# 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 $d N(t) / d t$, the rate of some events, e.g., photons per unit time interval. Task:

Determine the number of photons in the first second:

$$
\begin{equation*}
N(1)=\int_{0}^{1} \frac{d N(t)}{d t} d t \tag{1}
\end{equation*}
$$

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

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

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

$$
\begin{equation*}
\int_{a}^{b} f(x) d x=\lim _{h \rightarrow 0}\left[h \sum_{i=1}^{(b-a) / h} f\left(x_{i}\right)\right] \tag{3}
\end{equation*}
$$

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

$$
\begin{equation*}
\int_{a}^{b} f(x) d x \approx \sum_{i=1}^{N} f\left(x_{i}\right) w_{i} \tag{4}
\end{equation*}
$$

$\rightarrow$ problem: find appropriate sampling $f_{i} \equiv f\left(x_{i}\right)$, generally: result improves with $N$
some hints

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

$$
\begin{equation*}
\int_{-1}^{1} f(|x|) d x=\int_{-1}^{0} f(-x) d x+\int_{0}^{1} f(x) d x \tag{5}
\end{equation*}
$$

- or transformation/substitution

$$
\begin{equation*}
\int_{0}^{1} x^{1 / 3} d x=\int_{y(0)=0^{1 / 3}}^{y(1)=1^{1 / 3}} y 3 y^{2} d y \quad\left(y(x)=x^{1 / 3} \rightarrow d x=3 x^{2 / 3} d y=3 y^{2} d y\right) \tag{6}
\end{equation*}
$$

## 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 $h$ :

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

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

with average height $\left(f_{i}+f_{i+1}\right) / 2$ :

$$
\begin{equation*}
\int_{x_{i}}^{x_{i}+h} f(x) d x \simeq \frac{h\left(f_{i}+f_{i+1}\right)}{2}=\frac{1}{2} h f_{i}+\frac{1}{2} h f_{i+1} \tag{8}
\end{equation*}
$$

i.e. Eq. (4): $\int_{a}^{b} f(x) d x \approx \sum_{i=1}^{N} f\left(x_{i}\right) w_{i}$ for $N=2$ and $w_{i}=\frac{1}{2} h$

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

$$
\begin{equation*}
\int_{a}^{b} f(x) d x \approx \frac{h}{2} f_{1}+h f_{2}+h f_{3}+\ldots+h f_{N-1}+\frac{h}{2} f_{N} \tag{9}
\end{equation*}
$$

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

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

hence area for each interval:

$$
\begin{equation*}
\int_{x_{i}}^{x_{i}+h}\left(\alpha x^{2}+\beta x+\gamma\right) d x \tag{11}
\end{equation*}
$$

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


- need to determine $\alpha, \beta, \gamma$ for $f(x)$, so consider interval $[-1,1]$

$$
\begin{equation*}
\int_{-1}^{1}\left(\alpha x^{2}+\beta x+\gamma\right) d x=\frac{1}{3} \alpha x^{3}+\frac{1}{2} \beta x^{2}+\left.\gamma x\right|_{-1} ^{+1}=\frac{2 \alpha}{3}+2 \gamma \tag{12}
\end{equation*}
$$

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

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

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

$$
\begin{equation*}
\int_{-1}^{1}\left(\alpha x^{2}+\beta x+\gamma\right) d x=\frac{f(-1)}{3}+\frac{4 f(0)}{3}+\frac{f(1)}{3} \tag{14}
\end{equation*}
$$

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

$$
\begin{align*}
\int_{x_{i}-h}^{x_{i}+h} f(x) d x & =\int_{x_{i}-h}^{x_{i}} f(x) d x+\int_{x_{i}}^{x_{i}+h} f(x) d x  \tag{15}\\
& \simeq \frac{h}{3} f_{i-1}+\frac{4 h}{3} f_{i}+\frac{h}{3} f_{i+1} \tag{16}
\end{align*}
$$

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

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

$$
\begin{equation*}
\int_{a}^{b} f(x) d x \approx \frac{h}{3} f_{1}+\frac{4 h}{3} f_{2}+\frac{2 h}{3} f_{3}+\frac{4 h}{3} f_{4}+\ldots \frac{2 h}{3} f_{N-2}+\frac{4 h}{3} f_{N-1}+\frac{h}{3} f_{N} \tag{17}
\end{equation*}
$$

with $w_{i}=\left\{\frac{h}{3}, \frac{4 h}{3}, \frac{2 h}{3}, \frac{4 h}{3}, \ldots, \frac{4 h}{3}, \frac{h}{3}\right\} \rightarrow$ check: $\sum_{i=1}^{N} w_{i} \stackrel{!}{=}(N-1) h$
$\rightarrow$ 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 $h f^{(2)} \frac{h^{2}}{12}, \times$ number of subintervals $N=[b-a] / h$ :

$$
\begin{align*}
E_{\text {trap }} & =\mathcal{O}\left(\frac{[b-a]^{3}}{12 N^{2}}\right) f^{(2)}, \quad E_{\text {Simps }}=\mathcal{O}\left(\frac{[b-a]^{5}}{180 N^{4}}\right) f^{(4)}  \tag{18}\\
\epsilon_{\text {trap, Simps }} & \simeq \frac{E_{\text {trap, Simps }}}{f} \tag{19}
\end{align*}
$$

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 $\epsilon_{\mathrm{ro}} \approx \epsilon_{\text {appr }}$ ):

$$
\begin{align*}
& \epsilon_{\mathrm{tot}}=\epsilon_{\mathrm{ro}}+\epsilon_{\text {approx }} \approx \sqrt{N} \epsilon_{\mathrm{m}}+\epsilon_{\text {trap, Simps }}  \tag{20}\\
& \rightarrow \epsilon_{\mathrm{ro}} \stackrel{!}{=} \epsilon_{\text {trap, Simps }}=\frac{E_{\text {trap, Simps }}}{f} \tag{21}
\end{align*}
$$

Assuming some scale:

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

## Integration error III

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

$$
\begin{align*}
& \sqrt{N} \epsilon_{\mathrm{m}} \approx \frac{f^{(2)}(b-a)^{3}}{f N^{2}}=\frac{1}{N^{2}}  \tag{23}\\
& \Rightarrow N \approx \frac{1}{\left(\epsilon_{\mathrm{m}}\right)^{2 / 5}}=\left(\frac{1}{10^{-15}}\right)^{2 / 5}=10^{6}  \tag{24}\\
& \Rightarrow \epsilon_{\mathrm{ro}} \approx \sqrt{N} \epsilon_{\mathrm{m}}=10^{-12} \tag{25}
\end{align*}
$$

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

$$
\begin{align*}
\sqrt{N} \epsilon_{\mathrm{m}} & \approx \frac{f^{(4)}(b-a)^{5}}{f N^{4}}=\frac{1}{N^{4}}  \tag{26}\\
\Rightarrow N & \approx \frac{1}{\left(\epsilon_{\mathrm{m}}\right)^{2 / 9}}=\left(\frac{1}{10^{-15}}\right)^{2 / 9}=2154  \tag{27}\\
\Rightarrow \epsilon_{\mathrm{ro}} & \approx \sqrt{N} \epsilon_{\mathrm{m}}=5 \times 10^{-14} \tag{28}
\end{align*}
$$

We conclude:

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

So far: improvment 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 $\rightarrow$ interpolation) for same number of nodes $N$ $\rightarrow$ compute $N \times f\left(x_{i}\right)$.
$\rightarrow$ choose $w_{i}$ and $x_{i}$ such that integral is exact for
orthogonal polynomials $\times$ specific weight function $W(x)$

$$
\begin{equation*}
\int_{a}^{b} g(x) d x=\int_{a}^{b} W(x) f(x) d x \approx \int_{a}^{b} W(x) p_{n}(x) d x=\sum_{i=1}^{N} f\left(x_{i}\right) w_{i} \tag{29}
\end{equation*}
$$

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

$$
\begin{equation*}
\int_{a}^{b} f(x) d x \approx \frac{b-a}{2} \sum_{i=1}^{N} f\left(\frac{b-a}{2} x_{i}+\frac{a+b}{2}\right) w_{i} \tag{30}
\end{equation*}
$$

## Gaussian quadrature II

## Example: Chebyshev-Gauß quadrature

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

$$
\begin{equation*}
\int_{-1}^{+1} g(x) d x=\int_{-1}^{+1} \frac{f(x)}{\sqrt{1-x^{2}}} d x \approx \int_{a}^{b} \frac{T_{n}(x)}{\sqrt{1-x^{2}}} d x=\sum_{i=1}^{N} w_{i} f\left(x_{i}\right)=\sum_{i=1}^{N} w_{i} g\left(x_{i}\right) \sqrt{1-x_{i}^{2}} \tag{31}
\end{equation*}
$$

with analytic(!) $w_{i}=\frac{\pi}{N}$, and $x_{i}=\cos \left(\frac{2 i-1}{2 N} \pi\right)$ are the zeros of the associated Chebyshev polynomials of 1 st kind $T_{n}(x)$, with $T_{n+1}(x)=2 x T_{n}(x)-T_{n-1}, T_{0}(x)=1, T_{1}(x)=x$ and

$$
\begin{equation*}
\int_{-1}^{+1} T_{n}(x) w(x) T_{m}(x) d x=\delta_{n m} \tag{32}
\end{equation*}
$$

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

```
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 $f(x) / \sqrt{1-x^{2}}$

Most often: $W(x) \equiv 1 \rightarrow$ Legendre-Gauß 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

$$
\begin{array}{r}
\frac{d}{d x}\left[\left(1-x^{2}\right) \frac{d P_{n}(x)}{d x}\right]+n(n+1) P_{n}(x)=0 \\
\rightarrow P_{n}(x)=\frac{1}{2^{n} n!} \frac{d^{n}}{d x^{n}}\left(x^{2}-1\right)^{n} \quad \text { (Rodrigues' formula ) } \tag{34}
\end{array}
$$

so, $P_{0}(x)=1, P_{1}(x)=x, P_{2}(x)=\frac{1}{2}\left(3 x^{2}-1\right), \ldots$
Then, the $n$ weights (for the $n$ points of the interval)

$$
\begin{equation*}
w_{i}=\frac{2}{\left(1-x_{i}^{2}\right)\left[P_{n}^{\prime}\left(x_{i}\right)\right]^{2}} \tag{35}
\end{equation*}
$$

where $x_{i}$ are the $n$ zeros of $P_{n}(x)$

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

| $n$ | $P_{n}$ | $P_{n}^{\prime}$ | $x_{i}$ | $w_{i}$ |
| :---: | :---: | :---: | :---: | :---: |
| 2 | $\frac{1}{2}\left(3 x^{2}-1\right)$ | $3 x$ | $\pm \frac{1}{\sqrt{3}}$ | 1,1 |
| 3 | $\frac{1}{2}\left(5 x^{3}-3 x\right)$ | $\frac{1}{2}\left(15 x^{2}-3\right)$ | $0, \pm \sqrt{\frac{3}{5}}$ | $\frac{8}{9}, \frac{5}{9}, \frac{5}{9}$ |

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

$$
\begin{equation*}
x_{i} \approx \cos \left(\frac{4 i-1}{4 n+2} \pi\right) \tag{36}
\end{equation*}
$$

Then the values of $P_{n}(x)$ and $P_{n}^{\prime}(x)$ for Newton's method can be obtained via recursion:

$$
\begin{align*}
n P_{n}(x) & =(2 n-1) x P_{n-1}(x)-(n-1) P_{n-2}(x)  \tag{37}\\
\rightarrow P_{n}(x) & =\left[(2 n-1) x P_{n-1}(x)-(n-1) P_{n-2}(x)\right] / n  \tag{38}\\
\left(x^{2}-1\right) P_{n}^{\prime}(x) & =n x P_{n}(x)-n P_{n-1}(x)  \tag{39}\\
\rightarrow P_{n}^{\prime}(x) & =\left(n x P_{n}(x)-n P_{n-1}(x)\right) /\left(x^{2}-1\right) \tag{40}
\end{align*}
$$

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

$$
\begin{align*}
x_{i} & =t_{i} \frac{b-a}{2}+\frac{a+b}{2}  \tag{41}\\
w_{i, x} & =w_{i, t} \frac{b-a}{2} \tag{42}
\end{align*}
$$

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

| interval | midpoint | $x_{i}\left(t_{i}\right)$ | $w_{i, x}$ |
| :--- | :--- | :--- | :--- |
| $[0 ; \infty]$ | $a$ | $a \frac{1+t_{i}}{1-t_{i}}$ | $\frac{2 a}{\left(1-t_{i}\right)^{2}} w_{i, t}$ |
| $[-\infty ;+\infty]$ | scale a | $a \frac{t_{i}}{1-t_{i}^{2}}$ | $\frac{a\left(1+t_{i}^{2}\right)}{\left(1-t_{i}\right)^{2}} w_{i, t}$ |
| $[b ;+\infty]$ | $a+2 b$ | $\frac{a+2 b+a t_{i}}{1-t_{i}}$ | $\frac{2(b+a)}{\left(1-t_{i}\right)^{2}} w_{i, t}$ |
| $[0 ; b]$ | $a b /(b+a)$ | $\frac{a b\left(1+t_{i}\right)}{b+a-(b-a) t_{i}}$ | $\frac{2 a b^{2}}{\left(b+a-(b-a) t_{i}\right)^{2}} w_{i, t}$ |

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 | $e^{-x^{2}}$ |

In general, the Gauß quadrature is constructed from orthogonal polynomials $p_{n}(x)$ with

$$
\begin{equation*}
\int_{a}^{b} p_{n}(x) W(x) p_{n^{\prime}}(x) d x=\left\langle p_{n} \mid p_{n^{\prime}}\right\rangle=\mathcal{N}_{n} \delta_{n n^{\prime}} \tag{43}
\end{equation*}
$$

where $\mathcal{N}_{n}$ is a normalization constant. If we choose the roots $x_{i}$ of $p_{n}(x)=0$ and

$$
\begin{equation*}
w_{i}=\frac{-a_{n} \mathcal{N}_{n}}{p_{n}^{\prime}\left(x_{i}\right) p_{n+1}\left(x_{i}\right)} \tag{44}
\end{equation*}
$$

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

$$
\begin{equation*}
\int_{a}^{b} g(x) d x-\sum_{i=1}^{n} f\left(x_{i}\right) w_{i}=\frac{\mathcal{N}_{n}}{A_{n}^{2}(2 n)!} f^{(2 n)}\left(x_{0}\right) \tag{45}
\end{equation*}
$$

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 $a_{n}=(2 n+1) /(n+1)$ and $\mathcal{N}_{n}=2 /(2 n+1)$.


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.

Gaussian-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 $\epsilon$ small enough, recalculate all $f\left(x_{i}\right)$ for new degree $n \rightarrow$ disadvantage of Gaussian quadrature

Idea: trapezoid rule with subsequent calls with increasing $n$ to refine until precision $\epsilon$ reached:

```
    ...
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)) ;
}
```

void trap (double const \&a, double const \&b, double \&s, int const \&n)

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

$$
\begin{align*}
\int_{x_{1}}^{x_{n}} f(x) d x & =h\left[\frac{1}{2} f_{1}+f_{2} \ldots f_{n-1}+\frac{1}{2} f_{n}\right]  \tag{46}\\
& -\frac{B_{2} h^{2}}{2!}\left(f_{n}^{\prime}-f_{1}^{\prime}\right)-\ldots-\frac{B_{2 k} h^{2 k}}{(2 k)!}\left(f_{n}^{(2 k-1)}-f_{1}^{(2 k-1)}\right)-\ldots \tag{47}
\end{align*}
$$

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

$$
\begin{equation*}
s=\frac{4}{3} s_{2 n}-\frac{1}{3} s_{n} \tag{48}
\end{equation*}
$$

cancels leading error term, $1 / n^{4}$ remains $\rightarrow$ 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 $I\left(h_{k}\right)$ for series $h_{k}$
(2) extrapolate $\left(h_{k}^{2}, I\left(h_{k}\right)\right)$ with polynomial in $h^{2}$
e.g., $\int_{0}^{1} e^{-x} d x$

Note that polynomial $\left(a+b h^{2}\right)$ 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 $I(h)=h\left(\frac{1}{2} f(a)+\sum_{j=1}^{N-1} f\left(x_{j}\right)+\frac{1}{2} f(b)\right) \rightarrow$ recycle already calculated nodes for $h / 2$

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

$$
\begin{equation*}
f^{\prime}=\frac{d f(x)}{d x}:=\lim _{h \rightarrow 0} \frac{f(x+h)-f(x)}{h} \tag{49}
\end{equation*}
$$

Problem: for $h \rightarrow 0 \rightarrow f(x+h) \approx f(x)$
$\rightarrow$ subtractive cancelation for numerator
\& machine precision limit for denominator often better (e.g., for large noise): analytic approximation of function (see, e.g., $\rightarrow$ interpolation) and its derivative

## Numerical differentiation II

## Forward difference

Taylor series with step size $h$

$$
\begin{equation*}
f(x+h)=f(x)+h f^{\prime}(x)+\frac{h^{2}}{2} f^{\prime \prime}(x)+\frac{h^{3}}{6} f^{(3)}(x)+\ldots \tag{50}
\end{equation*}
$$

$\rightarrow$ forward difference by solving Eq. (50) for $f^{\prime}$

$$
\begin{equation*}
f_{\mathrm{fd}}^{\prime}(x):=\frac{f(x+h)-f(x)}{h} \simeq f^{\prime}(x)+\frac{h}{2} f^{\prime \prime}(x)+\ldots \tag{51}
\end{equation*}
$$

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

$$
\begin{equation*}
f_{\mathrm{fd}}^{\prime}(x) \approx \frac{f(x+h)-f(x)}{h}=2 b x+b h \quad \text { vs. exact } f^{\prime}=2 b x \tag{52}
\end{equation*}
$$

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

## Numerical differentiation III

## Central difference

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

$$
\begin{equation*}
f_{c d}^{\prime}:=\frac{f\left(x+\frac{h}{2}\right)-f\left(x-\frac{h}{2}\right)}{h} \tag{53}
\end{equation*}
$$

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

$$
\begin{equation*}
f_{\mathrm{cd}}^{\prime} \simeq f^{\prime}(x)+\frac{1}{24} h^{2} f^{(3)}(x)+\ldots \tag{54}
\end{equation*}
$$

$\rightarrow$ 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 $f(x)=a+b x^{2}$

$$
\begin{equation*}
f_{\mathrm{cd}}^{\prime}(x) \approx \frac{f\left(x+\frac{h}{2}\right)-f\left(x-\frac{h}{2}\right)}{h}=2 b x \quad \text { vs. exact } f^{\prime}=2 b x \tag{55}
\end{equation*}
$$



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

$$
\begin{equation*}
f_{\mathrm{ed}}^{\prime}(x) \simeq \lim _{h \rightarrow 0} f_{\mathrm{cd}}^{\prime} \tag{56}
\end{equation*}
$$

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

$$
\begin{equation*}
f_{\mathrm{cd}}^{\prime}(x, h / 2)=\frac{f(x+h / 4)-f(x-h / 4)}{h / 2} \approx f^{\prime}(x)+\frac{h^{2} f^{(3)}(x)}{96}+\ldots \tag{57}
\end{equation*}
$$

We elminate linear and quadratic error term by forming

$$
\begin{align*}
f_{\mathrm{ed}}^{\prime}(x) & :=\frac{4 \frac{f(x+h / 4)-f(x-h / 4)}{h / 2}-\frac{f(x+h / 2)-f(x-h / 2)}{h}}{3}  \tag{58}\\
& \approx f^{\prime}(x)-\frac{h^{4} f(5)(x)}{4 \cdot 16 \cdot 120}+\ldots \tag{59}
\end{align*}
$$

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

$$
\begin{equation*}
f_{\mathrm{ed}}^{\prime}(x)=\frac{1}{3 h}\left(8\left[f\left(x+\frac{h}{4}\right)-f\left(x-\frac{h}{4}\right)\right]-\left[f\left(x+\frac{h}{2}\right)-f\left(x-\frac{h}{2}\right)\right]\right) \tag{60}
\end{equation*}
$$

## Numerical differentiation VII

## Error analysis

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

$$
\begin{equation*}
f^{\prime} \approx \frac{f(x+h)-f(x)}{h} \approx \frac{\epsilon_{\mathrm{m}}}{h} \approx \epsilon_{\mathrm{ro}} \tag{61}
\end{equation*}
$$

and

$$
\begin{equation*}
\epsilon_{\mathrm{approx}}^{\mathrm{fd}} \approx \frac{f^{(2)} h}{2}, \quad \epsilon_{\mathrm{approx}}^{\mathrm{cd}} \approx \frac{f^{(3)} h^{2}}{24} \tag{62}
\end{equation*}
$$

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

$$
\begin{gather*}
\frac{\epsilon_{\mathrm{m}}}{h} \approx \epsilon_{\mathrm{approx}}^{\mathrm{fd}}=\frac{f^{(2)} h}{2}, \quad \frac{\epsilon_{\mathrm{m}}}{h} \approx \epsilon_{\mathrm{approx}}^{\mathrm{cd}}=\frac{f^{(3)} h}{24}  \tag{63}\\
\Rightarrow h_{\mathrm{fd}}^{2}=\frac{2 \epsilon_{\mathrm{m}}}{f^{(2)}} \quad \Rightarrow h_{\mathrm{cd}}^{3}=\frac{24 \epsilon_{\mathrm{m}}}{f^{(3)}} \tag{64}
\end{gather*}
$$

for $f^{\prime} \approx f^{(2)} \approx f^{(3)} \simeq 1$ (e.g., $\left.\exp (x), \cos (x)\right)$ and double precision $\left(\epsilon_{\mathrm{m}} \approx 10^{-15}\right)$ :

$$
\begin{array}{cc}
h_{\mathrm{fd}} \approx 4 \times 10^{-8} \quad \& \quad h_{\mathrm{cd}} \approx 3 \times 10^{-5} \\
\Rightarrow \epsilon_{\mathrm{fd}} \simeq \frac{\epsilon_{\mathrm{m}}}{h_{\mathrm{cd}}} \simeq 3 \times 10^{-8}, \quad \Rightarrow \epsilon_{\mathrm{cd}} \simeq \frac{\epsilon_{\mathrm{m}}}{h_{\mathrm{cd}}} \simeq 3 \times 10^{-11} \tag{66}
\end{array}
$$

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

## Numerical differentiation IX

## Second derivative

starting from first derivative with central difference method

$$
\begin{equation*}
f^{\prime}(x) \simeq \frac{f(x+h / 2)-f(x-h / 2)}{h} \tag{67}
\end{equation*}
$$

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

$$
\begin{align*}
f^{(2)}(x) & \simeq \frac{f^{\prime}(x+h / 2)-f^{\prime}(x-h / 2)}{h}  \tag{68}\\
& \simeq \frac{[f(x+h)-f(x)]-[f(x)-f(x-h)]}{h^{2}}  \tag{69}\\
& \simeq \frac{f(x+h)+f(x-h)-2 f(x)}{h^{2}} \tag{70}
\end{align*}
$$

$\rightarrow$ 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)

