# NUR A lecture 4

In this lecture:

Discretization
(Extended) trapezoid rule
(Extended) Simpson's rule
Higher orders
Open (extended) formulas/midpoint
Romberg integration and errors
Richardson extrapolation
Handling improper integrals
Integrating in log vs linear space
Basics of Gaussian quadrature
Multidimensional integration

# Numerical Recipes for Astrophysics A

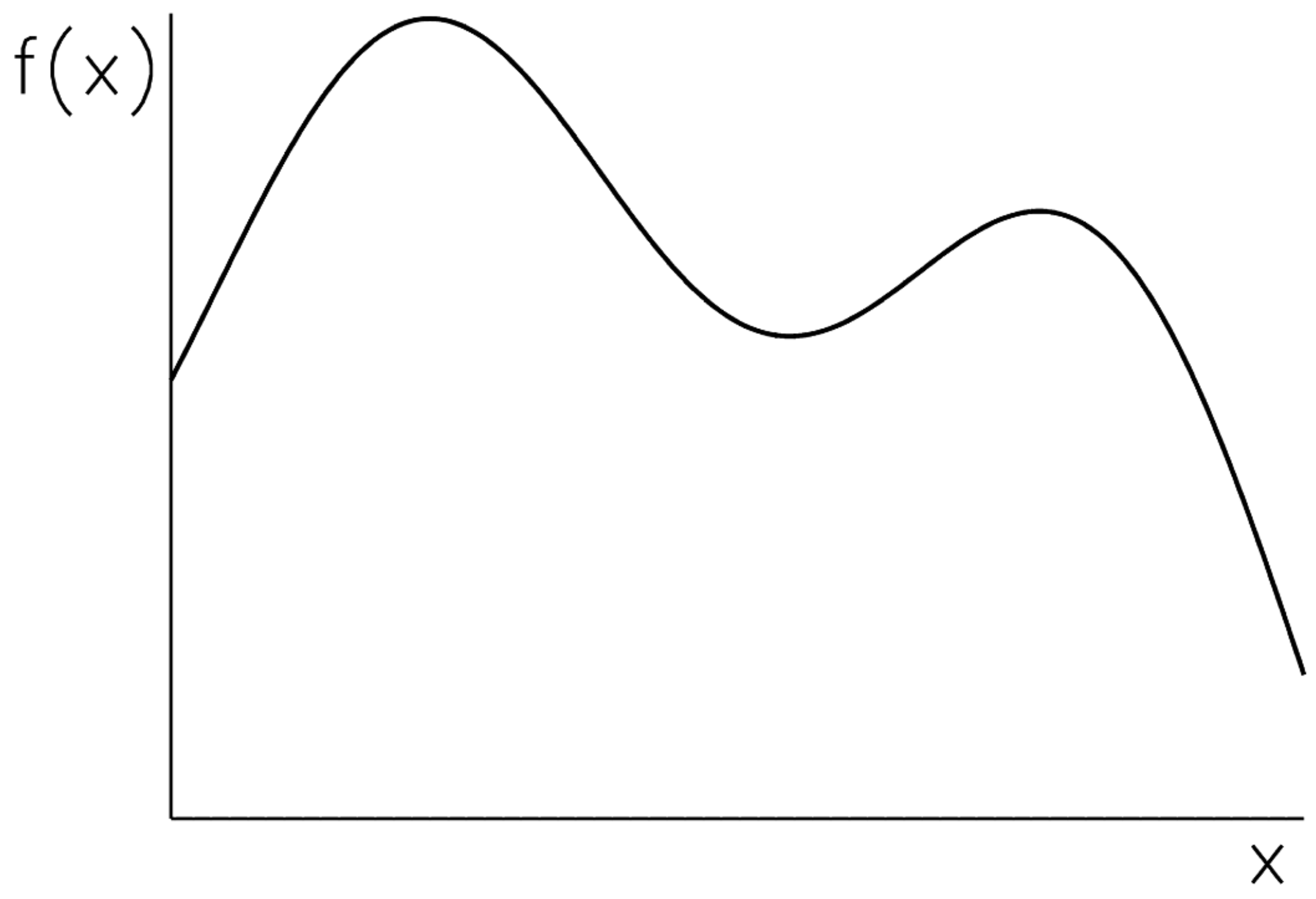
Lecture 4

# Questions about last week?

# Integrating functions

**NR Ch 4**

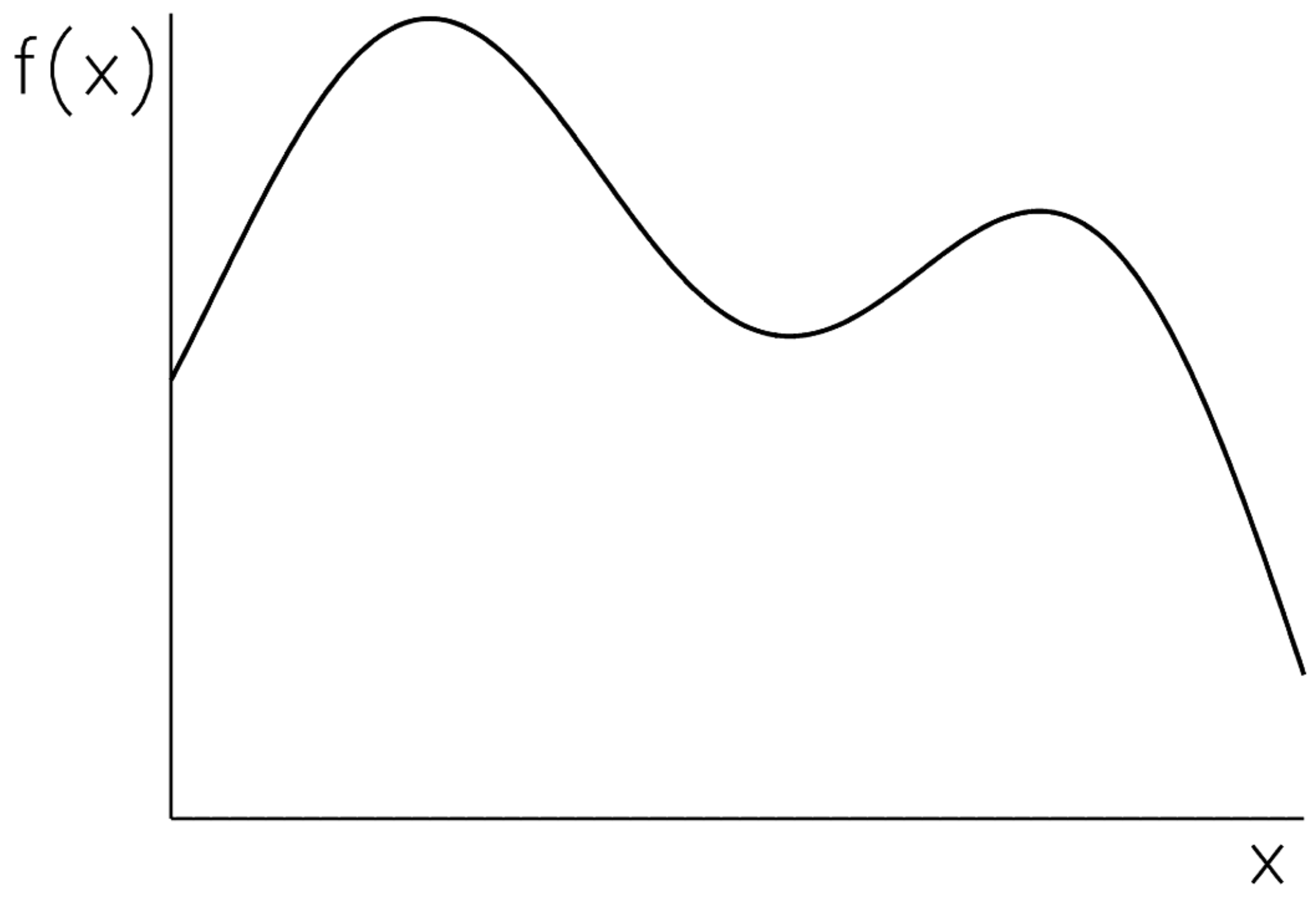
# Integrating functions




- Discretize and evaluate

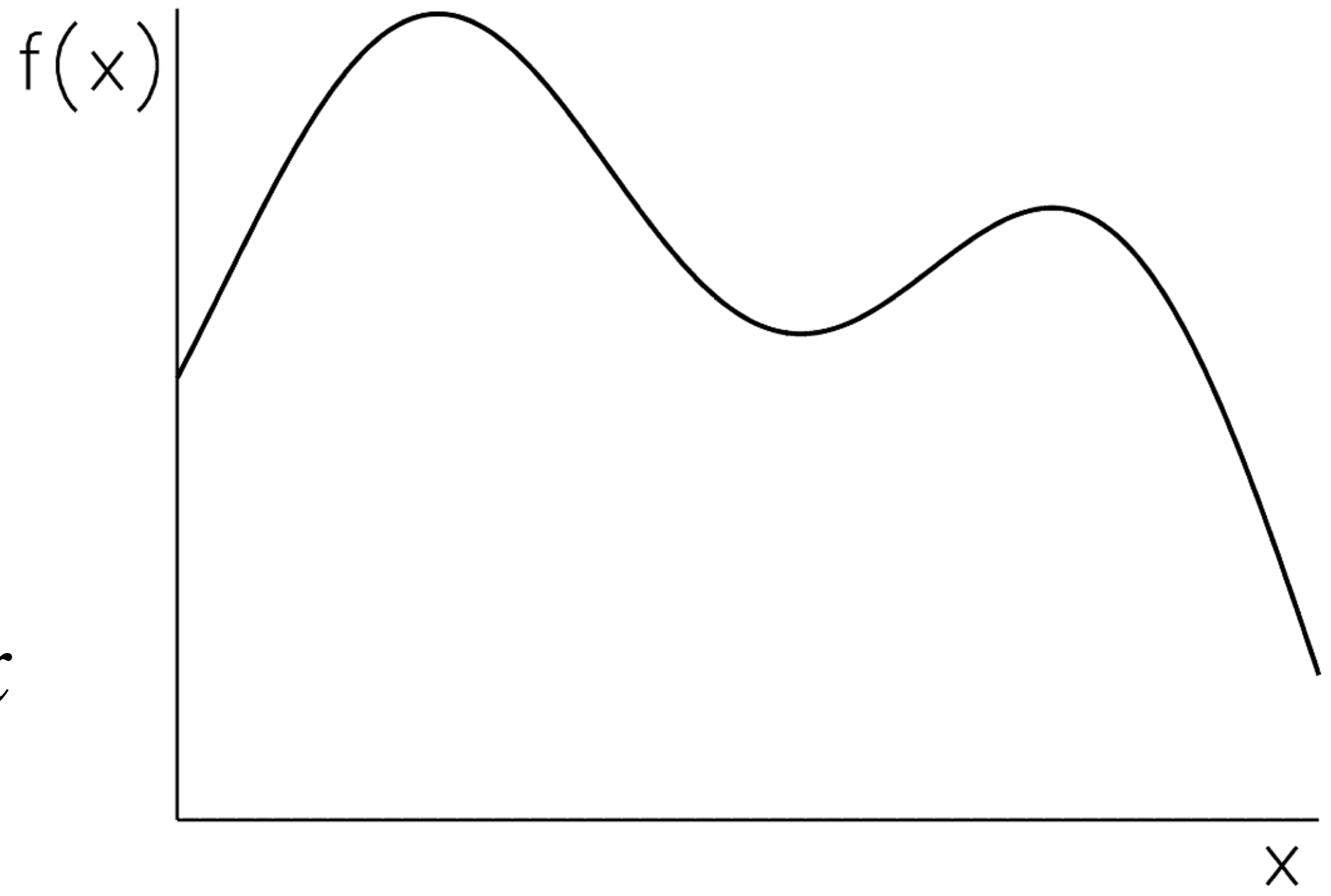
- Undefined $f(x)$/divergence

# Equally spaced abscissae




- Trapezoid rule and extension

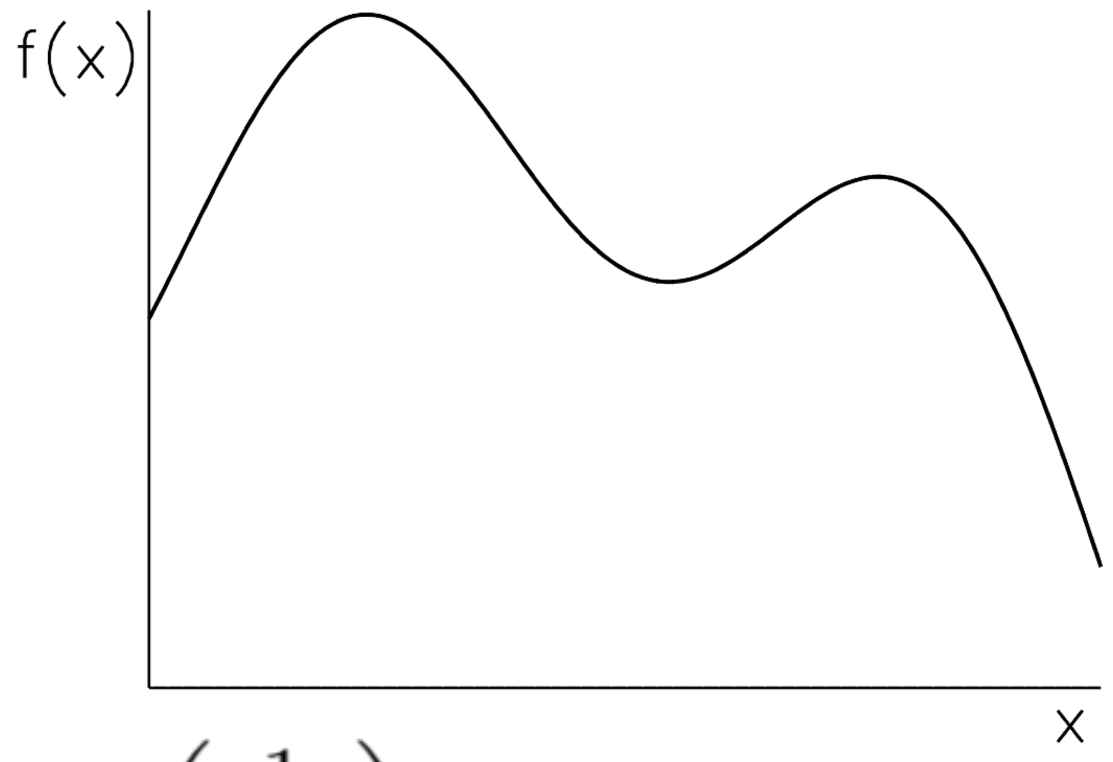
# Equally spaced abscissae




- Higher order: Simpson's rule

$$g(x) = ax^2 + bx + c \;\; \Rightarrow \;\; G(x) = \frac{1}{3}ax^3 + \frac{1}{2}bx^2 + cx$$

# Equally spaced abscissae




- Extended Simpson's rule

$$\int_{x_0}^{x_\mathrm{N}} f(x)\,\mathrm{d}x = \frac{h}{3}\left(f_0 + 4f_1 + 2f_2 + 4f_3 + \cdots + 2f_{\mathrm{N}-2} + 4f_{\mathrm{N}-1} + f_\mathrm{N}\right) + \mathcal{O}\left(\frac{1}{N^4}\right)$$

- Higher order still

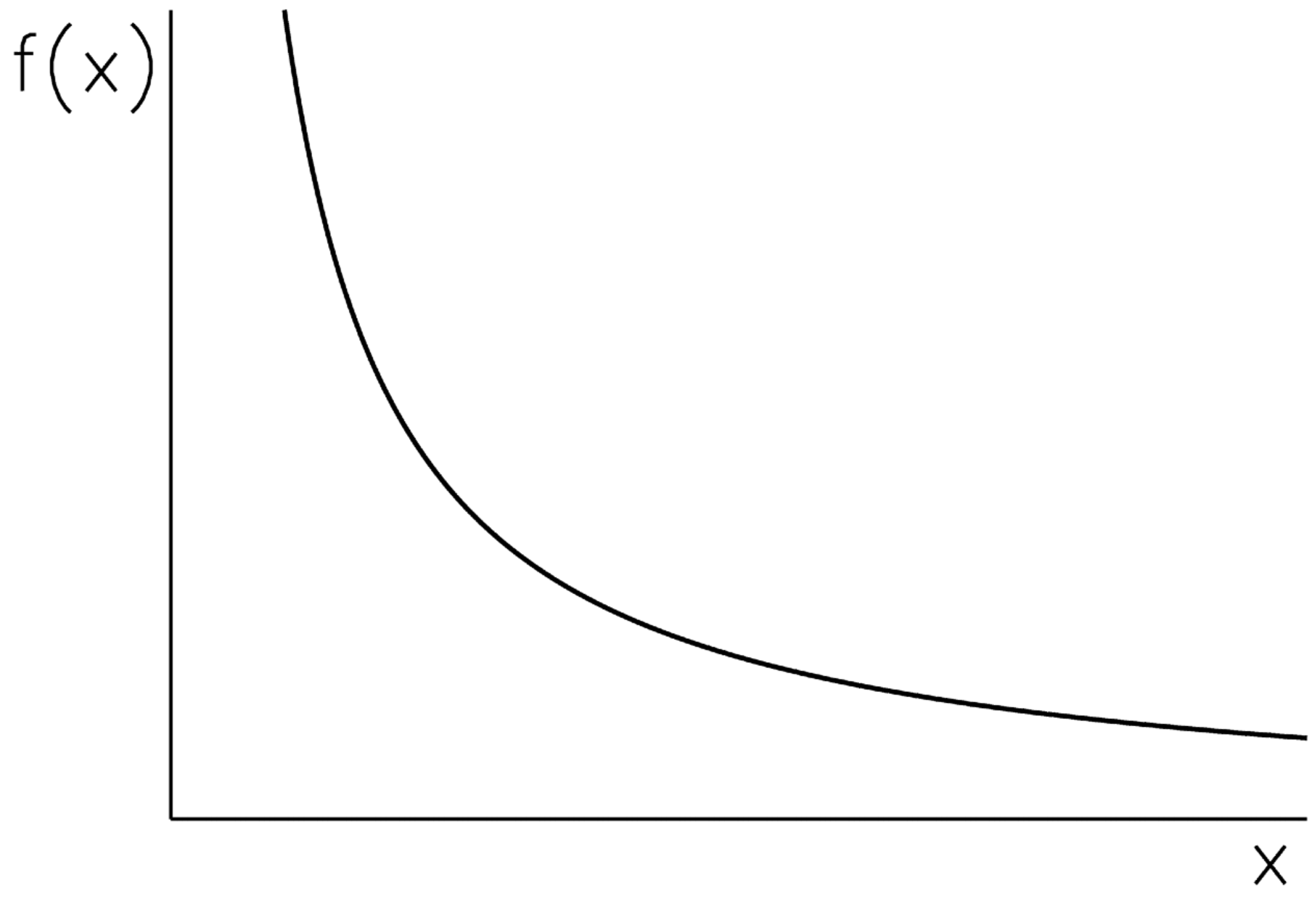
Simpson's $\frac{3}{8}$ rule:

$$\int_{x_0}^{x_3} f(x)\,\mathrm{d}x = \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3) + \mathcal{O}(h^5 f^{(4)})$$

Boole's rule:

$$\int_{x_0}^{x_4} f(x)\,\mathrm{d}x = \frac{2h}{45}(7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4) + \mathcal{O}(h^7 f^{(6)})$$

# Open formulas




- Deriving open formulas

- Open extended formulas

- Semi-open

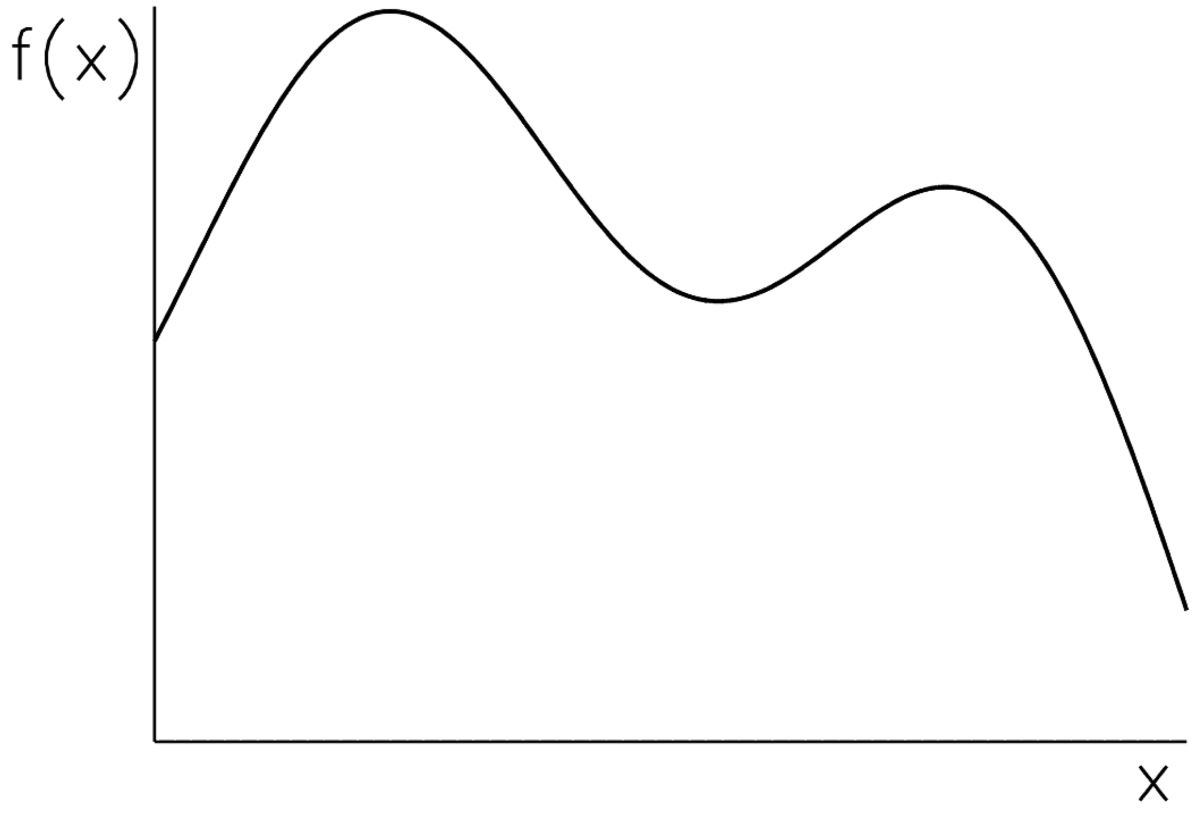
# Open formulas

- Second-order extended (Simpson's)

$$\int_{x_0}^{x_\mathrm{N}} f(x)\,\mathrm{d}x = \frac{h}{3}\left(\frac{27}{4}f_1 + \frac{13}{4}f_3 + 4f_4 + 2f_5 + 4f_6 + \cdots + 2f_{\mathrm{N}-5} + 4f_{\mathrm{N}-4} + \frac{13}{4}f_{\mathrm{N}-3} + \frac{27}{4}f_{\mathrm{N}-1}\right) + \mathcal{O}\left(\frac{1}{N^4}\right)$$

- Extended midpoint rule

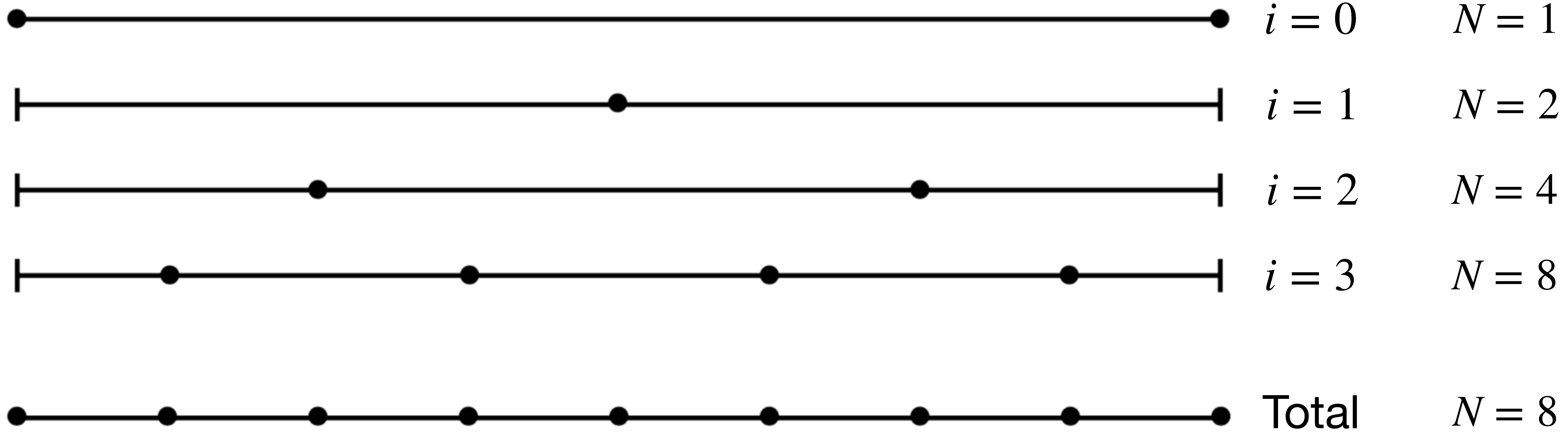
$$\int_{x_0}^{x_\mathrm{N}} f(x)\,\mathrm{d}x = h\left(f_{1/2} + f_{3/2} + f_{5/2} + \cdots + f_{\mathrm{N}-3/2} + f_{\mathrm{N}-1/2}\right) + \mathcal{O}\left(\frac{1}{N^2}\right)$$



# Romberg integration

- Combining trapezoids

# Romberg integration




$$S_{i+1} = \frac{1}{2}S_i + \frac{b-a}{N_{i+1}}\sum_j f_j = \frac{1}{2}\left(S_i + \Delta_{i+1}\sum_j f_j\right)$$

# Analogue to Neville's algorithm

$N+1$ evals: $h: \quad \mathcal{O}\left(\frac{1}{N^2}\right)$

$$\frac{1}{4}\mathcal{O}\left(\frac{1}{N^4}\right)$$

$2N+1$ evals: $h/2: \quad \frac{1}{4}\mathcal{O}\left(\frac{1}{N^2}\right) \qquad \frac{1}{64}\mathcal{O}\left(\frac{1}{N^6}\right)$

$$\frac{1}{64}\mathcal{O}\left(\frac{1}{N^4}\right) \qquad \frac{1}{4096}\mathcal{O}\left(\frac{1}{N^8}\right)$$

$4N+1$ evals: $h/4: \quad \frac{1}{16}\mathcal{O}\left(\frac{1}{N^2}\right) \qquad \frac{1}{4096}\mathcal{O}\left(\frac{1}{N^6}\right)$

$$\frac{1}{1024}\mathcal{O}\left(\frac{1}{N^4}\right)$$

$8N+1$ evals: $h/8: \quad \frac{1}{64}\mathcal{O}\left(\frac{1}{N^2}\right)$

# Analogue to Neville's algorithm

$$
\begin{array}{lllll}
h: & \mathcal{O}\left(\frac{1}{N^2}\right) & & & \\
 & & \frac{1}{4}\mathcal{O}\left(\frac{1}{N^4}\right) & & \\
h/2: & \frac{1}{4}\mathcal{O}\left(\frac{1}{N^2}\right) & & \frac{1}{64}\mathcal{O}\left(\frac{1}{N^6}\right) & \\
 & & \frac{1}{64}\mathcal{O}\left(\frac{1}{N^4}\right) & & \frac{1}{4096}\mathcal{O}\left(\frac{1}{N^8}\right) \\
h/4: & \frac{1}{16}\mathcal{O}\left(\frac{1}{N^2}\right) & & \frac{1}{4096}\mathcal{O}\left(\frac{1}{N^6}\right) & \\
 & & \frac{1}{1024}\mathcal{O}\left(\frac{1}{N^4}\right) & & \\
h/8: & \frac{1}{64}\mathcal{O}\left(\frac{1}{N^2}\right) & & &
\end{array}
$$

$$\boxed{S_{i,j} = \frac{4^j S_{i+1,j-1} - S_{i,j-1}}{4^j - 1}}$$

# Romberg integration

1. Decide on an initial step size h and an “order” $m$, for example $h = b - a$ and $m = 5$.
2. Make an array $r$ of size $m$ for your estimates, up to step size $h/2^{m-1}$; set these to $0$.
3. Calculate the initial estimate $r_0$: for $h = b - a$, it’s $r_0 = \frac{1}{2}h[f(a) + f(b)]$.
4. Set $N_\mathrm{p} = 1$, loop over $i$ from $1$ through $m - 1$:
5. Add in new function evaluations: $r_i = 0$, $\Delta = h$, $h = \frac{1}{2}h$, $x = a + h$, then $N_\mathrm{p}$ times do: $r_i = r_i + f(x)$, $x = x + \Delta$.
6. Now combine the new points with the already calculated ones for an estimate for $h/2^i$: $r_i = \frac{1}{2}[r_{i-1} + \Delta r_i]$, then double $N_\mathrm{p}$.
7. Finish the loop over $i$. We now have the initial “column” of estimations.
8. Reset $N_\mathrm{p}$ to $1$, start a new loop over $i$ from $1$ through $m - 1$:
9. Upgrade the previous results by combining them: multiply $N_\mathrm{p}$ by $4$, then for $j$ from $0$ up to $m - i$: $r_j = [N_\mathrm{p} r_{j+1} - r_j]/(N_\mathrm{p} - 1)$.
10. Finish the loops over $j$ and $i$; $r_0$ now contains the best estimate for the integral.

# The magic in practice: error function

$$\mathrm{erf}(1) = \frac{2}{\sqrt{\pi}} \int_0^1 e^{-x^2}\,\mathrm{d}x \approx 0.8427007929$$

$N = 1,\ h = 1:$

$N = 2,\ h = 1/2:$

$N = 4,\ h = 1/4:$

$N = 8,\ h = 1/8:$

$N = 16,\ h = 1/16:$

# The magic in practice: error function

$$\mathrm{erf}(1) = \tfrac{2}{\sqrt{\pi}} \int_0^1 e^{-x^2}\,\mathrm{d}x \approx 0.8427007929$$

$N = 1,\ h = 1:\quad 0.7717433323$

$N = 2,\ h = 1/2:\quad 0.8252629556$

$N = 4,\ h = 1/4:\quad 0.8383677774$

$N = 8,\ h = 1/8:\quad 0.8416192212$

$N = 16,\ h = 1/16:\quad 0.8424305055$

# The magic in practice: error function

$$\mathrm{erf}(1) = \frac{2}{\sqrt{\pi}} \int_0^1 e^{-x^2}\,\mathrm{d}x \approx 0.8427007929$$

$N = 1,\ h = 1:$ $\quad 0.7717433323$

$\qquad\qquad 0.8431028300$

$N = 2,\ h = 1/2:$ $\quad 0.8252629556$

$\qquad\qquad 0.8427360514$

$N = 4,\ h = 1/4:$ $\quad 0.8383677774$

$\qquad\qquad 0.8427030358$

$N = 8,\ h = 1/8:$ $\quad 0.8416192212$

$\qquad\qquad 0.8427009336$

$N = 16,\ h = 1/16:$ $\quad 0.8424305055$

# The magic in practice: error function

$$\mathrm{erf}(1) = \tfrac{2}{\sqrt{\pi}} \int_0^1 e^{-x^2}\,\mathrm{d}x \approx 0.8427007929$$

| | | | | | |
|---|---|---|---|---|---|
| $N=1,\ h=1:$ | $0.7717433323$ | | | | |
| | | $0.8431028300$ | | | |
| $N=2,\ h=1/2:$ | $0.8252629556$ | | $0.8427115995$ | | |
| | | $0.8427360514$ | | $0.8427006639$ | |
| $N=4,\ h=1/4:$ | $0.8383677774$ | | $0.8427008348$ | | $0.8427007933$ |
| | | $0.8427030358$ | | $0.8427007928$ | |
| $N=8,\ h=1/8:$ | $0.8416192212$ | | $0.8427007934$ | | |
| | | $0.8427009336$ | | | |
| $N=16,\ h=1/16:$ | $0.8424305055$ | | | | |

# Extrapolation

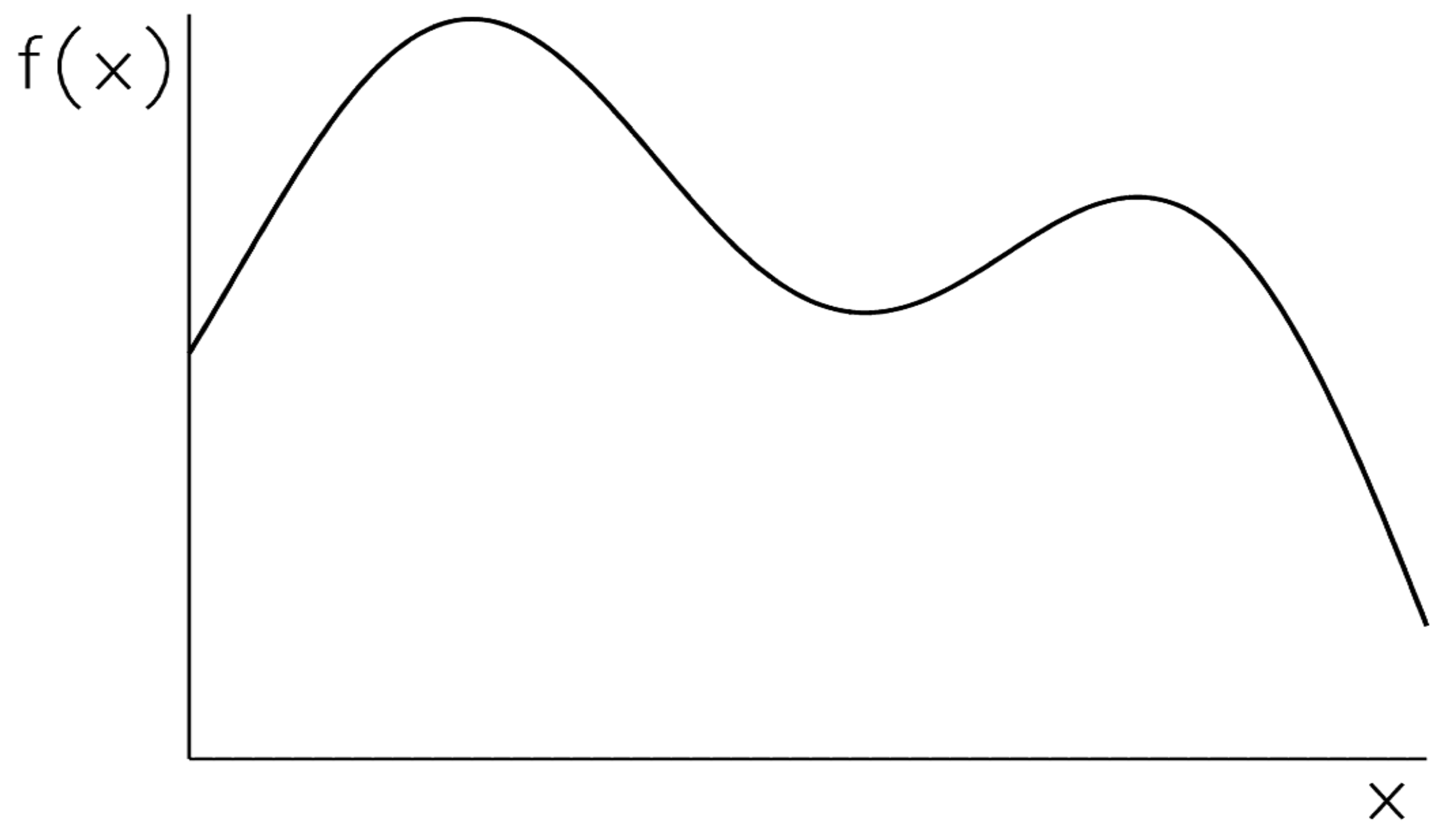
- Explicitly extrapolating to $h = 0$

- Where does this fail?

# Improper integrals

- Improper but not infinite or ill-defined:
  - The integrand is limited and has finite limits but cannot be evaluated at one of the limits (i.e. $\sin x/x$ at $x = 0$).
  - The upper or lower limit is $\pm\infty$.
  - It has an integrable singularity at either limit (e.g. $x^{-1/2}$ at $x = 0$).
  - It has an integrable singularity at some known place between the limits.
  - It has an integrable singularity at some unknown place between the limits.

- Extended midpoint Romberg



# Change of variables

- Limits to infinity

Example: substitute $x = \dfrac{1}{t}$ (when $ab > 0$ and $f(x)$ decreases faster than $x^{-2}$ as $x \to \pm\infty$)

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

- Slow power-law divergence

Example: substitute $x = a + t^{1/(1-\gamma)}$ (when $f(x)$ diverges as $(x-a)^{-\gamma}$ with $0 \le \gamma < 1$)

$$\Rightarrow \quad \int_a^b f(x)\,\mathrm{d}x = \int_0^{(b-a)^{1-\gamma}} t^{\gamma/(1-\gamma)} f\left(a + t^{1/(1-\gamma)}\right)\,\mathrm{d}t$$

- Many implementations exist!

# Breaking up the integral

- Splitting the limits

$$\int_a^b f(x)\,\mathrm{d}x = \int_a^m f(x)\,\mathrm{d}x + \int_m^b f(x)\,\mathrm{d}x$$

$$\left(= \int_a^{m_0} f(x)\,\mathrm{d}x + \int_{m_0}^{m_1} f(x)\,\mathrm{d}x + \cdots + \int_{m_\mathrm{N}}^{b} f(x)\,\mathrm{d}x\right)$$

- Basics of adaptive step sizes

# Linear vs logarithmic

- Range, space and measure

- Appropriate transformations

# Gaussian quadrature

- Additional freedom: unequal spacing

- Convergence

# Gaussian quadrature

- Default rule: Gauss-Legendre
    - Gauss-Chebyshev:
    - Gauss-Laguerre:
    - Gauss-Hermite:
- $w/x$-generation in NumPy

# Multidimensional integration

- Reducing the dimensionality

- Function evaluation = integral

- Pre-calculation and interpolation

# Next week:
# Differentiation and random numbers