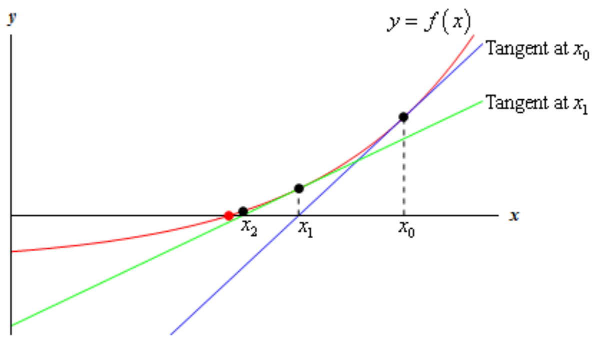
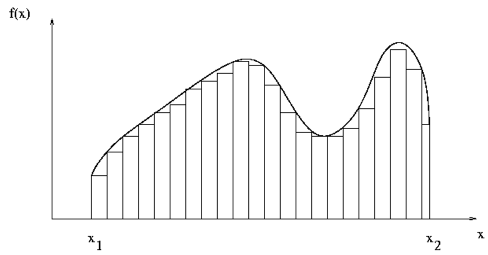
Lecture 5

Root finding & numerical integration



Root finding.

Credit: Paul Dawkins



Numerical integration.

Credit Michael Richmond (Tuffs)

Mathematical problem

Common problems in computational physics include *root finding* and *numerical integration*

- Root-finding: Find a (the) value('s) x, for which

$$f(x) = 0\,.$$

  usually within a range $x \in [a, b]$

- Numerical integration: evaluate

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

for a given function $f(x)$, where a and b are given

Both problems can occur in more than one dimension

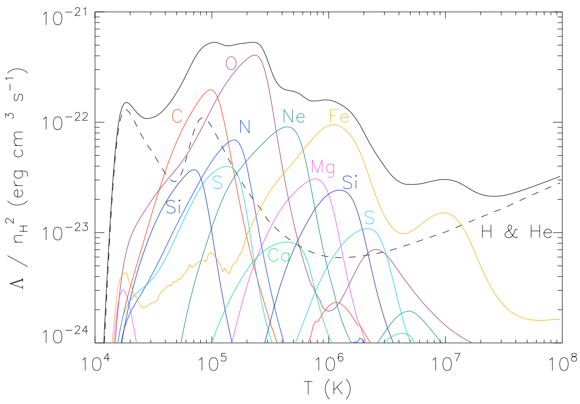
which significantly complicates matters

Here we only discuss the one-dimensional case.

Example: root finding

- Cooling in cosmological simulations: $\rho \frac{\mathrm{d}T}{\mathrm{d}t} = -\Lambda(T)\,\rho^2$ solved numerically (implicitly) as T is temperature, t is time, *rho* is density, Λ is cooling rate

$$\frac{T(t+\Delta t) - T(t)}{\Delta t} = -\Lambda(T+\Delta t)\rho$$



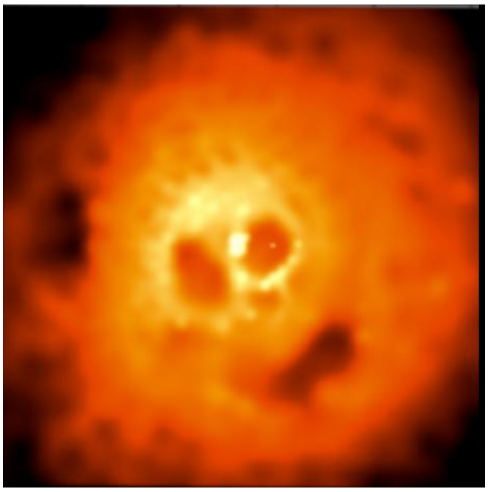
Cosmological gas cooling function $\Lambda(T)$. Different colours refer to different chemical elements.

Credit: Wiersma et al., 2009

Example: numerical integration

- The energy radiated by cosmic gas during an interval Δt

$$\Delta E = \int_t^{t+\Delta t} \Lambda(T)\,\rho^2\,\mathrm{d}t$$



X-ray image of the Perseus cluster, a massive cluster of galaxies.

Credit: Nasa

Root finding method 1: Newton-Raphson

Find value X for a given function $f(x)$, so that $f(X) = 0$

- Assume x_i starting point for root, develop f as a Taylor series expansion close to x_i

  $$f(x_i) + f'(x_i)(X - x_i) + \cdots \approx f(X) = 0\,,$$

  and solve for X

  $$X = x_i - \frac{f(x_i)}{f'(x_i)} \equiv x_{i+1}\,.$$

  x_{i+1} is improved estimate for root
- Newton-Raphson is the iterative scheme

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

Root finding method 1: Newton-Raphson

- $x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$
- Termination criterion for the iteration: $|x_{i+1} - x_i|$ is 'small enough'
- Method requires that f' be calculable
- Method needs a guess for start of iteration
- Which root is found if there is more than one?

Root finding method 1: Convergence of Newton-Raphson

- To estimate the error rewrite $x_{i+1} = X + \Delta x_{i+1}$ as

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

- Solve for Δx_{i+1} & expand last term in a Taylor series:

$$\begin{aligned} \Delta x_{i+1} &= \Delta x_i - \frac{f(X) + \Delta x_i f'(X) + \frac{1}{2}(\Delta x_i)^2 f''(X) + \ldots}{f'(X) + \Delta x_i f''(X) + \ldots} \\ &= \frac{f''(X)}{2f'(X)}(\Delta x_i)^2 + \mathcal{O}[(\Delta x_i)^3]\,. \end{aligned}$$

- Error term is quadratic in $\Delta x \to$ decreases quickly
  convergence rate depends on f' and f"

  f' small and/or f'' large $\to$ convergence is slow

Root finding method 2: Secant method

- If f' is not known, we can't apply Newton-Raphson scheme
- Instead use Secant method: compute f' numerically from actual and previous guesses

$$f'(x_i) \approx \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}} + \mathcal{O}[(x_i - x_{i-1})^2] \,.$$

- Use this estimate in Newton-Raphson method

$$x_{i+1} = x_i - f(x_i)\frac{x_i - x_{i-1}}{f(x_i) - f(x_{i-1})} \,.$$

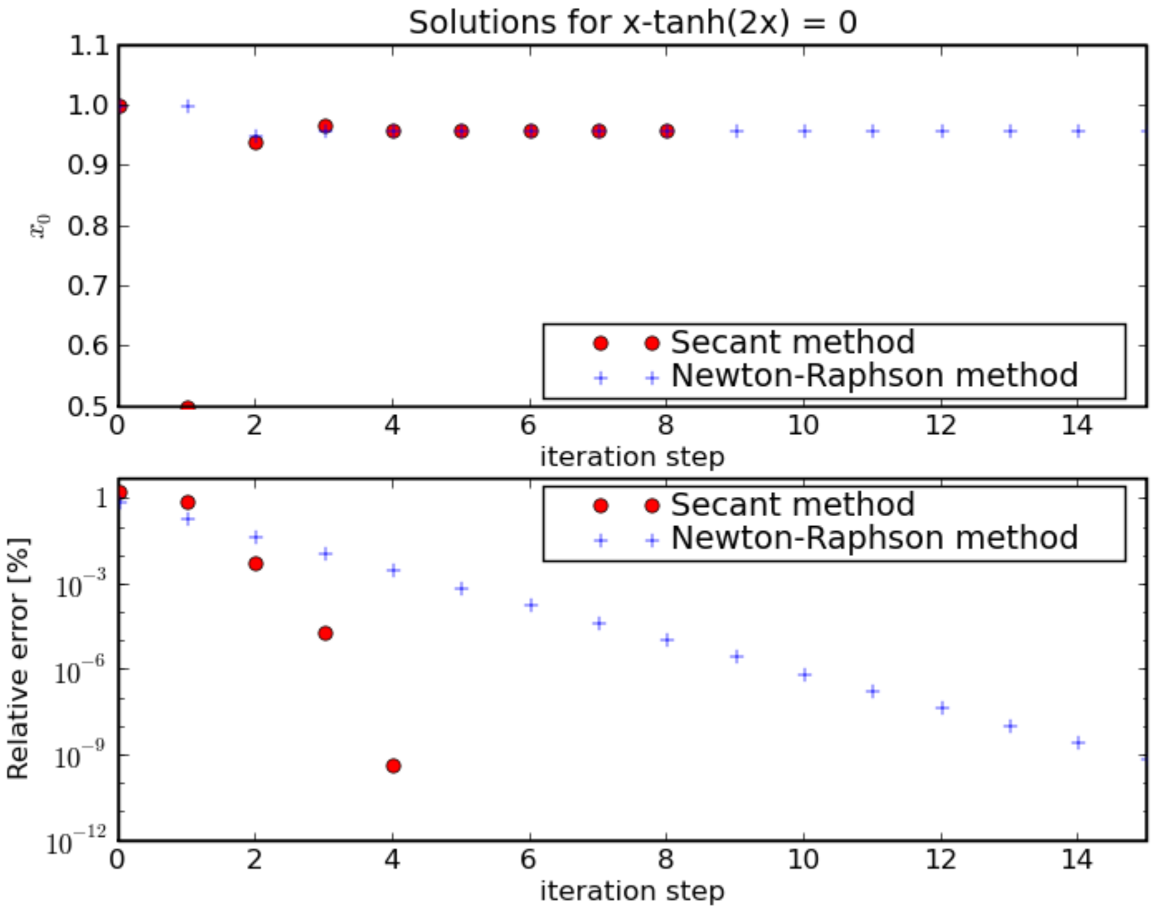
requires that we have two guesses to start iteration, x_1 and x_2

- Depending on smoothness of f, secant method may converge faster than Newton-Raphson. Asymptotically,

$$\lim_{i\to\infty} |\Delta x_{i+1}| \approx |\Delta x_i|^{1.618}$$

$\Delta x_i = X - x_i$. Exponent is called the 'golden ratio',$(\sqrt{5}+1)/2 \approx 1.618$

Root finding: Newton-Raphson vs. Secant method



Root finding method 3: Bisection

Robust method that relies on subdividing intervals

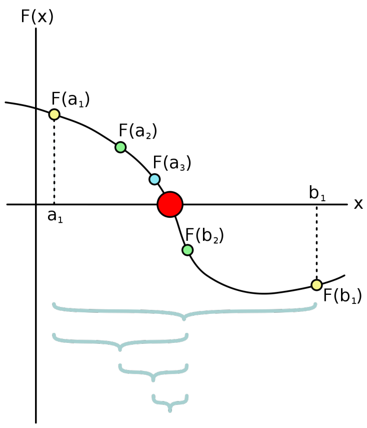
- Use: $f(x_0) \cdot f(x_1) < 0 \Longrightarrow \exists X \in [x_0, x_1] : f(X) = 0.$

  Provided f is continuous

- Find interval $[x_i, x_{i+1}]$ with $f(x_i)f(x_{i+1}) < 0$

  for example $f(x_i) < 0$ but $f(x_{i+1}) > 0$

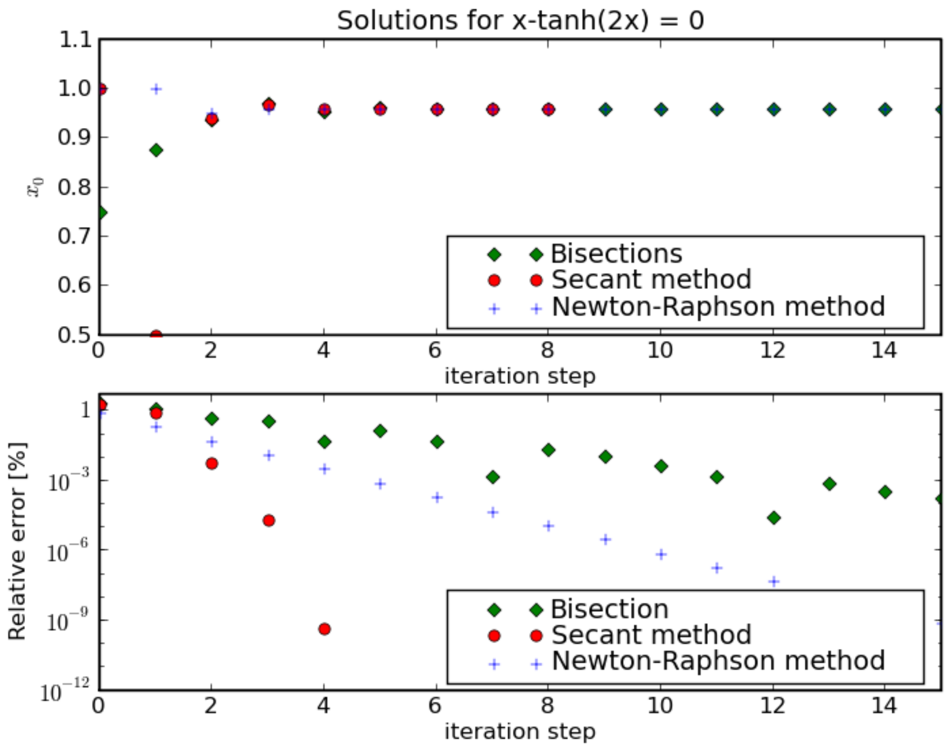
- Bisection: divide interval at $x_{i+2} = \frac{x_i + x_{i+1}}{2}$. Replace either x_i or x_{i+1} with x_{i+2} such that for new interval limits still one function value above and one below zero.



Bisection method.

Credit: wikipedia

Root finding: comparison of convergence



Root finding: summary

- We discussed *Iterative procedures* - must provide guess, and stop iteration when accuracy goal is reached. Typical condition (example):

$$\left|\frac{x_{i+1} - x_i}{x_{i+1} + x_i}\right| \leq p\,.$$

  can be absolute criterion as well, $|x_{i+1} - x_i| < q$
- Complications cases with several roots, extrema and saddle points, etc..
- Newton-Raphson: fastest convergence requires calculation of f'
- Secant method: fast compute f' numerically
- Bisections: slowest convergence but very robust
- In more than one dimension: very tricky business, would use gradient. Estimating convergence also tricky.

Numerical integration

- Evaluate

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

for given integration limits a and b, and a given function f

- Example: period of non-linear pendulum.

$$T = \sqrt{\frac{8l}{g}} \int_0^{\theta_{\max}} \frac{\mathrm{d}\theta}{\sqrt{\cos\theta - \cos\theta_{\max}}}$$

Elliptic integral, closed form analytic solution not known

Numerical integration: Newton-Cotes method

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

- Newton-Cotes: divide interval $[a, b]$ in N subintervals of size $\Delta x = (b - a)/N$ and approximate integral by a sum:

$$\int_a^b f(x)\ \mathrm{d}x \approx \sum_{i=0}^{N-1} f(x_i)\Delta x = \sum_{i=0}^{N-1} f(a + i\Delta x)\Delta x\,.$$

- Replace integration by sum over rectangular segments

approximate f as being piece-wise constant when segments are 'small enough'

Numerical integration: convergence of Newton-Cotes method

- The Euler-Maclaurin summation formula is:

sum over integers, requires that **all** derivatives of F exist

$$\sum_{i=1}^{N-1} F(i) = \int_0^N F(u)\,\mathrm{d}u - \frac{1}{2}\left[F(0) + F(N)\right] + \sum_{k=1}^{\infty}\left\{\frac{B_{2k}}{(2k)!}\left[F^{(2k-1)}(N) - F^{(2k-1)}(0)\right]\right\}.$$

$F^{(n)}(u) = n^{\mathrm{th}}$ derivative of F

B_{2k} are the Bernoulli numbers e.g. $B_2 = 1/6$, $B_4 = -1/30$

Numerical integration: convergence of Newton-Cotes

- Setting $u = \frac{x-a}{\Delta x}$, $F(u) = f(x)$ E-M summation formula becomes

$$\sum_{i=1}^{N-1} f(x_i) = \frac{1}{\Delta x}\int_a^b f(x)\,\mathrm{d}x - \frac{1}{2}\left[f(a) + f(b)\right]$$

$$+ \sum_{k=1}^{\infty}\left\{\frac{B_{2k}}{(2k)!}\left[f^{(2k-1)}(b) - f^{(2k-1)}(a)\right](\Delta x)^{2k-1}\right\}.$$

- Rearrange and adjust the summation index:

$$\int_a^b f(x)\,\mathrm{d}x = \sum_{i=0}^{N-1} f(x_i)\Delta x + \frac{\Delta x}{2}\left[f(b) - f(a)\right]$$

$$-\frac{(\Delta x)^2}{12}\left[f'(b) - f'(a)\right] + \mathcal{O}[(\Delta x)^4].$$

Numerical integration: trapezoidal rule

- Improve convergence of N-C by including the term $[f(b) - f(a)]/2$ that appears in the Euler-MacLaurin formula:

$$\int_a^b f(x)\,\mathrm{d}x = \sum_{i=0}^{N-1} f(x_i)\Delta x + \frac{\Delta x}{2}[f(b) - f(a)] + \ldots$$

- Trapezoidal rule accurate up to second order in Δx - Newton-Cotes accurate to first order in Δx.

Numerical integration: trapezoidal rule

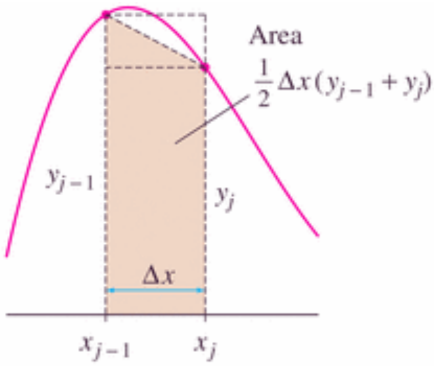


FIGURE 3 The area of a trapezoid is equal to the average of the areas of the left- and right-endpoint rectangles.

Illustration of the 'trapezoidal rule'.

Credit: Andy Long

Numerical integration: Simpson's rule

- Use higher-order interpolation rather than linear interpolation of trapezoidal rule
- Simpson's rule: Fit parabolic segments through the top edges of two neighbouring segments. If A_i is the area of the segment between x_i and x_{i+1} in the parabolic fit, then

$$A_i + A_{i+1} = \frac{\Delta x}{3}\left[f(x_i) + 4f(x_{i+1}) + f(x_{i+2})\right] .$$

- This can be seen by using

$$A_i + A_{i+1} = \int_{x_i}^{x_{i+2}} \left(ax^2 + bx + c\right) \, \mathrm{d}x$$

and the parabolic fit

$$f(x_{j=i,i+1,i+2}) = ax_j^2 + bx_j + c\,.$$

Numerical integration: Simpson's rule

- From the area $A_i + A_{i+1}$ of two neighbouring segments in the parabolic fit we have

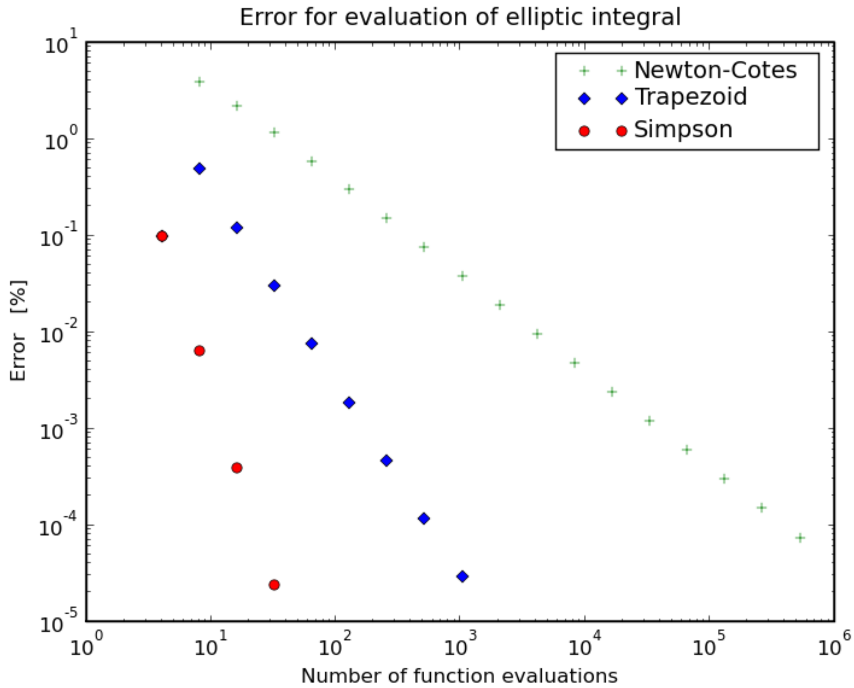
$$\int_a^b f(x)\,\mathrm{d}x \approx \frac{\Delta x}{3}\Big[f(a) + 4f(x_1) + 2f(x_2) + 4f(x_3) + \ldots + \cdots + 2f(x_{N-2}) + 4f(x_{N-1}) + f(b)\Big]$$

- Convergence of Simpson's rule: $\propto (\Delta x)^4$.

Numerical integration: comparison of methods

- Trivial test: Elliptic integral

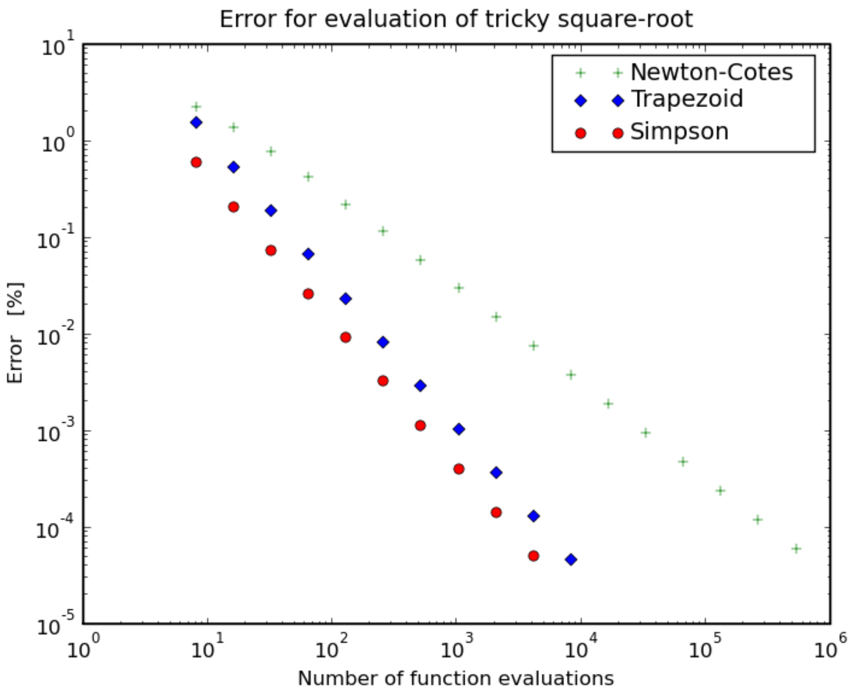
$$I = \int_0^{\pi/2} \left(1 - k^2 \sin^2\theta\right)^{1/2} \, \mathrm{d}\theta \xrightarrow{k\to 1} 1$$



Numerical integration: comparison of methods

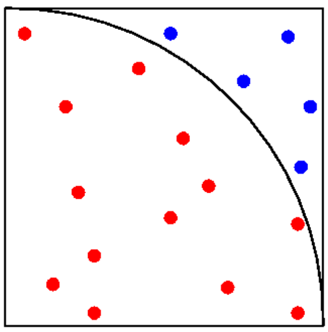
- Harder test - function with diverging derivative at $x = 2$:

$$I = \int_0^2 \left(4 - x^2\right)^{1/2} \, \mathrm{d}x = \pi$$



Numerical integration: Monte Carlo integration

- Example: calculating π. Compare surface area of sphere ($S = \pi r^2$) to that of a square with length $2r$ ($S = 4\,r^2$)
- Use pseudo-random number generator



$$\frac{\text{Hits}}{\text{Misses} + \text{Hits}} \longrightarrow \frac{\pi}{4}$$

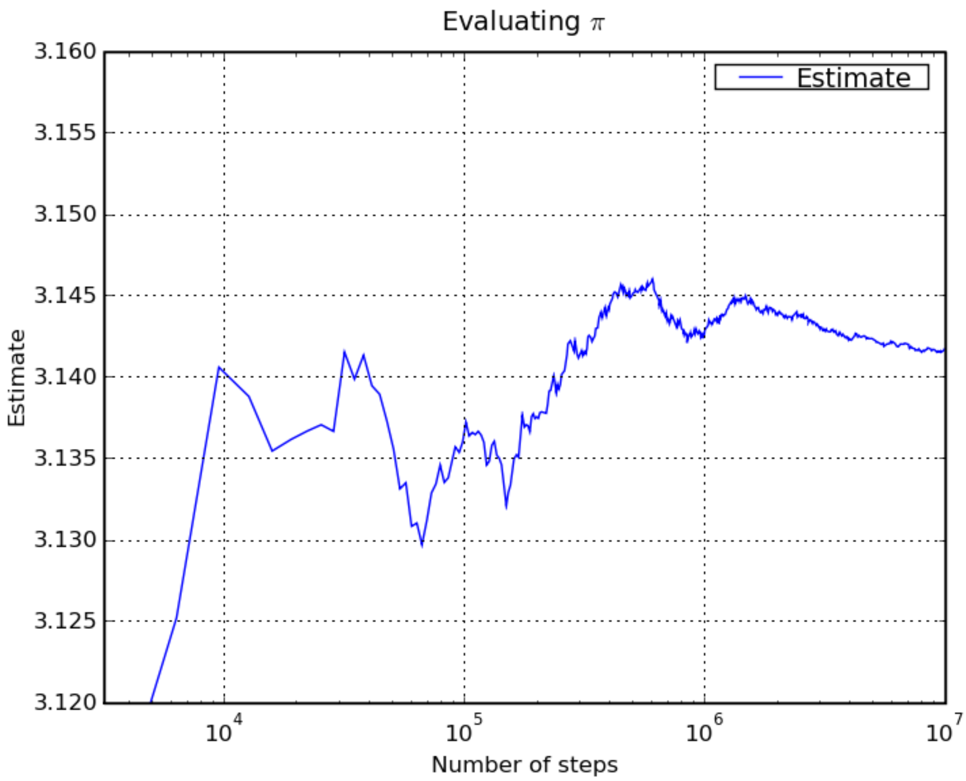
Throw random points (x,y), with x, y in [0,1]

For hits: $(x^2 + y^2) < r^2 = 1$

Ratio of surface of quarter circle ($S = \pi r^2/4$) over that of square ($S = r^2$) is fraction of points that land inside the circle

Numerical integration: Monte Carlo integration

Example: evaluating π



Monte Carlo integration: convergence

- MC integration: Estimate integral by N probes

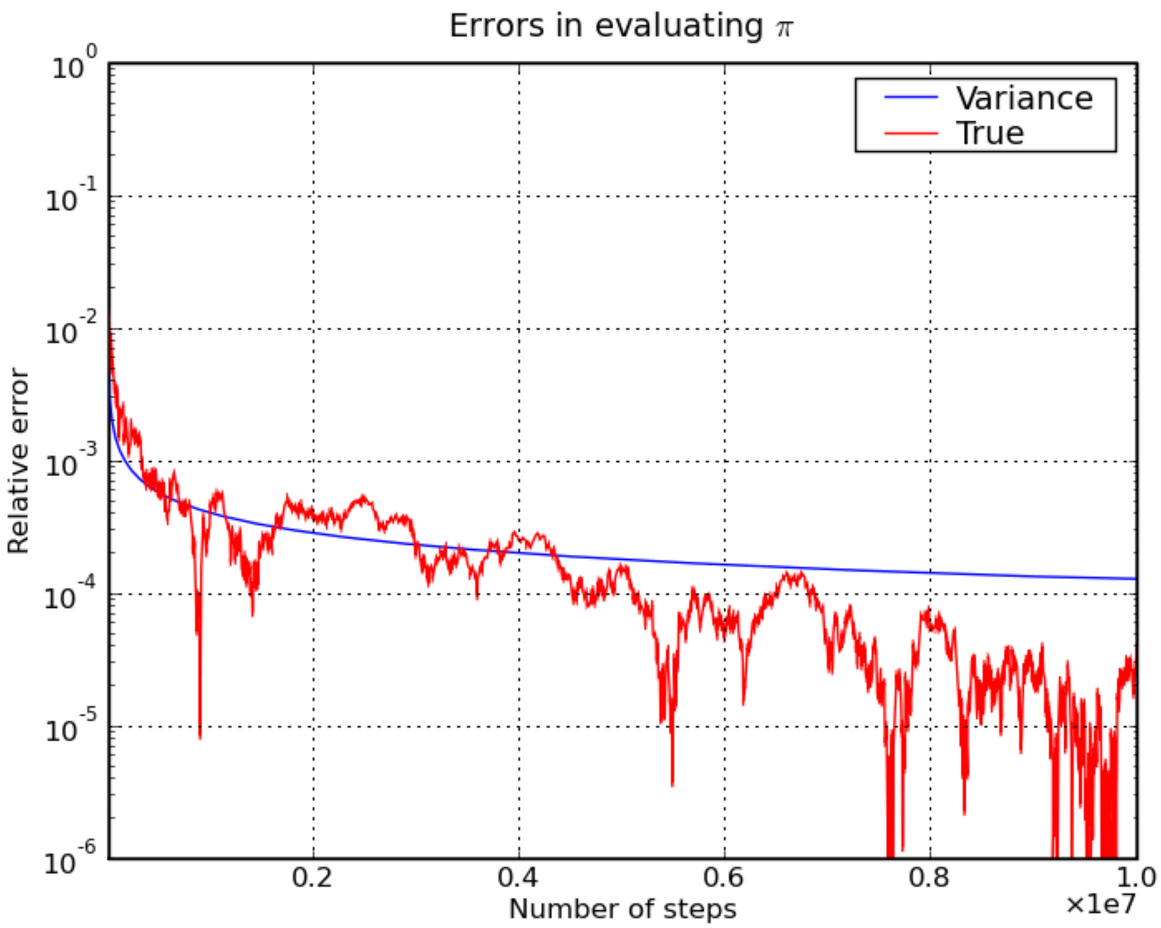
$$I = \int_a^b f(x)\,\mathrm{d}x \longrightarrow \langle I \rangle = \frac{b-a}{N}\sum_{i=1}^{N} f(x_i) = \langle f \rangle_{a,b}\,,$$

  where x_i are random numbers homogeneously distributed in $[a,\ b]$

- Basic idea for error estimate: statistical sample
  $\Longrightarrow$ use standard deviation as error estimate

$$\langle E_f(N) \rangle = \sigma = \left[\frac{\langle f^2 \rangle_{a,b} - \langle f \rangle_{a,b}^2}{N}\right]^{1/2}$$

Monte Carlo integration: convergence



Comparing convergence rates in numerical integration

- Interesting question: How do error estimates scale with the number of function calls?
- May become crucial, if function calls "expensive"
- Trapezium: $\sim N^{-2/d}$, Simpson: $\sim N^{-4/d}$, MC: $\sim N^{-1/2}$ for d dimensions.
- Therefore: For $d \geq 8$ dimensions MC wins!
- Method of choice for high-dimensional integration.

Numerical integration: summary

- When to favour higher-order over lower-order and vice versa?
  - Integral needed only once: knowing accuracy important

    convergence
  - Integral needs evaluating many times

    e.g. with small changes of integration limits

    in general: smooth function $\rightarrow$ use higher-order method
    non-smooth function $\rightarrow$ use low-order method

    for best accuracy with minimum computational cost

    similar to Lecture 2: (non)-smooth functions: use (lower)higher-order
- Very smooth function: use Gaussian integration not discussed here

Numerical integration application: Hyperspheres

Hypersphere is a sphere in $d > 3$ dimensions

- Volume in spherical coordinates:

$$V_d = \int_0^R r^{d-1}\mathrm{d}r \int d\Omega_n = \frac{R^d}{d} \int d\Omega_n$$

R is radius of the sphere, $\int d\Omega_n$ is the 'angular bit'

- Here: want to have fun - calculate volume numerically

Hypersphere volume: analytical calculation

difficult way: using d-dimensional polar coordinates

- Transform to d-dimensional polar coordinates

$$
\begin{aligned}
x_1 &= r \sin\theta_1 \sin\theta_2 \ldots \sin\theta_{d-3} \sin\theta_{d-2} \sin\theta_{d-1} \\
x_2 &= r \sin\theta_1 \sin\theta_2 \ldots \sin\theta_{d-3} \sin\theta_{d-2} \cos\theta_{d-1} \\
x_3 &= r \sin\theta_1 \sin\theta_2 \ldots \sin\theta_{d-3} \cos\theta_{d-2} \\
\vdots &\ \ \vdots \ \ \vdots \\
x_{d-1} &= r \sin\theta_1 \cos\theta_1 \\
x_d &= r \cos\theta_1
\end{aligned}
$$

- Volume element:

$$
\mathrm{d}V_d = \int_0^R r^{d-1}\,\mathrm{d}r \left[\prod_{i=1}^{d-2} \int_0^\pi \sin^{d-1-i}\theta_i\,\mathrm{d}\theta_i\right] \int_0^{2\pi} \mathrm{d}\theta_{d-1}
$$

Hypersphere volume: analytical calculation

- For integral above, use (with $\beta = -1/2$)

$$\int_0^{\pi} \sin^{2\alpha+1}(x)\cos^{2\beta+1}(x)\,\mathrm{d}x = \frac{\Gamma(\alpha+1)\Gamma(\beta+1)}{\Gamma(2+\alpha+\beta)}$$

- Therefore volume of d-dimension hypersphere

$$V_d = \frac{\pi^{d/2} R^d}{\Gamma\left(1+\frac{d}{2}\right)}\,.$$

Hypersphere volume: analytical calculation

the clever way: use integration of Gaussians

- Remember Gaussian integral: $\int_{-\infty}^{\infty} \exp(-x^2)\,\mathrm{d}x = \pi^{1/2}$
- Therefore

$$\begin{aligned}\left(\int_{-\infty}^{\infty} \exp(-x^2)\,\mathrm{d}x\right)^n &= \pi^{n/2} \\ &= \int_0^{\infty} r^{n-1} \exp(-r^2)\mathrm{d}r \int d\Omega_n\end{aligned}$$

use n-dimensional spherical coordinates

- But $\int_0^{\infty} r^{n-1} \exp(-r^2)\mathrm{d}r = \Gamma(n/2)/2$
- Therefore

$$\int \mathrm{d}\Omega_n = \frac{2\pi^{n/2}}{\Gamma(n/2)}$$

The Γ-function

- Properties:
  - $\Gamma(x+1) = x\Gamma(x)$, for $n \in N$: $\Gamma(n+1) = n!$
  - $\Gamma(1/2) = \sqrt{\pi}$, $\Gamma(1+n/2) = \sqrt{\pi/2^{n+1}}\, n!!$
- Integral representation:

$$\Gamma(z) = \int_0^\infty t^{z-1} e^{-t}\, \mathrm{d}t = \int_0^1 \left(\ln \frac{1}{u}\right)^{z-1} \mathrm{d}u$$

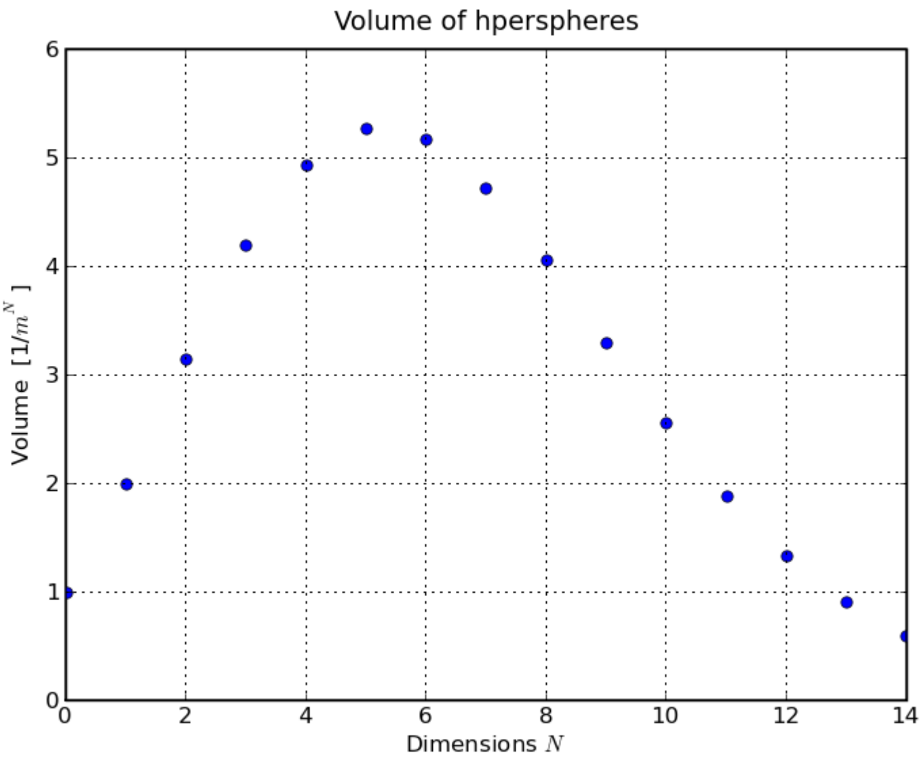
- First derivative:

$$\Gamma'(z) = \Gamma(z)\psi^{(0)}(z) = \Gamma(z)\left[\int_0^1 \mathrm{d}t \frac{1-t^{z-1}}{1-t} - \gamma_E\right] ,$$

where Euler-Mascheroni number $\gamma_E = 0.577215665$.

Volume of unit hyperspheres

'unit' means radius $= 1$



Summary

- Discussed different methods for root-finding,
  i.e. for solving $f(x) = 0$:
  Newton-Raphson, secant and bisection method
- Methods for numerical integration, based on segments:
  Newton-Cotes, trapezium and Simpson's rule.
- Another method, based on random numbers: Monte Carlo
  alternative way for error estimate through statistics