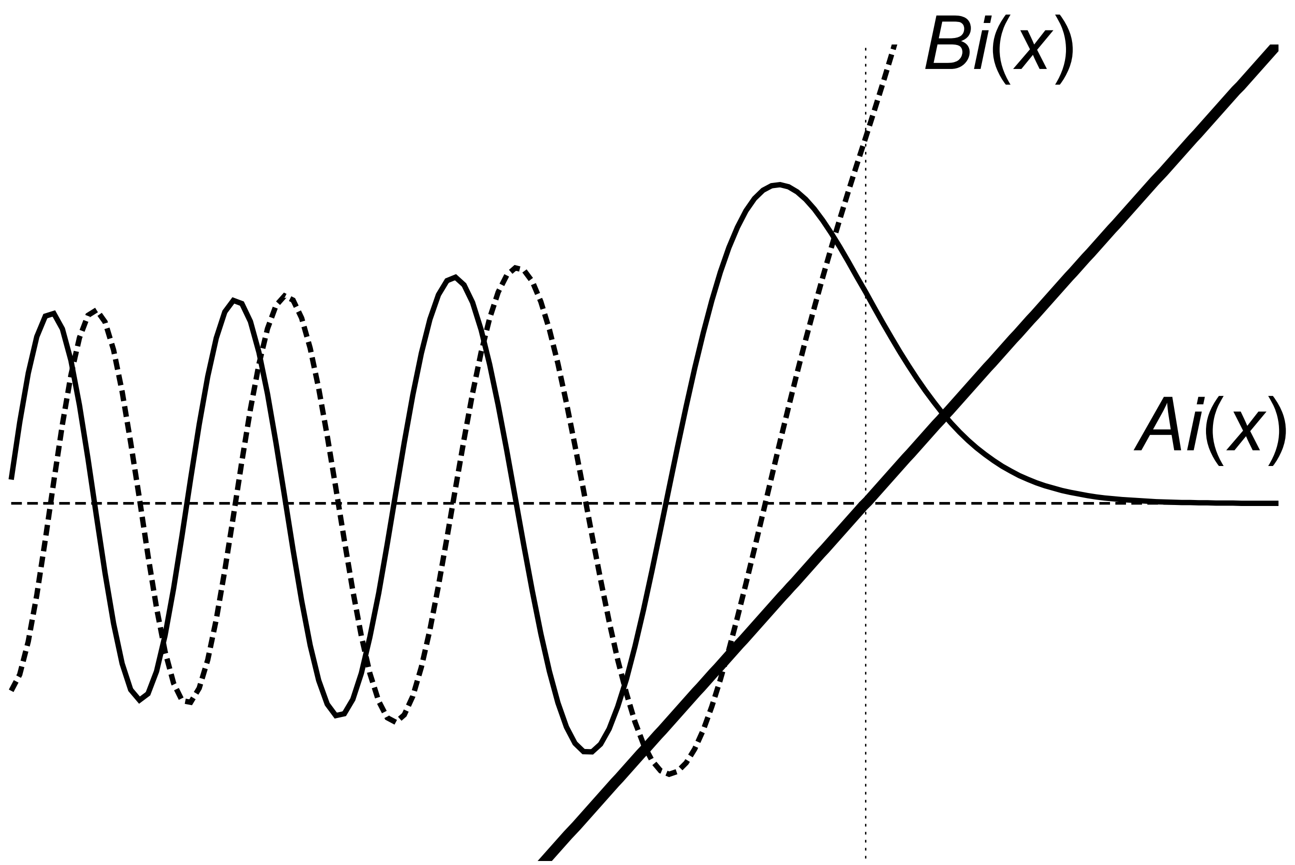
homogeneous field



$$-\frac{d^2\varphi}{dx^2} + x\,\varphi = E\varphi$$

$$\varphi(x) = Ai(x-E)$$
$$\varphi(x) = Bi(x-E)$$

asymptotics

$$\mathrm{Ai}(-x) \sim \frac{\cos\left(\frac{2}{3}(-x)^{3/2} + \pi/4\right)}{\sqrt{\pi\sqrt{x}}} \qquad \mathrm{Ai}(x) \sim \frac{\exp\left(-\frac{2}{3}x^{3/2}\right)}{2\sqrt{\pi\sqrt{x}}}$$

$$\mathrm{Bi}(-x) \sim -\frac{\sin\left(\frac{2}{3}(-x)^{3/2} - \pi/4\right)}{\sqrt{\pi\sqrt{x}}} \qquad \mathrm{Bi}(x) \sim \frac{\exp\left(+\frac{2}{3}x^{3/2}\right)}{\sqrt{\pi\sqrt{x}}}$$

NIST Handbook of Mathematical Functions

DLMF: 9 Airy and Related Functions

http://dlmf.nist.gov/9

work Ref local Comp Journals conf Lect priv News 2Papers GReaderShare ReadLater Readability

DLMF: 9 Airy and Related Functions

Digital Library of Mathematical Functions

- Index
- Notations
- Search
- Need Help?
- How to Cite
- Customize
- Annotate

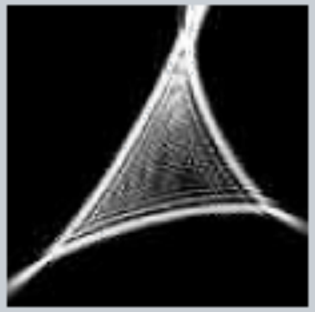
About the Project

NIST National Institute of Standards and Technology

Chapter 9. Airy and Related Functions

F. W. J. Olver

Institute for Physical Science and Technology and Department of Mathematics, University of Maryland, College Park, Maryland.



http://dlmf.nist.gov/

numerical differentiation

task: evaluate *f'(x)*, only knowing *f(x)* at some specified abscissae x_i

idea: approximate *f* by a function that can be easily differentiated, e.g., a Taylor expansion. Then combine the $f(x_i)$ such that – except for the desired derivative – as many terms as possible are cancelled.

example: first derivative

$$\begin{aligned} f(x_0+h) &= f(x_0) + h\,f'(x_0) + \frac{h^2}{2}\,f''(x_0) + \frac{h^3}{6}\,f'''(x_0) + \mathcal{O}(h^4) \\ f(x_0) &= f(x_0) \\ f(x_0-h) &= f(x_0) - h\,f'(x_0) + \frac{h^2}{2}\,f''(x_0) - \frac{h^3}{6}\,f'''(x_0) + \mathcal{O}(h^4) \end{aligned}$$

Then $\quad f(x_0+h) - f(x_0-h) = 2h\,f'(x_0) + \frac{h^3}{3}\,f'''(x_0) + \mathcal{O}(h^4)$

or $\quad f'(x_0) = \frac{f(x_0+h) - f(x_0-h)}{2h} + \mathcal{O}(h^3)$

numerical differentiation

Approximations to 1st derivative:

$$f'(x_0) = \frac{f(x_0+h)-f(x_0)}{h} + \mathcal{O}(h)$$

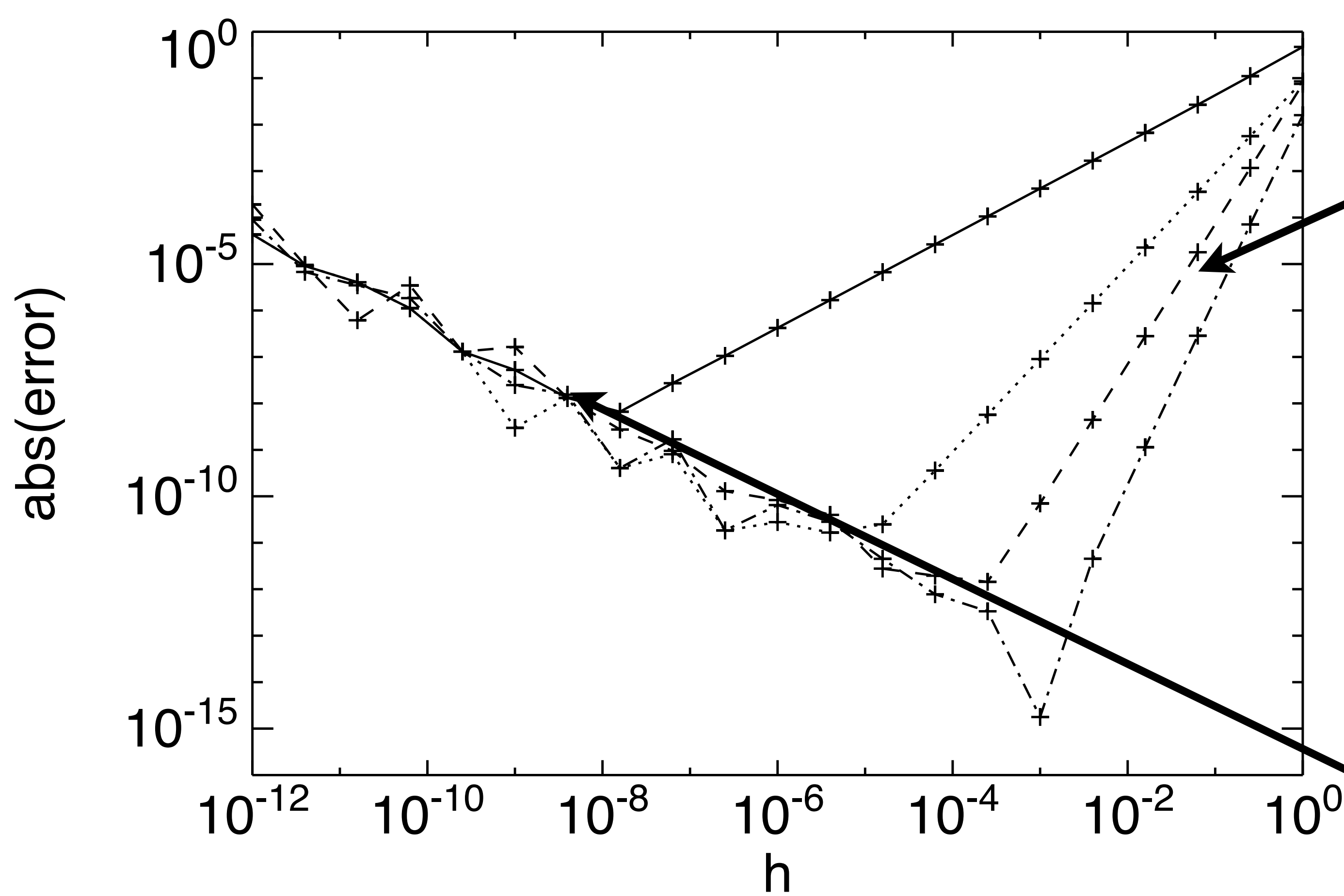
$$f'(x_0) = \frac{f(x_0+h)-f(x_0-h)}{2h} + \mathcal{O}(h^2)$$

$$f'(x_0) = \frac{-f(x_0+2h)+6f(x_0+h)-3f(x_0)-2f(x_0-h)}{6h} + \mathcal{O}(h^3)$$

$$f'(x_0) = \frac{-f(x_0+2h)+8f(x_0+h)-8f(x_0-h)+f(x_0-2h)}{12h} + \mathcal{O}(h^4)$$

differences of similar numbers in numerator & small denominator

example: $\sin(x)$, $x_0 = 1$



O(h^n) error from approximation

ε/h error from finite machine accuracy *ε*

method of undetermined coefficients

idea: given a set of abscissae x_n, e.g., $x_n=x_0+nh$, n=-1, 0, 1, 2, make an ansatz with undetermined coefficients, e.g.,:

$$f'(x_0) = \frac{\alpha_{-1} f(x_{-1}) + \alpha_0 f(x_0) + \alpha_1 f(x_1) + \alpha_2 f(x_2)}{h}$$

determine the coefficients α_i by requiring that the formula differentiates polynomials of order, e.g., 0 to 3 exactly by solving the resulting system of linear equations

Maple session:

```
> with(linalg):
> n := 1: # formula for nth derivative
> mesh := [x0-h, x0, x0+h, x0+2*h]; p := nops(mesh): # abscissae x_i
```

$$mesh := [x0-h, x0, x0+h, x0+2h]$$

```
> f_x := array([seq(map(x -> x^k, mesh), k=0..p-1)]); # evaluate monomials on mesh
```

$$f\_x := \begin{bmatrix} 1 & 1 & 1 & 1 \\ x0-h & x0 & x0+h & x0+2h \\ (x0-h)^2 & x0^2 & (x0+h)^2 & (x0+2h)^2 \\ (x0-h)^3 & x0^3 & (x0+h)^3 & (x0+2h)^3 \end{bmatrix}$$

```
> der_f := array([seq(binomial(k, n)*n!*x0^(k-n), k=0..p-1)]);
     # derivative of monomials
```

$$der\_f := \begin{bmatrix} 0 & 1 & 2\,x0 & 3\,x0^2 \end{bmatrix}$$

```
> coefficients := linsolve(f_x, der_f); # coefficients alpha_i
```

$$coefficients := \begin{bmatrix} -\frac{1}{3h} & -\frac{1}{2h} & \frac{1}{h} & -\frac{1}{6h} \end{bmatrix}$$

Numerov method

one-dimensional Schrödinger equation

$$u''(x) + k^2(x)u(x) = 0 \quad \text{where } k^2(x) = \frac{2m}{\hbar^2}(E - V(x))$$

numerical derivative

$$f''(x_0) = \frac{f(x_0+h) - 2f(x_0) + f(x_0-h)}{h^2} - \frac{h^2}{12} f^{(4)}(x_0) + \mathcal{O}(h^4)$$

two-point iteration of wave function *u(x$_j$)*:

$$u_{j+1} = (2 - h^2 k_j^2)\, u_j - u_{j-1} + \mathcal{O}(h^4)$$

Numerov trick:

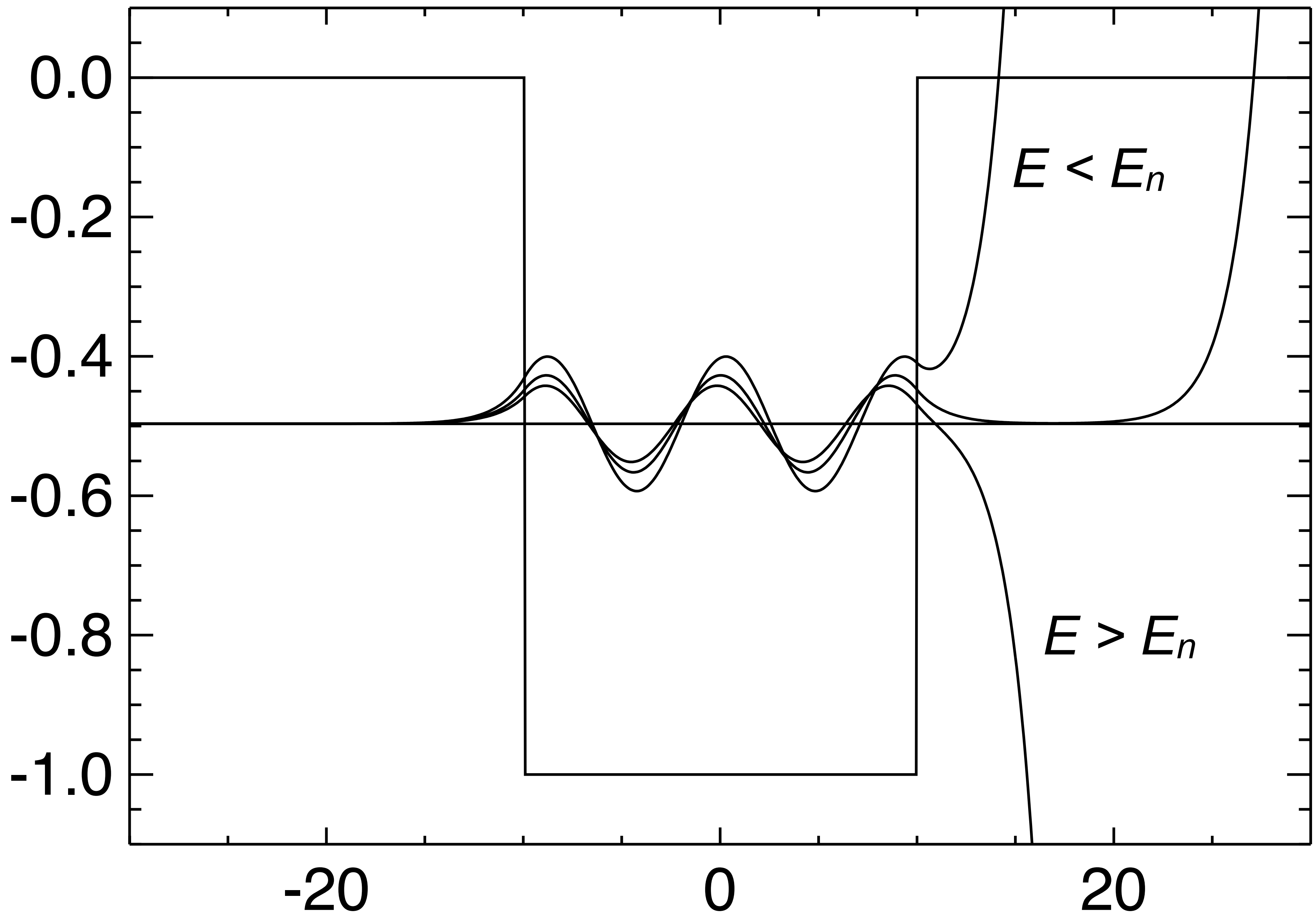
remove leading error in derivative formula by using Schrödinger equation

$$-\frac{h^2}{12} u^{(4)}(x_j) + \mathcal{O}(h^4) = +\frac{h^2}{12}\frac{d^2}{dx^2}\left(k^2(x_j)u(x_j)\right) + \mathcal{O}(h^4) = \frac{k_{j+1}^2 u_{j+1} - 2k_j^2 u_j + k_{j-1}^2 u_{j-1}}{12} + \mathcal{O}(h^4)$$

Numerov iteration:

$$u_{j+1} = \frac{2(1 - 5h^2 k_j^2/12)u_j - (1 + h^2 k_{j-1}^2/12)u_{j-1}}{1 + h^2 k_{j+1}^2/12} + \mathcal{O}(h^6)$$

Numerov iteration close to eigenvalue



$E > V(x)$
φ convex

$E > V(x)$
φ concave

(in)stability of Numerov iteration