DISCRETIZATION

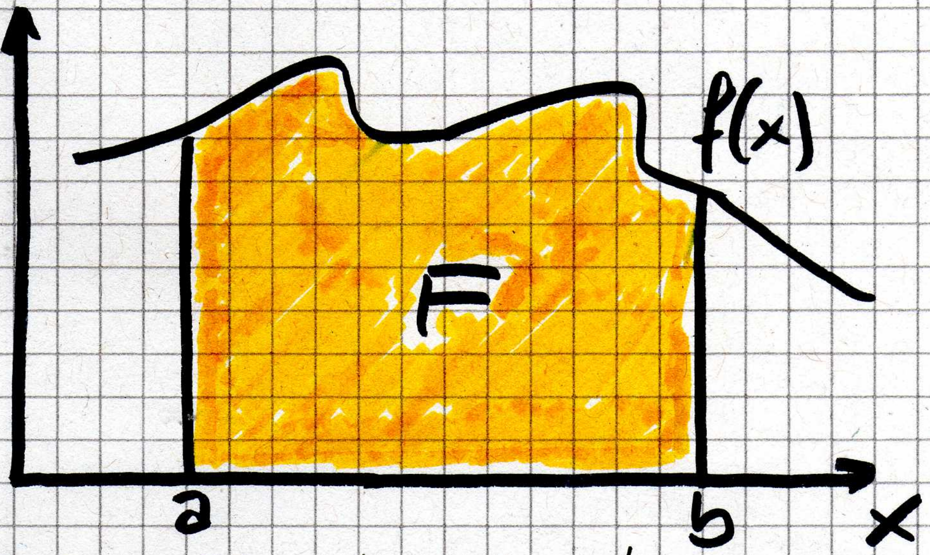
- Numerical integration
- Numerical differentiation
- Num. int. of differential eqs.

Numerical Integration of functions

- Aim: obtain an accurate value of definite integrals with the smallest number of function evaluations

- Start from the geometrical interpretation of definite integrals:

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



- Divide the interval into many "small" sub-intervals

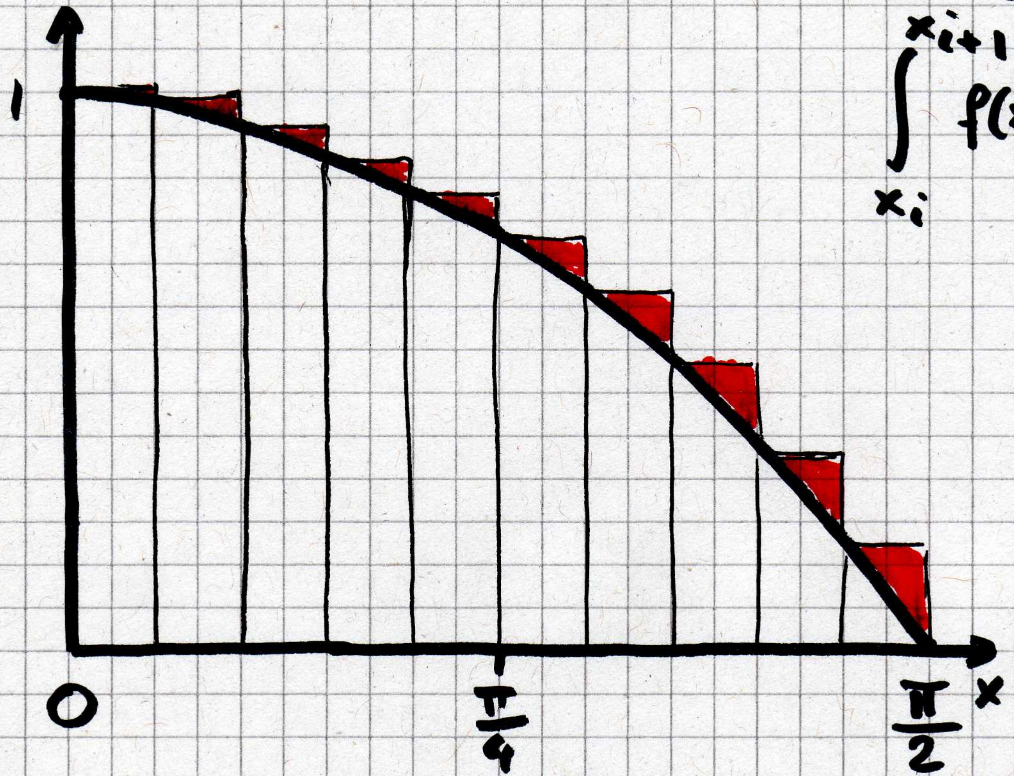
  - equispaced points

$$h = \frac{b-a}{N} \qquad x_0 = a$$

$$x_i = x_0 + i\,h \qquad i = 1, 2, \dots, N$$

  - NB: other choices can be more apropriate

Numerical Integration: Rectangular rule



The rectangular approximation for $f(x) = \cos(x)$ for $0 \le x \le \frac{\pi}{2}$

In one interval

$$\int_{x_i}^{x_{i+1}} f(x)\,dx = h\,f(x_i)$$

with an error

$$\mathcal{O}(h^2 f') \propto 1/N^2$$

when applied iteratively over consecutive intervals

$$F_N \simeq \sum_{i=0}^{N-1} f(x_i)\,h$$

with total error

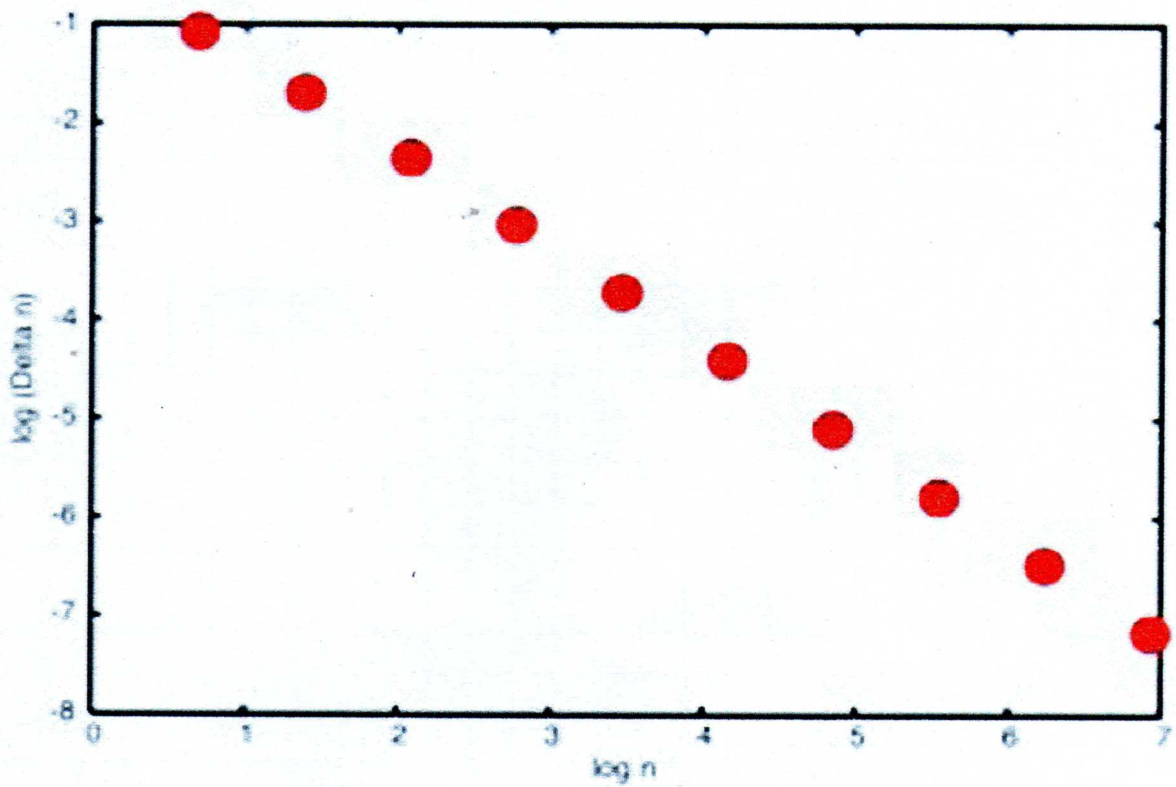
$$\mathcal{O}(h f') \propto 1/N$$

Rectangular rule : error

$$I = \int_0^{\pi/2} \cos(x)\,dx = 1 \qquad F_N = \frac{\pi}{2N}\sum_{i=0}^{N-1}\cos(x_i)\ ;\quad x_i = i\frac{\pi}{2N}$$

$$\Delta_N = F_N - I$$

n	F_n	Δ_n
2	1.34076	0.34076
4	1.18347	0.18347
8	1.09496	0.09496
16	1.04828	0.04828
32	1.02434	0.02434
64	1.01222	0.01222
128	1.00612	0.00612
256	1.00306	0.00306
512	1.00153	0.00153
1024	1.00077	0.00077



Numerical Integration: Trapezoidal rule

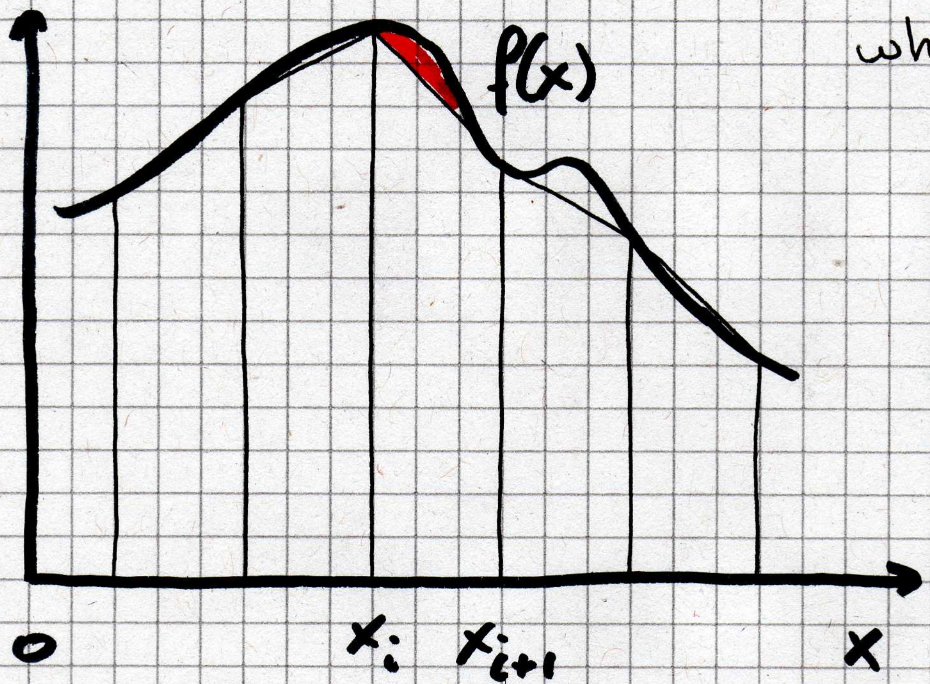
linear interpolation in each sub-interval

In one interval

$$\int_{x_i}^{x_{i+1}} f(x)\,dx = h\,\frac{f_i + f_{i+1}}{2}$$

with error

$$\mathcal{O}(h^3 f'') \propto 1/N^3$$



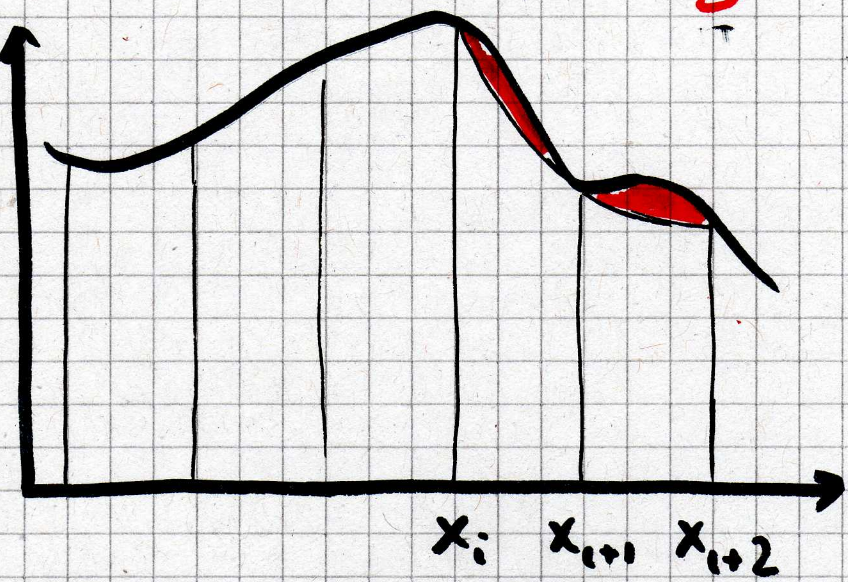
when applied iteratively

$$F_N = \left[\frac{1}{2} f_0 + \sum_{i=1}^{N-1} f_i + \frac{1}{2} f_N\right] h$$

with total error

$$\mathcal{O}(h^2 f'') \propto 1/N^2$$

Numerical Integration: Simpson's rule



parabolic interpolation between triplets of adjacent points

In one interval

$$\int_{x_i}^{x_{i+2}} f(x)\,dx = h\left[\frac{f_i + 4f_{i+1} + f_{i+2}}{3}\right]$$

with error

$$\mathcal{O}(h^5 f^{iv}) \propto \frac{1}{N^5}$$

when applied iteratively over consecutive intervals
(requires an **odd** number of points)

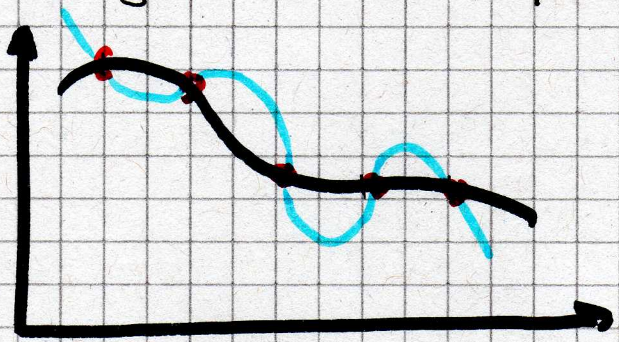
$$F_N = \left[\frac{1}{3}f_0 + \frac{4}{3}f_1 + \frac{2}{3}f_2 + \frac{4}{3}f_3 + \dots + \frac{2}{3}f_{N-2} + \frac{4}{3}f_{N-1} + \frac{1}{3}f_N\right]h$$

with error

$$\mathcal{O}(h^4 f^{iv}) \propto \frac{1}{N^4}$$

Summary

- Constant interpolation $\rightarrow$ 1 point $\rightarrow$ Rectangular rule
- Linear interpolation $\rightarrow$ 2 points $\rightarrow$ Trapezoidal rule
- Quadratic interpolation $\rightarrow$ 3 points $\rightarrow$ Simpson's rule
- ....
- higher-order polynomial $\rightarrow$ many points $\rightarrow$ ....



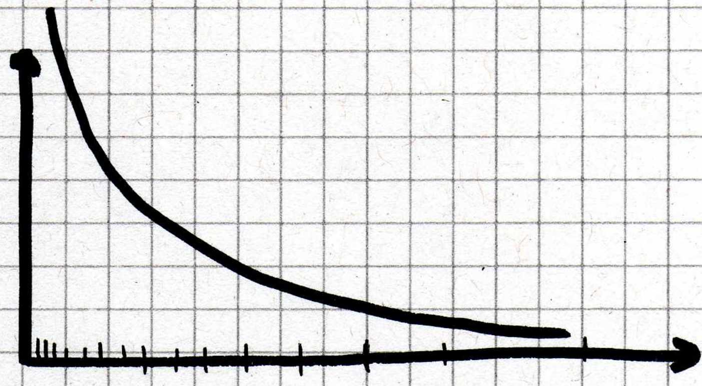
NOT CONVENIENT !

Higher order : possible strong oscillations between consecutive $(x_i, f(x_i))$ giving bad interpolation of $f(x)$.
Very sensitive to possible numerical errors in $f(x)$

Extensions

- Non uniformly spaced intervals

$$\int_a^b f(x)\,dx = \int_{s(a)}^{s(b)} f(x(s))\,\frac{dx}{ds}\,ds$$



$\Rightarrow$ uniform sub-intervals in a scaled variable s

- Divergent integrand $\Rightarrow$ subtract (and add) an analytically integrable term with the same divergence

$$\int f(x)\,dx = \underbrace{\int \left[f(x) - f_{easy}(x)\right] dx}_{\text{not divergent}} + \underbrace{\int f_{easy}(x)\,dx}_{\text{analytic}}$$

- Many dimension (D)

Straightforward generalization but the cost grows like N^D

a different strategy is needed $\rightarrow$ Monte Carlo

Numerical differentiation

Given a function (possibly known only numerically on a grid) we often need its derivative

$$f'(x) = \frac{df}{dx} = \lim_{\Delta x \to 0} \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

The obvious discretized version is

$$f'(x) \simeq \frac{f(x+h) - f(x)}{h}$$

$$= \frac{\cancel{f(x)} + f'(x)h + f''\frac{h^2}{2} + \dots - \cancel{f(x)}}{h}$$

with error $\quad O(hf'')$

numerical accuracy

$$\varepsilon(h) \sim \frac{\varepsilon_{roundoff}\,|f|}{h} + h\,|f''|$$

$$\min \varepsilon(h) \implies \frac{\partial \varepsilon(h)}{\partial h} = -\frac{\varepsilon_r\,|f|}{h} + |f''| = 0$$

$$\Downarrow$$

$$h = \sqrt{\varepsilon_r}\,\sqrt{\frac{|f|}{|f''|}}$$

$$\varepsilon \sim \sqrt{\varepsilon_{roundoff}}\,\sqrt{|f|\,|f''|}$$

single precision $\varepsilon_{roundoff} \sim 10^{-8}$ $\varepsilon \sim 10^{-4}$

double precision $\varepsilon_{roundoff} \sim 10^{-16}$ $\varepsilon \sim 10^{-8}$

Numerical Differentiation : symmetric difference

If one extra function evaluation is affordable (or stored)

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h}$$

$$= \Big[\cancel{f(x)} + f'h + \cancel{\tfrac{1}{2} f'' h^2} + \tfrac{1}{3!} f''' h^3 + \cancel{\tfrac{1}{4!} f^{iv} h^4} + \cdots \Big]$$

$$- \Big[\cancel{f(x)} - f'h + \cancel{\tfrac{1}{2} f'' h^2} - \tfrac{1}{3!} f''' h^3 + \cancel{\tfrac{1}{4!} f^{iv} h^4} + \cdots \Big] / 2h$$

with error $\mathcal{O}(h^2 f''')$

numerical accuracy (sym. diff.)

$$\varepsilon(h) \sim \frac{\varepsilon_{roundoff}\,|f|}{h} + h^2 |f'''|$$

$$\frac{\partial \varepsilon(h)}{\partial h} = -\frac{\varepsilon_r\,|f|}{h^2} + 2h\,|f'''| = 0$$

$$\Downarrow$$

$$h \sim \left(\varepsilon_r \left|\frac{f}{f'''}\right|\right)^{1/3}$$

$$\varepsilon \sim \varepsilon_{roundoff}^{2/3} \left(|f|^2 |f'''|\right)^{1/3}$$

single precision $\varepsilon_r \sim 10^{-8}$ $\varepsilon \sim 10^{-6}$

double precision $\varepsilon_r \sim 10^{-16}$ $\varepsilon \sim 10^{-10}$

Second order derivative

$$f(x+h) = f(x) + f'(x)\,h + \frac{1}{2} f'' h^2 + \frac{1}{3!} f''' h^3 + \frac{1}{4!} f^{iv} h^4 + \cdots$$

$$f(x-h) = f(x) - f'(x)\,h + \frac{1}{2} f'' h^2 - \frac{1}{3!} f''' h^3 + \frac{1}{4!} f^{iv} h^4 + \cdots$$

$$f(x) = f(x)$$

$$\frac{f(x+h) + f(x-h) - 2f(x)}{h^2} = f''(x) + \mathcal{O}(h^2)$$

numerical accuracy (2nd derivative)

$$\varepsilon(h) \sim \frac{\varepsilon_{roundoff}\,|f|}{h^2} + h^2 |f^{iv}|$$

$$\frac{\partial \varepsilon(h)}{\partial h} = -\frac{2\,\varepsilon_r}{h^3}|f| + 2h|f^{iv}| = 0$$

$$\Downarrow$$

$$h \sim \left(\varepsilon_r \left|f/f^{iv}\right|\right)^{1/4}$$

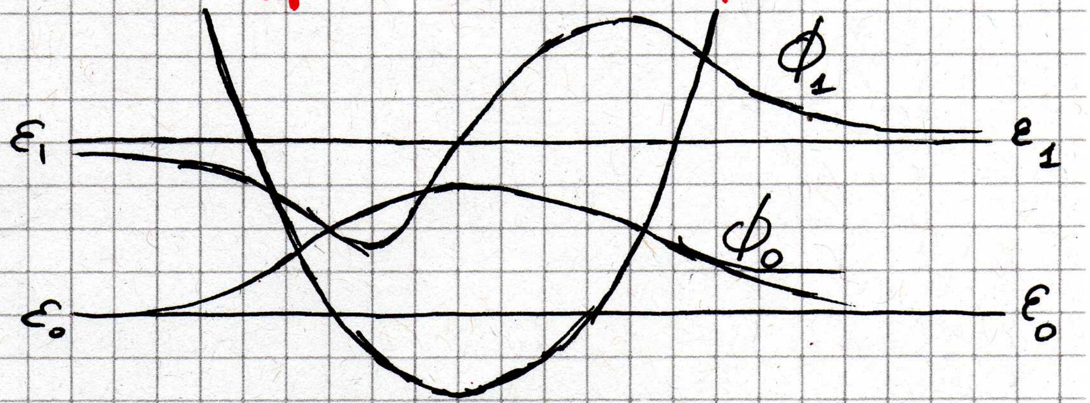
$$\varepsilon \sim \sqrt{\varepsilon_{roundoff}}\,\sqrt{|f|\,|f^{iv}|}$$

single precision $\varepsilon_r \sim 10^{-8}$ $\varepsilon \sim 10^{-4}$

double precision $\varepsilon_r \sim 10^{-16}$ $\varepsilon \sim 10^{-8}$

Numerical Integration of a Differential Equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\phi(x) + \left[V(x) - \varepsilon\right]\phi(x) = 0$$



$V(x) \to +\infty$ when $x \to \pm\infty$

looking for Bound States

$\phi_n(x) \to 0$ when $x \to \pm\infty$

ε_n **Discrete spectrum of energy levels**

- Hydrogen Atom

$$V(|r|) = -\frac{e^2}{|r|} \qquad \varepsilon_{n\ell m} = -\frac{e^2}{2a_0}\frac{1}{n^2} \qquad \phi_{n\ell m}(\vec{r}) = f_{n\ell}(r)\,Y_{\ell m}(\hat{r})$$

- Harmonic Oscillator

$$V(x) = \frac{1}{2}m\omega_0^2 x^2 \qquad \varepsilon_n = \hbar\omega_0\left(n+\frac{1}{2}\right) \qquad \phi_n(x) = H_n(x)\,e^{-\alpha x^2}$$

- .... and for a generic $V(x)$?

K1

Numerical Integration of an ODE

- use atomic (scaled) units

$$\left[\begin{array}{ll} \hbar = 1 & \omega^2 = 1 \\ m = 1 & \end{array}\right]$$

$$-\frac{\hbar^2}{2m}\frac{d^2\phi(x)}{dx^2} + \left[\frac{m\omega^2}{2}x^2 - \varepsilon\right]\phi(x) = 0$$

$$\tilde{x} = \sqrt{\frac{m\omega}{\hbar}}\,x \qquad \tilde{\varepsilon} = \frac{\varepsilon}{\hbar\omega}$$

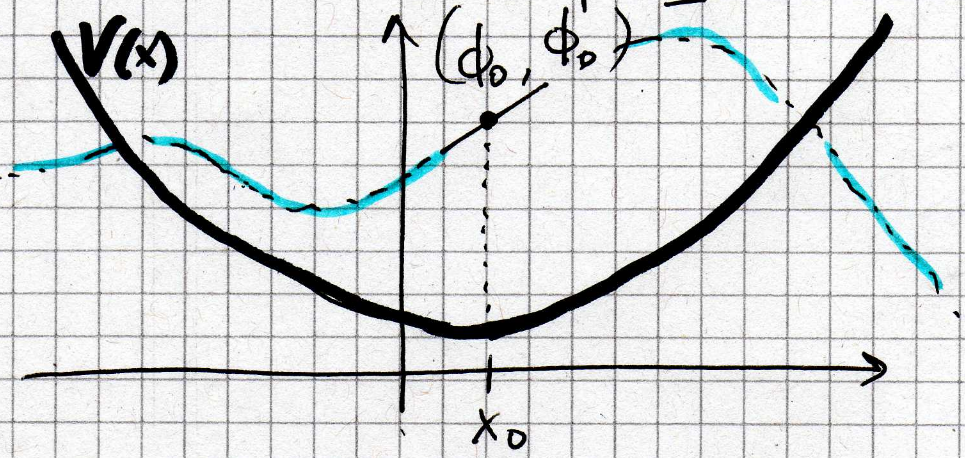
$$\frac{\partial}{\partial\tilde{x}} = \sqrt{\frac{\hbar}{m\omega}}\,\frac{\partial}{\partial x}$$

$$-\frac{1}{2}\frac{d^2}{d\tilde{x}^2}\phi + \left[\frac{\tilde{x}^2}{2} - \tilde{\varepsilon}\right]\phi = 0$$

It is a good idea to scale the position an energy units so not to deal with exceedingly large (or small) quantities

$$\phi''(x) = 2\left[V(x) - \varepsilon\right]\phi$$

linear homogeneous 2^{nd} order differential equation



$\forall \varepsilon$ there are two linearly independent mathematical solutions (an all their linear combinations)

We are interested in the discrete set of ε_n for which a solution exists that is NOT diverging for $x \to -\infty$ AND $x \to +\infty$

in case of Symmetry: $V(x) = V(-x)$
$\Longrightarrow \phi(x) = \pm \phi(-x)$

ε_0 GS is nodeless — ϕ symmetric

ε_1 1st excited state has 1 node — ϕ antisymmetric — 1 node in 0

ε_2 2nd excited state has 2 nodes — ϕ symmetric — 1 node in $(0, +\infty)$

ε_3 3rd excited state has 3 nodes — ϕ antisymmetric — 1 node in 0, 1 node in $(0, +\infty)$

$\vdots$

If ε is known

$$\left[V(x) = \frac{m\omega^2}{2} x^2 \qquad \varepsilon_n = \hbar\omega\left(n+\frac{1}{2}\right) \right]$$

$$\phi''(x) = 2\left[V(x) - \varepsilon\right]\phi(x)$$

$x_i = i\,\Delta x \qquad \phi_i = \phi(x_i) \qquad V_i = V(x_i) \qquad i = 0, 1, \dots, N \quad X_{MAX} = N\Delta x$

$$\frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2} = 2(V_i - \varepsilon)\,\phi_i + O(\Delta x^2)$$

$$\phi_{i+1} - 2\phi_i + \phi_{i-1} = 2\,\Delta x^2 (V_i - \varepsilon)\,\phi_i + \cancel{O(\Delta x^4)}$$ local error

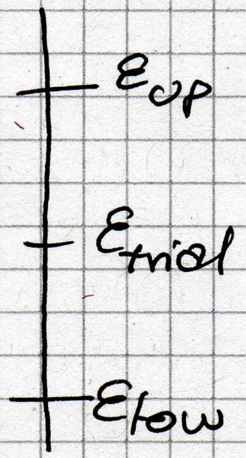
three-point recurrence: given initial conditions in 2 points $\left(\begin{matrix}\phi_0\ \phi'_0 \ \underline{\text{or}} \\ \phi_0\ \phi_1\end{matrix}\right)$
one can integrate outward the solution

INITIAL CONDITIONS

Antisymmetric Solution	Symmetric Solution
$\phi_0 = 0$ (a node in 0!)	$\phi_0 = 1$ (or anything to be rescaled later)
$\phi_1 = \Delta x$ (or anything to be rescaled later)	feed $\phi_1 = \phi_{-1}$ into $3pt$ recurrence
	$\phi_1 = \phi_0 + \Delta x^2 (V_0 - \varepsilon)\,\phi_0$

And if ε is NOT known?

- **shooting method**: given a trial ε integrate the eq.
  - if the # of nodes in the interval $(0, +x_{MAX})$ is larger than expected, ε is too large: reduce it
  - if the # of nodes is smaller than desired (or correct but the solution does NOT decay for $x \to x_{MAX}$), ε is too small: increase it
- **bisection**: 0) start by defining an upper and a lower bound for ε



1) define $\varepsilon_{trial} = \dfrac{\varepsilon_{up} + \varepsilon_{low}}{2}$

2) integrate and count the nodes

3) redefine the bounds according to node count

$n_{node} > n \to \varepsilon_{up} = \varepsilon_{trial}$

$n_{node} \leq n \to \varepsilon_{low} = \varepsilon_{trial}$

4) Iterate (go back to 1) until

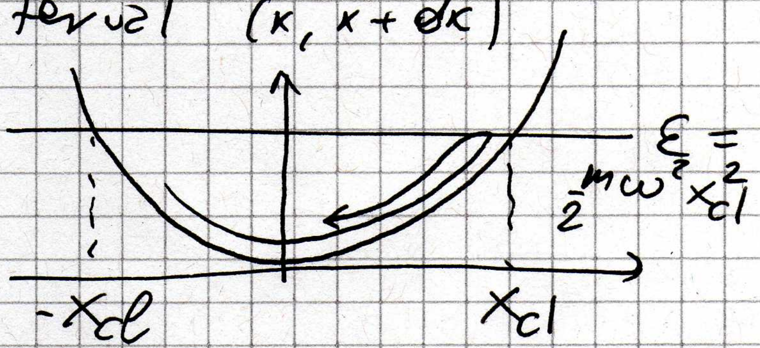
$|\varepsilon_{up} - \varepsilon_{low}| < \text{Epsilon}$

Renormalize and Compare with Classical result

- Renormalize: compute the integral by trapezoidal rule and rescale the solution by $1/\sqrt{\int |\phi|^2 dx}$
Less trivial than you think...

- Classical probability

$p(x)\,dx$ = fraction of time spent in the interval $(x, x+dx)$



$$p(x)\,dx \propto \frac{dt}{dx}\,dx \sim \frac{dx}{|v|}$$

$$p(x)\,\Delta x = \frac{\Delta t}{T/2} = \frac{2}{T}\frac{1}{|v|}\Delta x$$

$$\frac{mv^2}{2} + \frac{m\omega^2 x^2}{2} = \varepsilon = \frac{m\omega^2}{2} x_{cl}^2$$

$$p(x) = \frac{1}{\pi}\frac{1}{\sqrt{x_{cl}^2 - x^2}}$$

$$|v| = \omega\sqrt{x_{cl}^2 - x^2}$$

$$\omega = \frac{2\pi}{T}$$

Integrate with a better local error

Numerov's method

$$\phi''(x) = f(x)\,\phi(x) \qquad \left[f(x) = 2\,(V(x) - \varepsilon) \right]$$

$$\phi_{i+1} = \phi_i + \phi_i'\,\Delta x + \phi_i''\,\frac{\Delta x^2}{2} + \phi_i'''\,\frac{\Delta x^3}{3!} + \phi_i^{IV}\,\frac{\Delta x^4}{4!} + \phi_i^{V}\,\frac{\Delta x^5}{5!} + O(\Delta x^6)$$

$$\phi_{i-1} = \phi_i - \phi_i'\,\Delta x + \phi_i''\,\frac{\Delta x^2}{2} - \phi_i'''\,\frac{\Delta x^3}{3!} + \phi_i^{IV}\,\frac{\Delta x^4}{4!} - \phi_i^{V}\,\frac{\Delta x^5}{5!} + O(\Delta x^6)$$

$$\phi_{i+1} + \phi_{i-1} - 2\phi_i = \Delta x^2 \phi_i'' + \phi_i^{IV}\,\frac{\Delta x^4}{12} + O(\Delta x^6)$$

$$\downarrow$$

$$\left(\frac{\phi_{i+1}'' + \phi_{i-1}'' - 2\phi_i''}{\Delta x^2} + O(\Delta x^2) \right)$$

$$\phi_{i+1} + \phi_{i-1} - 2\phi_i = \Delta x^2 f_i\,\phi_i + \left(\frac{\Delta x^2 f_{i+1}}{12}\,\phi_{i+1} + \frac{\Delta x^2 f_{i-1}}{12}\,\phi_{i-1} - \frac{2\Delta x^2 f_i \cdot \phi_i}{12} \right) + O(\Delta x^6)$$

$$\phi_{i+1}\,\tilde{f}_{i+1} + \phi_{i-1}\,\tilde{f}_{i-1} = \left[12 - 10\tilde{f}_i \right] \phi_i \qquad \tilde{f}_i = 1 - \frac{\Delta x^2}{12} f_i$$

three-point recurrence with a smaller local error (Δx^6)