Integration, differentiation, and root finding

Phys 750 Lecture 6

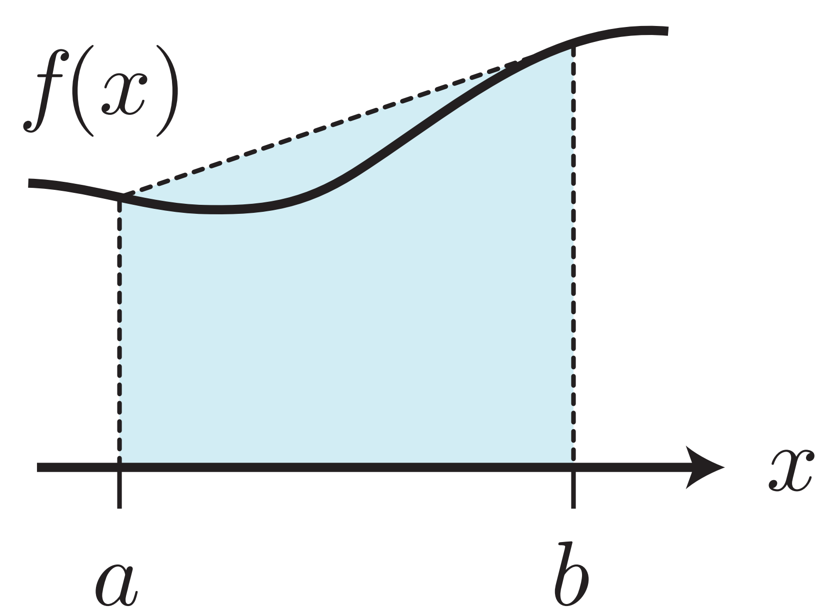
Numerical integration

- Compute an approximation to the definite integral

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

- Find area under the curve $f(x)$ in the interval $[a, b]$
- Trapezoid Rule: simplest geometric approximation

$$I \approx (b - a) \times \frac{1}{2}\big(f(b) + f(a)\big)$$



Numerical integration

- What is the quality of the approximation?
- Construct a power series from the left:

$$f(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f'''(a)}{3!}(x-a)^3 + \cdots$$

$$= f(a) + f'(a)(x-a) + \frac{f''(\xi)}{2!}(x-a)^2$$

exact equality

true for some choice of $\xi \in [a, b]$

Numerical integration

- Integrating term by term (with $H = b - a$) gives

$$I = f(a)H + \frac{f'(a)}{2!}H^2 + \frac{f''(\xi)}{3!}H^3$$

$$I_{\text{trap}} = \frac{f(a)}{2}H + \frac{f(b)}{2}H$$

error: $I - I_{\text{trap}} = O(H^3)$

$$= \frac{f(a)}{2}H + \frac{1}{2}\left(f(a) + f'(a)H + \frac{f''(\xi)}{2!}H^2\right)H$$

$$= f(a)H + \frac{f'(a)}{2}H^2 + \frac{f''(\xi)}{8}H^3$$

Numerical integration

- How to improve the estimate?

1. Find an approximation that matches to higher order: e.g., trapezoid is the best linear fit; Simpson's rule is the best quadratic fit through three points

$$I_{\text{Simp}} = \frac{H}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$$

$$I - I_{\text{Simp}} = O(H^5)$$

2. Make H small by subdividing the interval

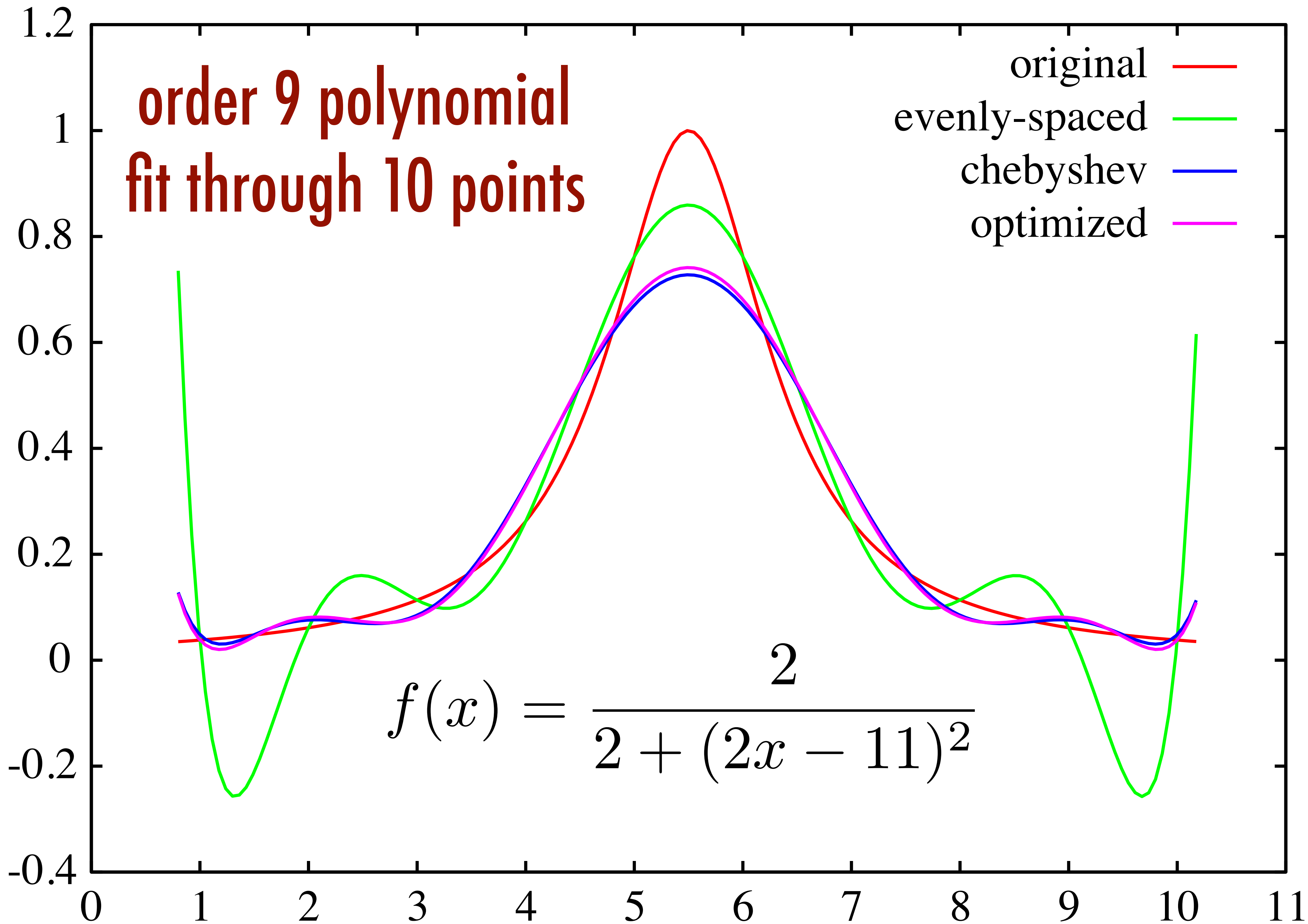
Polynomial fitting

- Newton-Cotes formulas:

$$\frac{H}{2}(f(b) - f(a))$$
$$\frac{H}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$$
$$\frac{H}{8}\left[f(a) + 3f\left(\frac{a+2b}{3}\right) + 3f\left(\frac{2a+b}{3}\right) + f(b)\right]$$
$$\frac{H}{90}\left[7f(a) + 32f\left(\frac{3a+b}{4}\right) + 12f\left(\frac{a+b}{2}\right) + 32f\left(\frac{a+3b}{4}\right) + 7f(b)\right]$$

- Polynomial fitting over a uniformly spaced set of points
- At high order, prone to Runge’s phenomenon

Runge's phenomenon



Interpolation error

- Suppose $n+1$ ordered points $x_0 < x_1 < \cdots < x_n$ evaluate to $f(x_i) = y_i$
- Order-n interpolating polynomial satisfying $P(x_i) = y_i$ is related to the original function by

$$f(x) = P(x) + \frac{f^{(n+1)}(\xi)}{(n+1)!} \prod_{i=0}^{n} (x - x_i)$$

for some $\xi \in [x_0, x_n]$

Interpolation error

- Overall fitting error controlled by

$$\mathcal{E} = \int_{x_0}^{x_n} dx\, \epsilon(x)^2 \qquad \epsilon(x) = \prod_{i=0}^{n} (x - x_i)$$

- Formal minimization $\partial\mathcal{E}/\partial x_i = 0$ gives

$$x_i = \frac{\int_{x_0}^{x_n} dx'\, x' \prod_{j\neq i}(x' - x_j)^2}{\int_{x_0}^{x_n} dx''\, \prod_{k\neq i}(x'' - x_k)^2}$$

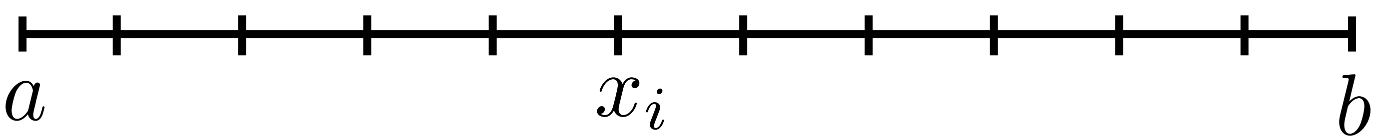
- Chebyshev nodes provide a good approximate solution:

$$x_i = \frac{1}{2}\left[x_0 + x_n - (x_n - x_0)\cos\left(\frac{(i+1/2)\pi}{n+1}\right)\right]$$

Integrating piecewise

- Break the integral into N disjoint intervals covering $[a, b]$

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



$$= \int_a^{x_1} f(x)\,dx + \int_{x_1}^{x_2} f(x)\,dx + \cdots + \int_{x_{N-1}}^{b} f(x)\,dx$$

- Treat the integrals piecewise using, e.g., trapezoid rule

global error: $N \times O\left(\frac{H}{N}\right)^3 = O\left(\frac{1}{N}\right)^2$

- Becomes exact in the limit $N \to \infty$

Romberg integration

- Break the interval $[a, b]$ of width $H = b - a$ into 2^n subintervals of width $h_n = H/2^n$
- By recursive construction, define

$$\mathcal{R}_{0,0} = \frac{H}{2}(f(a) + f(b))$$

$$\mathcal{R}_{n,0} = \frac{1}{2}\mathcal{R}_{n-1,0} + h_n \sum_{j=1}^{2^n-1} f(a + (2k-1)h_n)$$

$$\mathcal{R}_{n,m} = \frac{4^m \mathcal{R}_{n,m-1} - \mathcal{R}_{n-1,m-1}}{4^m - 1}$$

Romberg integration

$$
\begin{array}{cccc}
\mathcal{R}_{0,0} & & & \\
\mathcal{R}_{1,0} & \mathcal{R}_{1,1} & & \\
\mathcal{R}_{2,0} & \mathcal{R}_{2,1} & \mathcal{R}_{2,1} & \\
\mathcal{R}_{3,0} & \mathcal{R}_{3,1} & \mathcal{R}_{3,2} & \mathcal{R}_{3,3} \\
\vdots & & & \ddots
\end{array}
$$

$$\frac{2}{\sqrt{\pi}} \int_0^1 dx\, e^{-x^2}$$

$$\doteq 0.842700792949714 9$$

```
0.77174333
0.82526296  0.84310283
0.83836778  0.84273605  0.84271160
0.84161922  0.84270304  0.84270083  0.84270066
0.84243051  0.84270093  0.84270079  0.84270079  0.84270079
```

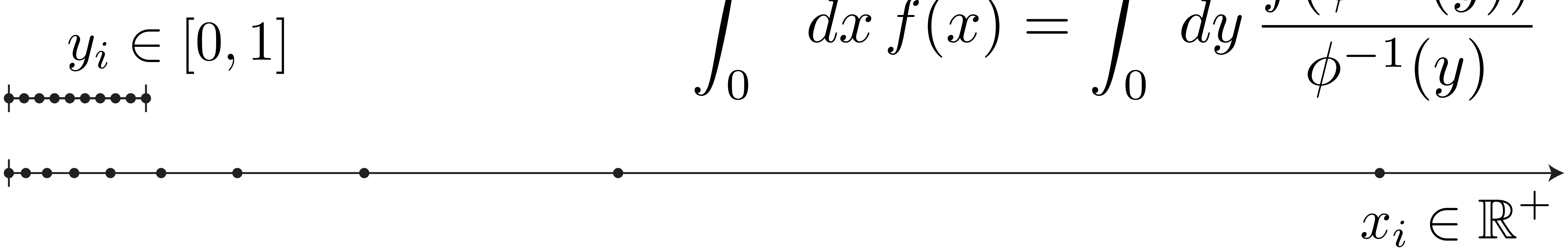
Troublesome cases

- There are additional complications if
  - the region of integration is infinite or semi-infinite
  - the integrand is otherwise badly behaved: e.g.,
    1. it diverges
    2. has discontinuities
    3. oscillates infinitely often in some finite region

Semi-infinite integral

- Choose a monotonic increasing function $\phi : [0, \infty] \to [0, 1]$
- 1-1 map between $\mathbb{R}^+$ and the unit interval
- E.g., $y = \phi(x) = \dfrac{x}{1+x}, \quad x = \phi^{-1}(y) = \dfrac{y}{1-y}$
- Conventional integration in transformed coordinates:

$$\int_0^\infty dx\, f(x) = \int_0^1 dy\, \frac{f(\phi^{-1}(y))}{\phi^{-1}(y)}$$

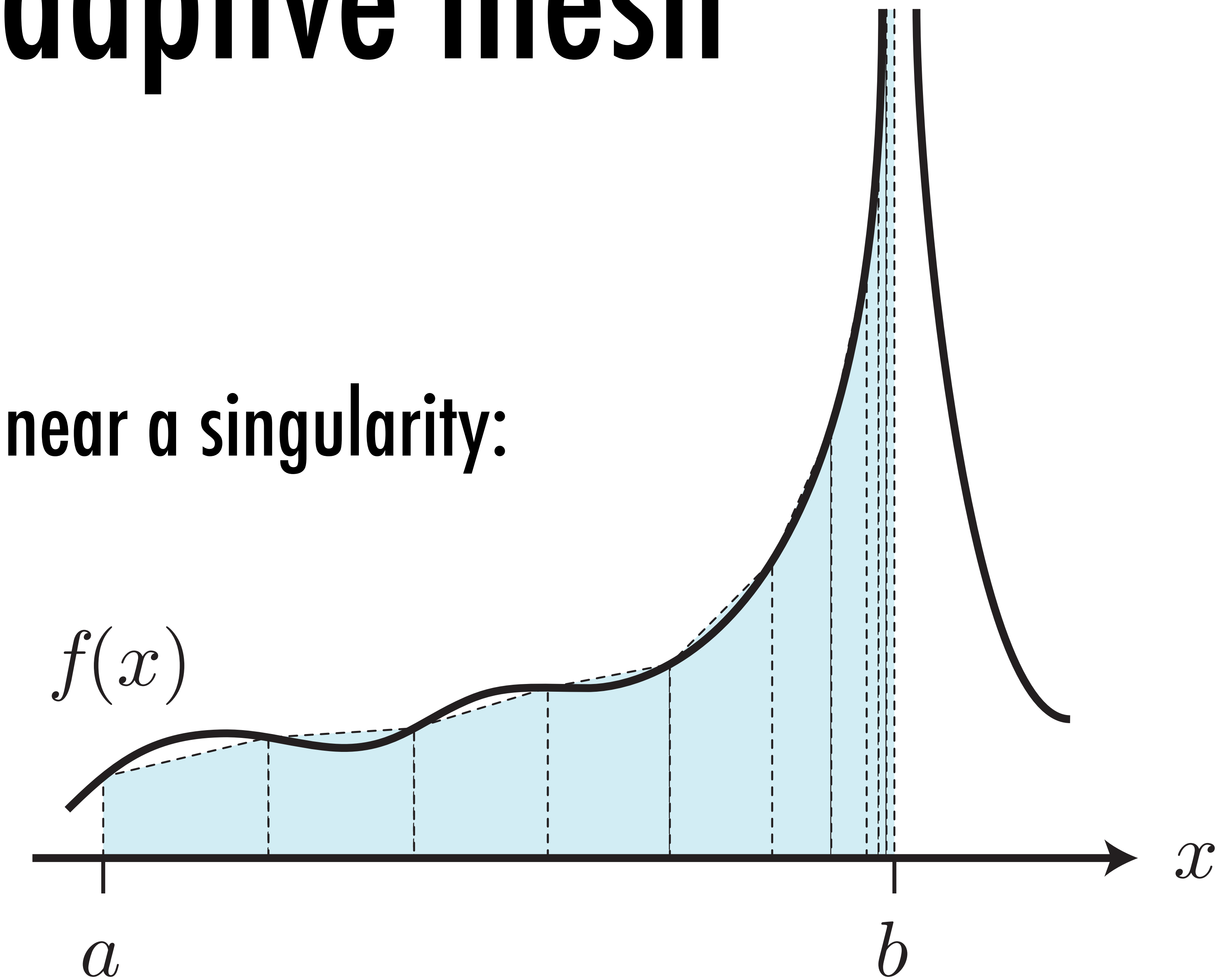


Nonuniform mesh

- Many problems can be addressed by the proper choice of mesh
- the points $a, x_1, x_2, \ldots, x_{N-1}, b$ do not have to be uniformly spaced:
  - Gaussian quadrature
  $$\int dx\, f(x) \doteq \sum_i f(x_i) w_i$$
  - Clenshaw-Curtis quadrature
  - choose an adaptive mesh to keep the piecewise areas roughly constant

Adaptive mesh

- Adaptive mesh near a singularity:



- Rule of thumb: $(x_{i+1} - x_i) \times \frac{1}{2}\big(f(x_i) + f(x_{i+1})\big) \approx \text{const.}$

Numerical Calculus

- Most physical phenomena evolve continuously and are described in terms of time rates of change and spatial gradients

$$\frac{\partial}{\partial t},\ \frac{\partial^2}{\partial t^2},\ \vec{\nabla},\ \nabla^2,\ \ldots$$

- On the computer we have only floating point approximations to real numbers and no proper sense of a continuous function and its derivatives

Numerical Calculus

- Recall: integration can be implemented as a limiting process of ever smaller discretization
- Numerical differentiation can be done in similar fashion
- E.g., breaking the real line into a fine grid $x_1, x_2, x_3, \ldots$ leads to the lowest-order approximation

$$f'(x_i) = \lim_{\delta x \to 0} \frac{f(x_i + \delta x) - f(x_i)}{\delta x}$$

$$\approx \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}$$

Numerical Calculus

- We must always consider how the “finite-difference” scheme scales with the grid spacing $h = x_{i+1} - x_i$
- Taylor expansion around x_i yields

$$f(x_{i+1}) - f(x_i) = f'(x_i)h + \frac{1}{2!}f''(x_i)h^2 + \frac{1}{3!}f'''(x_i)h^3 + \cdots$$

- We find that the error scales rather badly

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} + O(h)$$

asymmetric

Numerical Calculus

- Instead, expand to the right and left around x_i

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{1}{2!}f''(x_i)h^2 + \cdots$$
$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{1}{2!}f''(x_i)h^2 + \cdots$$

- Difference gives the symmetric "three-point formula"

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} + O(h^2)$$

Numerical Calculus

- Procedure can be generalized to higher order
- A “five-point” formula can be derived by including expansions for $f(x_{i+2}), f(x_{i-2})$:

$$f(x_{i+1}) - f(x_{i-1}) = 2hf'(x_i) + \frac{1}{3}f'''(x_i)h^3 + O(h^5)$$
$$f(x_{i+2}) - f(x_{i-2}) = 4hf'(x_i) + \frac{8}{3}f'''(x_i)h^3 + O(h^5)$$

- Eliminating the f''' term yields

$$f'(x_i) = \frac{1}{12h}\Big(f_{i-2} - 8f_{i-1} + 8f_{i+1} - f_{i+2}\Big) + O(h^5)$$

Richardson extrapolation

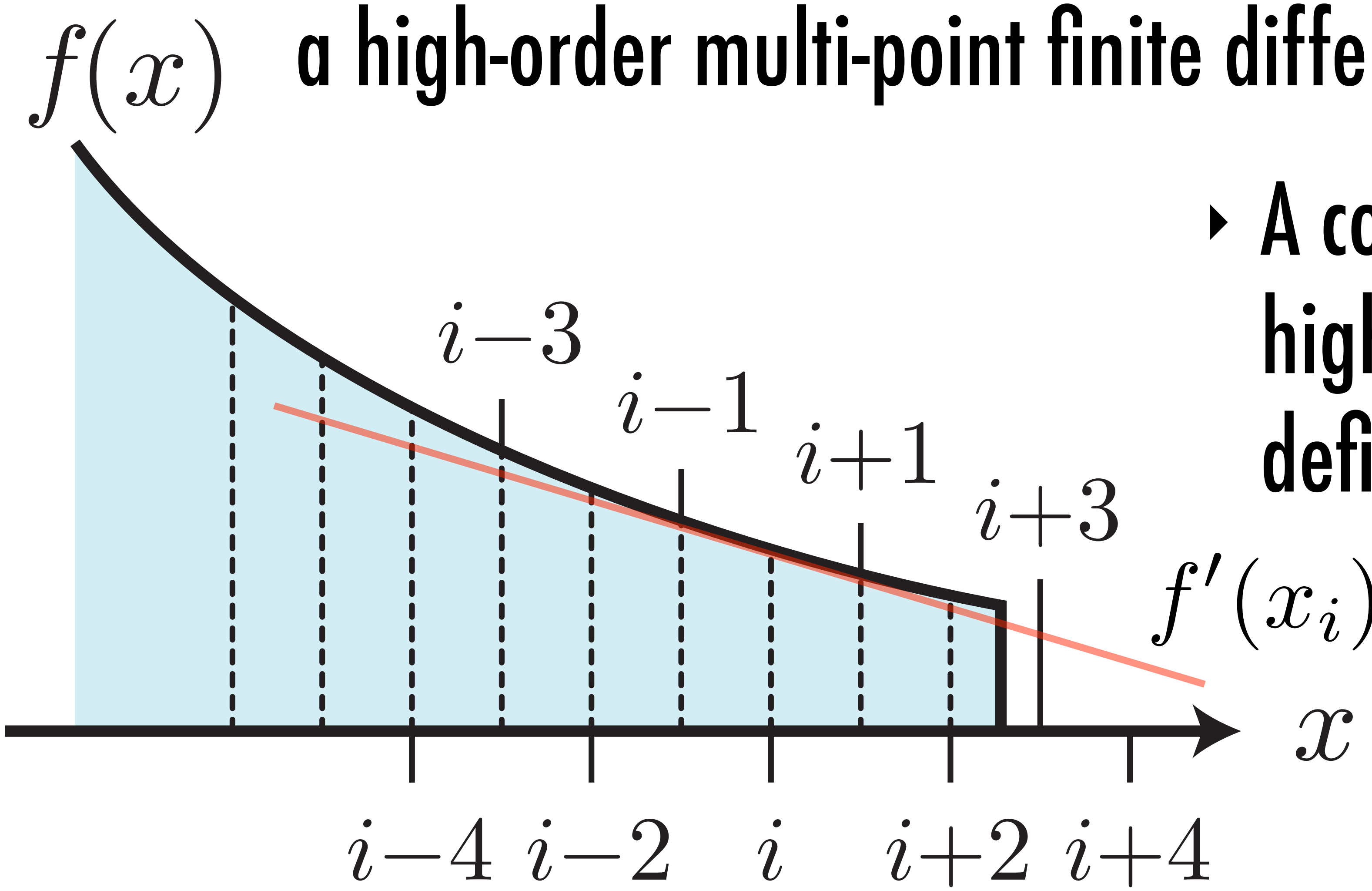
- Method to automate these order-by-order improvements
- Numerical derivatives built from function evaluations at $x, \quad x+h, \quad x+h/\xi, \quad x+h/\xi^2, \ldots$ for $\xi > 1$
- Recursive definition:

$$D^{(1)}(h) = \frac{f(x+h) - f(x)}{h}$$

$$D^{(n+1)}(h) = \frac{\xi^n D^{(n)}(h/\xi) - D^{(n)}(h)}{\xi^n - 1}$$

Numerical Calculus

- The three-point formula is often good enough
- Sometimes necessary to take h small rather than to use a high-order multi-point finite difference formula

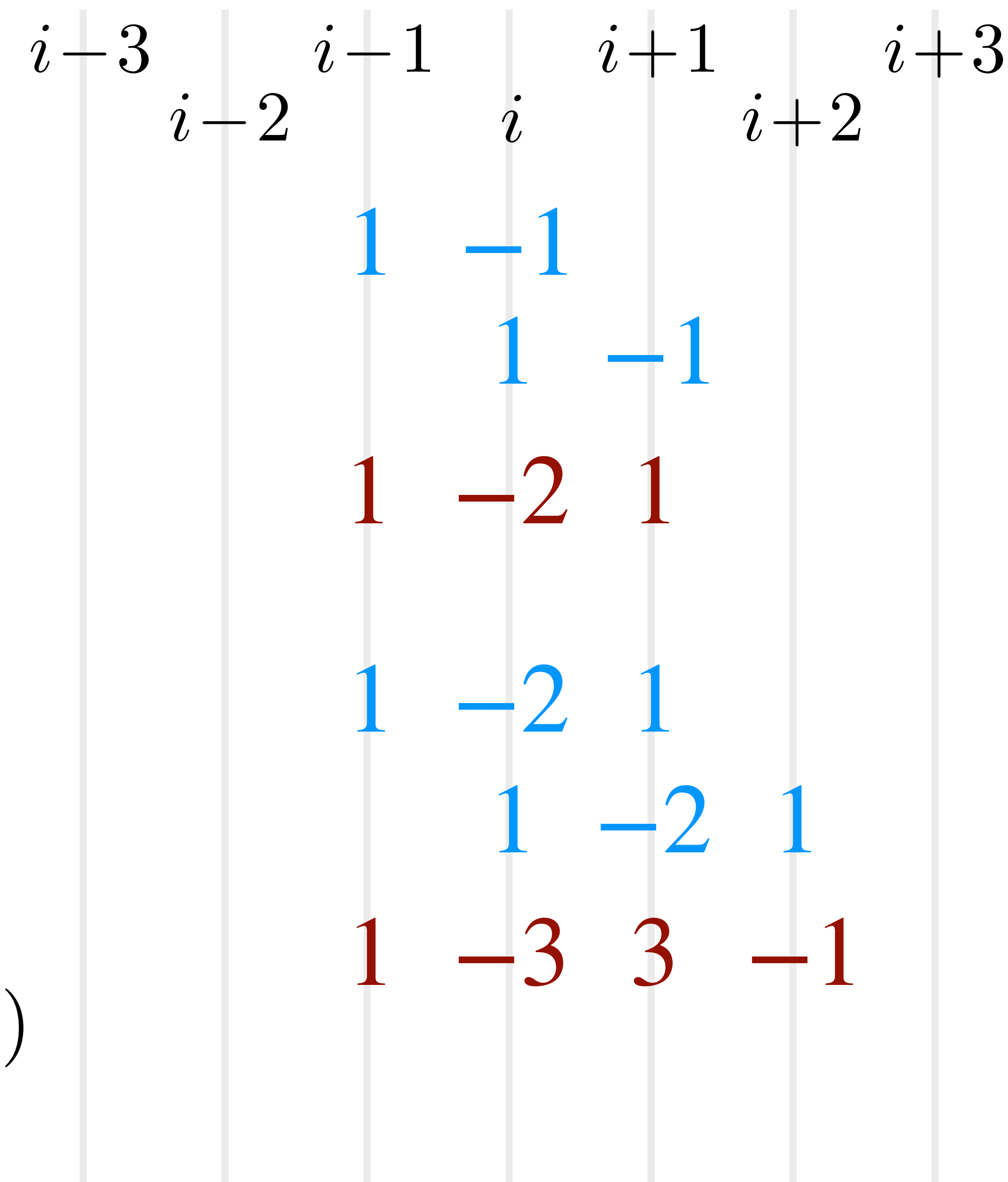


- A common problem is that high-order formulas are ill-defined near boundaries

Numerical Calculus

- Finite difference is a well-defined "shift and subtract" operation
- Derivatives at arbitrary order have weights that are binomial coefficients:

$$\Delta^n[f(x_i)] = \sum_{k=0}^{n} (-1)^k \binom{n}{k} f(x_{i+n-2k})$$



Root finding

- How to find the solution(s) of the equation $f(x) = 0$?
- Choice of method depends on whether $f'(x)$ is known analytically
- If we have knowledge of the derivative, a common and efficient scheme is the Newton-Raphson method

Root finding

- Suppose there is a root at $x^{\dagger}$ and we guess that its position is x_n
- Expansion in terms of the deviation $\Delta x_n = x_n - x^{\dagger}$ yields

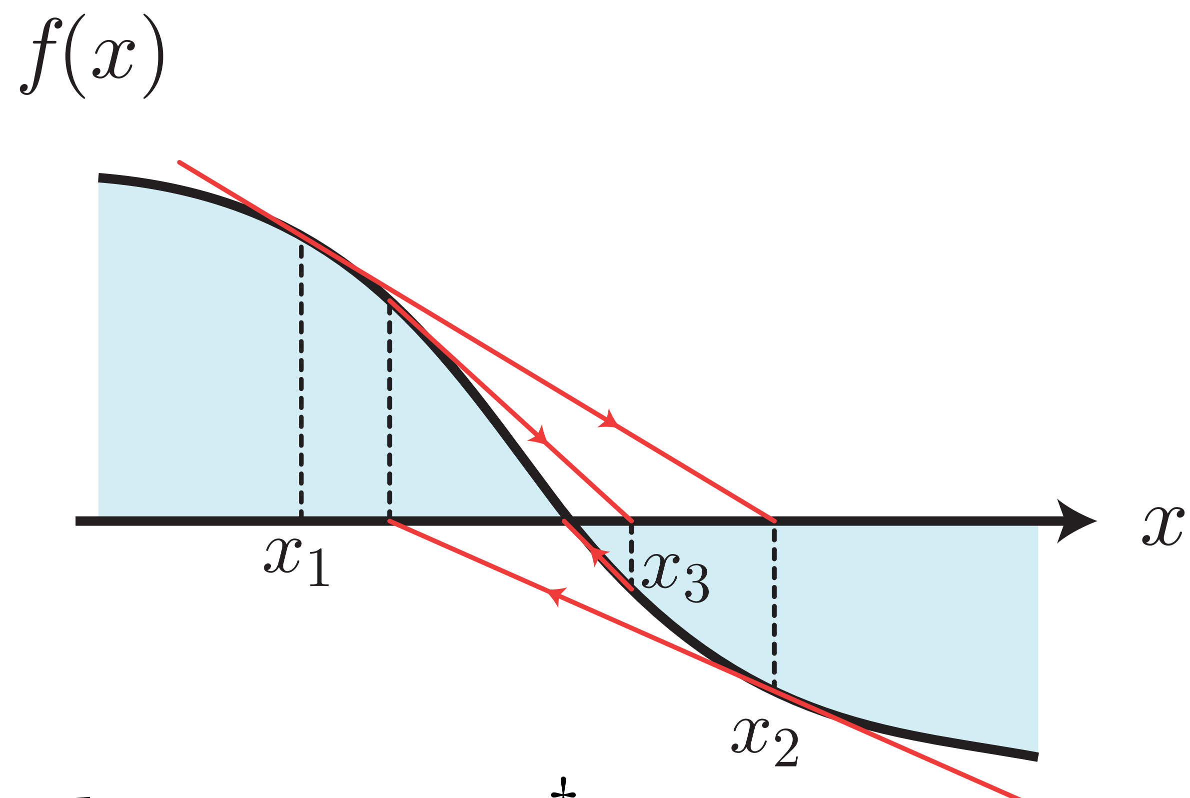
$$f(x^{\dagger}) = f(x_n) - f'(x_n)\Delta x_n + O\big([\Delta x_n]^2\big) = 0$$

- View approximate solution as a refined guess, x_{n+1}:

$$x^{\dagger} \approx x_{n+1} \equiv x_n - \frac{f(x_n)}{f'(x_n)}$$

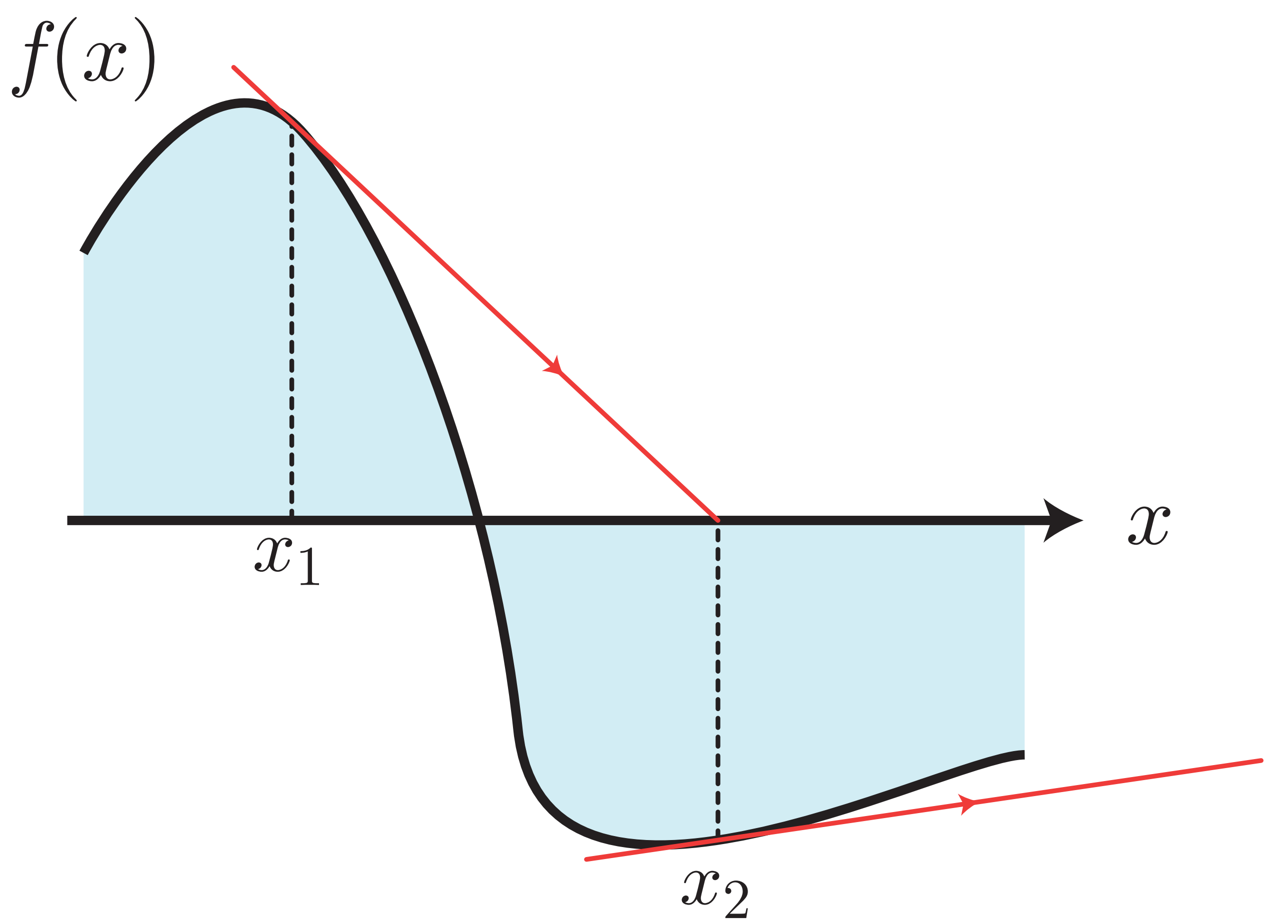
Newton-Raphson iterations

- Example of a successful Newton-Raphson search
- Each iteration brings us closer to the true root
- If $f(x)$ is smooth and the initial guess is close to the root, convergence is very fast



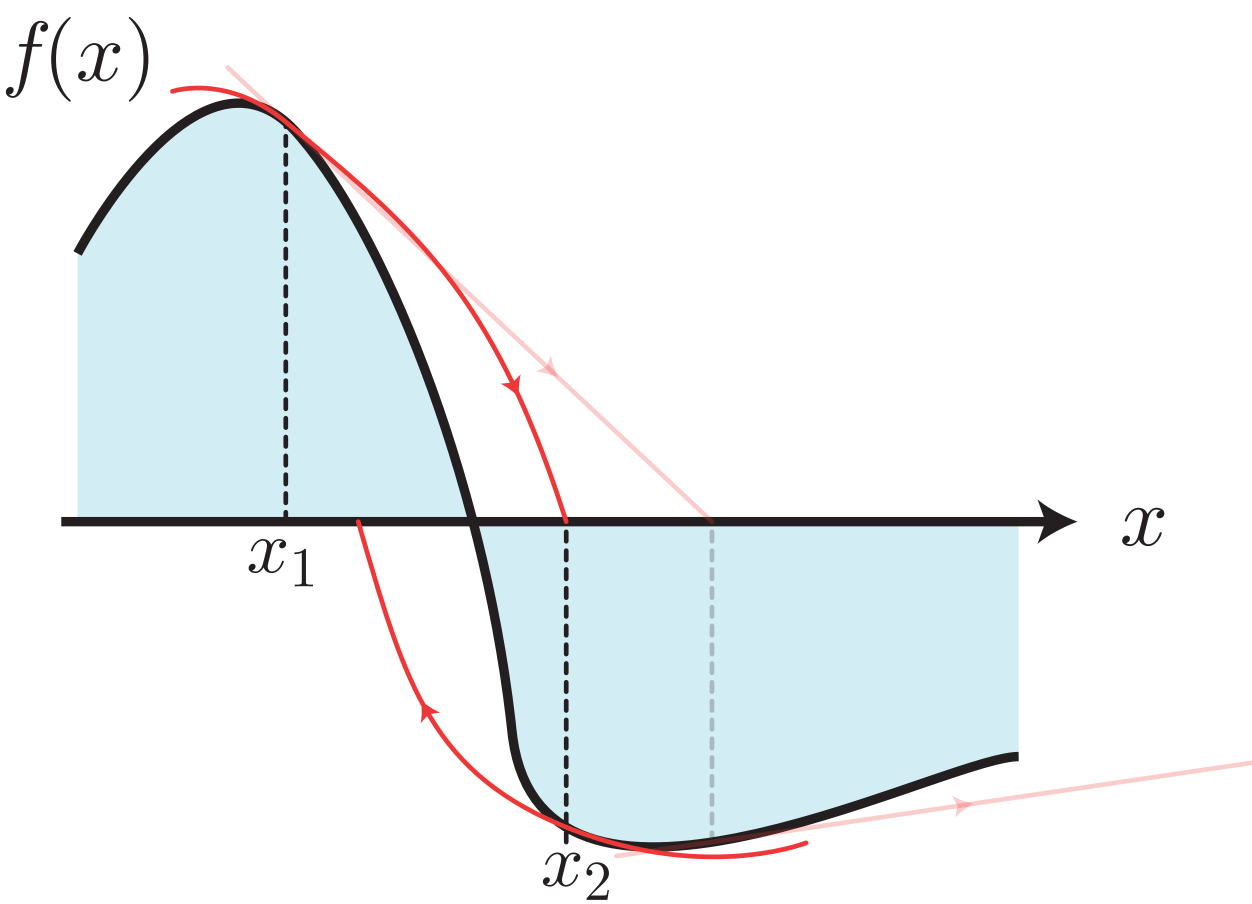
$$\lim_{n\to\infty} x_n = x^\dagger$$

Convergence region



- Failure to find the root can result if the initial guess is not sufficiently close to the true root
- Linear extrapolation from the local slope may be a bad approximation

Convergence region



- The region in which initial guesses converge to the correct solution can be expanded with a quadratic estimate of the y-axis crossing

$$x_{n+1} := x_n - \frac{f(x_n)}{f'(x_n)}\left[1 - \frac{f''(x_n)f(x_n)}{2(f'(x_n))^2}\right]^{-1}$$

Common variants

- Infer the direction from the slope but use a much smaller step size than demanded by Newton-Raphson

$$x_{n+1} := x_n - \operatorname{sgn}\left(\frac{f(x_n)}{f'(x_n)}\right) \times h \qquad h \ll \left|\frac{f(x_n)}{f'(x_n)}\right|$$

- Use a randomly generated distribution of step sizes