \alpha > -1$
$(-\infty;+\infty)$	Hermite	e^{-x^2}

Gaussian quadrature IX

In general, the Gauß quadrature is constructed from orthogonal polynomials $p_n(x)$ with

$$\int_a^b p_n(x)\, W(x)\, p_{n'}(x) dx = \langle p_n | p_{n'} \rangle = \mathcal{N}_n\, \delta_{nn'} \tag{43}$$

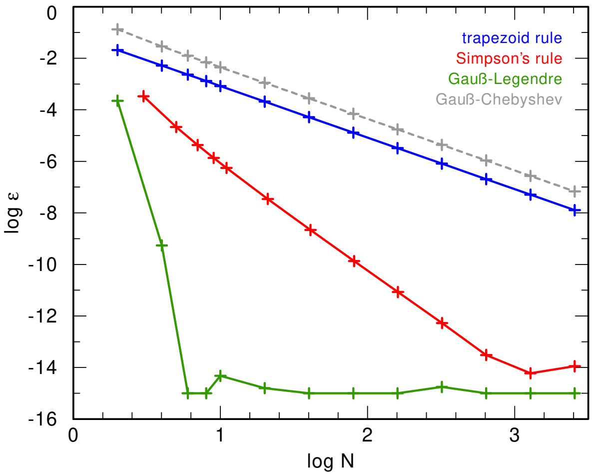
where $\mathcal{N}_n$ is a normalization constant. If we choose the roots x_i of $p_n(x) = 0$ and

$$w_i = \frac{-a_n \mathcal{N}_n}{p_n'(x_i)\, p_{n+1}(x_i)} \tag{44}$$

with $i = 1, \ldots, n$, then the error in the quadrature is

$$\int_a^b g(x) dx - \sum_{i=1}^{n} f(x_i) w_i = \frac{\mathcal{N}_n}{A_n^2 (2n)!}\, f^{(2n)}(x_0) \tag{45}$$

where x_0 is some value in $[a, b]$, A_n a coefficient of the x^n term in the polynomial $p_n(x)$, $a_n = A_{n+1}/A_n$, e.g, for the Legendre polynomials $a_n = (2n+1)/(n+1)$ and $\mathcal{N}_n = 2/(2n+1)$.



Numerical integration of $\exp(-x)$ on $[0, 1]$ with different methods and number of integration points. Note that for Simpson's rule N must be odd.

Gauß-Legendre quadrature with $W(x) \equiv 1$ is superior to simple methods with fixed integration step width. Gauß-Chebyshev is not optimal, as $W(x) = \frac{1}{\sqrt{1-x^2}}$

Romberg integration I

Ideally: choose required accuracy $\epsilon \rightarrow$ know n for Gaussian quadrature (e.g, from Eq. (45)). Unfortunately, usually impossible. Therefore: increase n until ϵ small enough, recalculate all $f(x_i)$ for new degree $n \rightarrow$ disadvantage of Gaussian quadrature

Idea: trapezoid rule with subsequent calls with increasing n to refine until precision ϵ reached:

```
void trap (double const &a, double const &b, double &s, int const &n)
  ...
if (n == 1) s = 0.5 * (b-a) * (f(a)+f(b)) ;
else {
 it = pow(2,(n-2)) ;
 delx = (b-a) / double(it) ;
 x = a + 0.5 * delx ;
 sum = 0. ;
 for (int j=1 ; j <= it ; ++j) {
  sum += f(x) ; x += delx ; }
 s = 0.5 * (s + (b-a) * sum / double(it)) ;
}
```

Romberg integration II

For the trapezoid rule the approximation error (starting with $\frac{1}{n^2}$ has only even powers of $\frac{1}{n}$):

$$\int_{x_1}^{x_n} f(x)dx = h\left[\frac{1}{2}f_1 + f_2 \ldots f_{n-1} + \frac{1}{2}f_n\right] \tag{46}$$

$$- \frac{B_2 h^2}{2!}(f_n' - f_1') - \ldots - \frac{B_{2k} h^{2k}}{(2k)!}(f_n^{(2k-1)} - f_1^{(2k-1)}) - \ldots \tag{47}$$

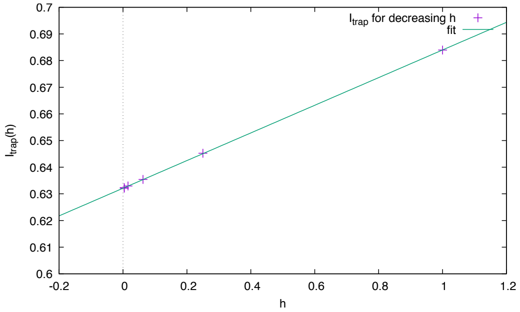
If compute Eq. (47) (without the error terms) for n and get s_n and once more with $2n$ and get s_{2n}, then leading error term in 2nd call is 1/4 of error in 1st call, hence

$$s = \frac{4}{3}s_{2n} - \frac{1}{3}s_n \tag{48}$$

cancels leading error term, $1/n^4$ remains → recovers Simpson's rule

Romberg integration III

Often better: trapezoid rule for different N (or $h = \frac{b-a}{N}$) + extrapolation for $h \rightarrow 0$ (cf. Richardson extrapolation) $\rightarrow$ Romberg integration



1. calculate $I(h_k)$ for series h_k
2. extrapolate $(h_k^2, I(h_k))$ with polynomial in h^2

e.g., $\int_0^1 e^{-x} dx$

Note that polynomial $(a + bh^2)$ in h^2 is plotted, although h is used for the trapezoid rule $\rightarrow$ extrapolate polynomial in h^2

$\rightarrow$ trapezoid rule ideal: expansion in even powers of h (each refinement $\rightarrow$ 2 orders accuracy) and $I(h) = h(\frac{1}{2}f(a) + \sum_{j=1}^{N-1} f(x_j) + \frac{1}{2}f(b)) \rightarrow$ recycle already calculated nodes for $h/2$

Numerical differentiation I

Sometimes numerical derivative needed, e.g., for minimization algorithms, Newton method for root finding, so

$$f' = \frac{df(x)}{dx} := \lim_{h \to 0} \frac{f(x+h) - f(x)}{h} \tag{49}$$

Problem: for $h \to 0 \to f(x+h) \approx f(x)$
$\to$ subtractive cancelation for numerator
& machine precision limit for denominator

often better (e.g., for large noise): analytic approximation of function (see, e.g., $\to$ interpolation) and its derivative

Forward difference

Taylor series with step size h

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{6} f^{(3)}(x) + \ldots \tag{50}$$

$\rightarrow$ forward difference by solving Eq. (50) for f'

$$f'_{\text{fd}}(x) := \frac{f(x+h) - f(x)}{h} \simeq f'(x) + \frac{h}{2} f''(x) + \ldots \tag{51}$$

approximate function by straight line through two points, error $\sim h$, e.g, consider $f(x) = a + bx^2$

$$f'_{\text{fd}}(x) \approx \frac{f(x+h) - f(x)}{h} = 2bx + bh \quad \text{vs. exact } f' = 2bx \tag{52}$$

$\rightarrow$ only good for small $h \ll 2x$

Central difference

modify Eq. (49) by stepping forward $h/2$ and backward $h/2$

$$f'_{\mathrm{cd}} := \frac{f(x+\frac{h}{2}) - f(x-\frac{h}{2})}{h} \tag{53}$$

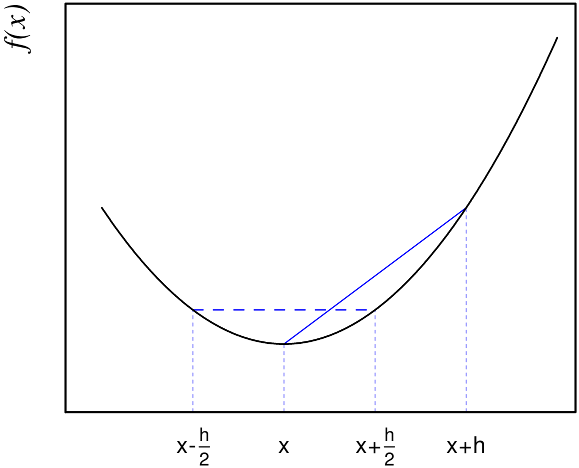
So, if we insert Taylor series for $f(x + \pm\frac{h}{2})$ in to Eq. (53)

$$f'_{\mathrm{cd}} := \frac{\left[f(x) + \frac{h}{2}f'(x) + \frac{h^2}{8}f''(x) + \right] - [\ldots]}{h} \simeq f'(x) + \frac{1}{24}h^2 f^{(3)}(x) + \ldots \tag{54}$$

$\rightarrow$ all terms with odd power of h cancel $\rightarrow$ accuracy is of order h^2
if function well behaved, i.e., $f^{(3)}h^2/24 \ll f^{(2)}h/2 \rightarrow$ error for central difference method $\ll$ forward difference method, e.g., for $f(x) = a + bx^2$

$$f'_{\mathrm{cd}}(x) \approx \frac{f(x+\frac{h}{2}) - f(x-\frac{h}{2})}{h} = 2bx \quad \text{vs. exact } f' = 2bx \tag{55}$$

Numerical differentiation IV



Forward difference (solid line) and central difference (dashed)
$\rightarrow$ central difference more accurate

Extrapolated difference

try to make also h^2 vanish by *algebraic exatrapolation*

$$f'_{\mathrm{ed}}(x) \simeq \lim_{h \to 0} f'_{\mathrm{cd}} \tag{56}$$

$\rightarrow$ need additional information for extrapolation by central difference with step size $h/2$:

$$f'_{\mathrm{cd}}(x, h/2) = \frac{f(x + h/4) - f(x - h/4)}{h/2} \approx f'(x) + \frac{h^2 f^{(3)}(x)}{96} + \ldots \tag{57}$$

We elminate linear and quadratic error term by forming

$$f'_{\mathrm{ed}}(x) := \frac{4\frac{f(x+h/4)-f(x-h/4)}{h/2} - \frac{f(x+h/2)-f(x-h/2)}{h}}{3} \tag{58}$$

$$\approx f'(x) - \frac{h^4 f^{(5)}(x)}{4 \cdot 16 \cdot 120} + \ldots \tag{59}$$

Numerical differentiation VI

for $h = 0.4$ and $f^{(5)} \simeq 1 \rightarrow$ approximation error close to ϵ_m. To minimize subtractive cancelation write Eq. (58) as

$$f'_\mathrm{ed}(x) = \frac{1}{3h}\left(8\left[f\left(x+\frac{h}{4}\right) - f\left(x-\frac{h}{4}\right)\right] - \left[f\left(x+\frac{h}{2}\right) - f\left(x-\frac{h}{2}\right)\right]\right) \tag{60}$$

Error analysis

→ usually decreasing h reduces approximation error but increases roundoff error (e.g., more calculation steps needed), moreover: subtractive cancelation. Hence, difference

$$f' \approx \frac{f(x+h) - f(x)}{h} \approx \frac{\epsilon_{\mathrm{m}}}{h} \approx \epsilon_{\mathrm{ro}} \tag{61}$$

and

$$\epsilon_{\mathrm{approx}}^{\mathrm{fd}} \approx \frac{f^{(2)} h}{2}, \qquad \epsilon_{\mathrm{approx}}^{\mathrm{cd}} \approx \frac{f^{(3)} h^2}{24} \tag{62}$$

Therefore $\epsilon_{\mathrm{ro}} \approx \epsilon_{\mathrm{approx}}$ for

$$\frac{\epsilon_m}{h} \approx \epsilon^{fd}_{approx} = \frac{f^{(2)}h}{2}, \qquad \frac{\epsilon_m}{h} \approx \epsilon^{cd}_{approx} = \frac{f^{(3)}h}{24} \tag{63}$$

$$\Rightarrow h^2_{fd} = \frac{2\epsilon_m}{f^{(2)}} \qquad \Rightarrow h^3_{cd} = \frac{24\epsilon_m}{f^{(3)}} \tag{64}$$

for $f' \approx f^{(2)} \approx f^{(3)} \simeq 1$ (e.g., $\exp(x)$, $\cos(x)$) and double precision ($\epsilon_m \approx 10^{-15}$):

$$h_{fd} \approx 4 \times 10^{-8} \qquad \& \qquad h_{cd} \approx 3 \times 10^{-5} \tag{65}$$

$$\Rightarrow \epsilon_{fd} \simeq \frac{\epsilon_m}{h_{cd}} \simeq 3 \times 10^{-8}, \qquad \Rightarrow \epsilon_{cd} \simeq \frac{\epsilon_m}{h_{cd}} \simeq 3 \times 10^{-11} \tag{66}$$

$\rightarrow$ can choose 1000× larger h for *central difference* $\rightarrow$ error is 1000× smaller for *central difference*

Second derivative

starting from first derivative with *central difference* method

$$f'(x) \simeq \frac{f(x+h/2) - f(x-h/2)}{h} \tag{67}$$

the 2nd derivative $f^{(2)}(x)$ is central difference from 1st derivative

$$f^{(2)}(x) \simeq \frac{f'(x+h/2) - f'(x-h/2)}{h}, \tag{68}$$

$$\simeq \frac{[f(x+h) - f(x)] - [f(x) - f(x-h)]}{h^2} \tag{69}$$

$$\simeq \frac{f(x+h) + f(x-h) - 2f(x)}{h^2} \tag{70}$$

$\rightarrow$ Eq. (69) better in terms of subtractive cancelation

Literature I

Landau, R. H., Páez, M. J., & Bordeianu, C. C., eds. 2007, Computational Physics (Wiley-VCH)