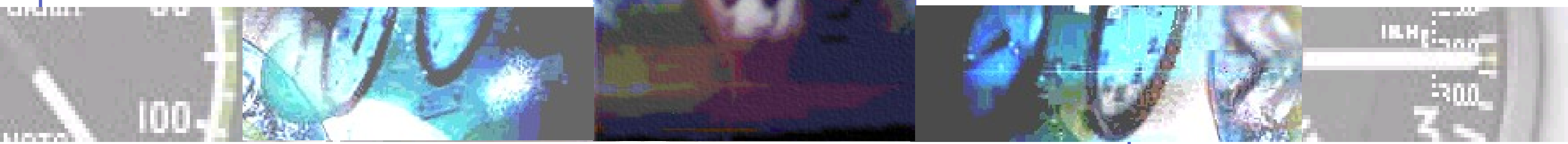
Numerical Differentiation

A Short Introduction



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Numerical Differentiation / Derivatives

- **Content**
  - Basic Definitions and Formulas
  - Error terms and optimal step size
  - Some difference formulas
  - Partial derivatives
  - Higher derivatives
  - Lagrange Interpolation
  - Richardson‘s extrapolation
  - Complex-step approximate derivatives
  - Example

  - Automated differentiation
  - Symbolic differentiation
  - Software

Numerical Derivatives in General

- **What**

  Numerical differentiation computes (or estimates) the derivatives or ‘slope‘ of a function by calculating function values at only a set of discrete points.

- **Why**

  Derivative in explicit functional form may not be available:

  - error prone differentiation by hand, or functions as variables
  - using functions with unknown derivatives, or available only as finite sets of points
  - blackbox functions (i.e. engineering procedures)

- **When**

  The evaluation or approximation of derivatives plays a central part in many applications:

  - design engineering
  - simulation of dynamical systems (e.g. weather forecast)
  - numerically solving differential equations
  - non-linear optimization problems (Kuhn-Tucker conditions, Hessian)

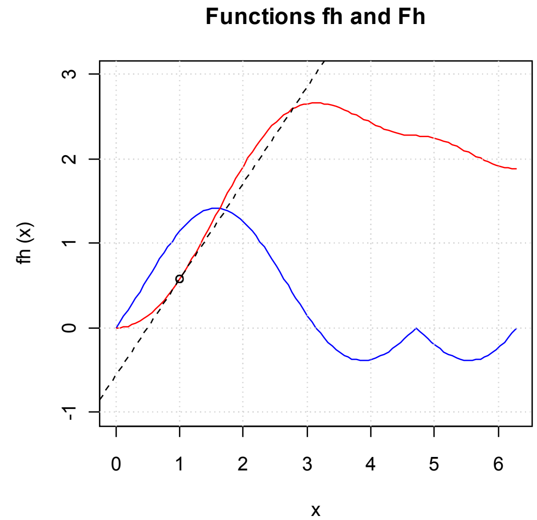
Example

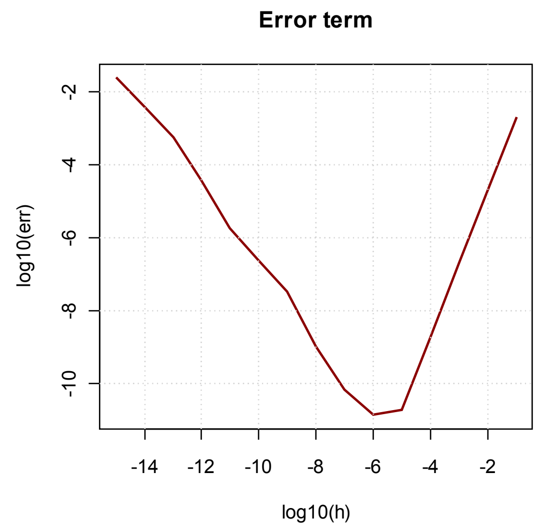
$$Fh(x) = \int_0^x \sin(t)\sqrt{1+\sin(t)}\,dt$$

is the antiderivative of

$$fh(x) = \sin(x)\sqrt{1+\sin(x)}$$

Determine as exactly as possible the derivative at $x_0 = 1$.





Method	Value	Difference
True value	1.14188294271546	$1.0\ 10^{-15}$
Forward difference formula	1.14188298816487	$4.5\ 10^{-8}$
Central difference formula	1.14188294264572	$0.7\ 10^{-10}$
Forward three point	1.14188294486617	$2.0\ 10^{-9}$
Central four point	1.14188294246069	$2.5\ 10^{-10}$
Richardson	1.14188294271225	$3.0\ 10^{-12}$
Complex-step		

Basic Formulas and Error terms

- **Forward difference formula**

$$f'(x_0) \approx \frac{f(x_0+h)-f(x_0)}{h}, 0<h<<1$$

- **Central difference formula**

$$f'(x_0) \approx \frac{f(x_0+h)-f(x_0-h)}{2h}, 0<h<<1$$

- **Four-point central difference formula**

$$f'(x_0) \approx \frac{-f(x_0+2h)+8f(x_0+h)}{12h} + \frac{-8f(x_0-h)+f(x_0-2h)}{12h} + O(h^4),$$
$$0<h<<1$$

- **Optimal step size and accuracy of forward difference formula**

$\varepsilon_m, \varepsilon_f$ machine, function accuracy

$$h \sim \sqrt{\varepsilon_f}\sqrt{\frac{|f|}{|f''|}} \sim \sqrt{\varepsilon_f}$$ step size

e_t, e_r truncation, roundoff error

$$e_t + e_r \sim 2\sqrt{\varepsilon_f}\sqrt{|f||f''|} \sim \sqrt{\varepsilon_f}$$

- **and central difference formula**

$$h \sim \varepsilon_f^{1/3}$$
$$e_t + e_r \sim \varepsilon_f^{2/3}$$

Higher Derivatives

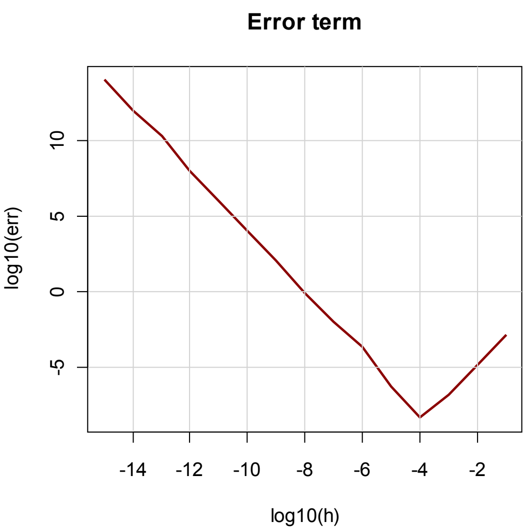
- **Centered Difference Formulas**

$$f''(x_0) \approx \frac{1}{h^2}[f(x_0+h) - 2f(x_0) + f(x_0-h)]$$

$$f'''(x_0) \approx \frac{1}{2h^3}[f(x_0+2h) - 2f(x_0+h) + 2f(x_0-h) - f(x_0-2h)]$$

$$f^{(4)}(x_0) \approx \frac{1}{h^4}[f(x_0+2h) - 4f(x_0+h) + 6f(x_0) - 4f(x_0-h) + f(x_0-2h)]$$

These formulas are all $O(h^2)$ and are easily verified by applying the Taylor series.



$h = 10^{-4}$
error = $4.5\ 10^{-9}$

Partial Derivatives

- **Usages**
  - Partial derivative

$$\frac{\partial f}{\partial x_i} \approx \frac{f(x_1,\dots,x_i+h,\dots,x_n)-f(x_1,\dots,x_i-h,\dots,x_n)}{2h}$$

  - Jacobian matrix $\left(\frac{\partial f_i}{\partial x_j}\right)_{1\le i\le m, 1\le j\le m}$
  - Laplacian operator

$$\nabla^2 f = f_{xx} + f_{yy}$$

  - Biharmonic operator

$$\nabla^4 f = f_{xxxx} + f_{xxyy} + f_{yyyy}$$

  - Hessian matrix

$$H(f)_{ij}(x) = \frac{\partial^2 f}{\partial x_i \partial x_j}(x)$$

$$f(x+\Delta x) \approx f(x) + J(x)\Delta x + \frac{1}{2}\Delta x^T H(x)\Delta x$$

- **Higher partial derivatives**

$$u_{xx}(x_0, y_0) \approx ¿$$

$$¿\frac{1}{h^2}[u(x_0-h, y_0) - 2u(x_0, y_0) + u(x_0+h, y_0)]$$

$$u_{xy}(x_0, y_0) \approx \frac{1}{4h^2}[$$

$$-u(x_0-h, y_0+h) + u(x_0+h, y_0+h)$$

$$+u(x_0-h, y_0-h) - u(x_0+h, y_0-h)]$$

$$\nabla^2 u(x_0, y_0) \approx \frac{1}{h^2}[$$

$$u(x_0, y_0+h) +$$

$$u(x_0-h, y_0) - 4u(x_0, y_0) + u(x_0+h, y_0) +$$

$$u(x_0, y_0-h)]$$

Discretized Functions

- **Lagrange interpolation**

$$(x_1, y_1), (x_2, y_2), (x_3, y_3)$$
$$f(x_i) = y_i$$
$$L(x) = L_1(x)\, y_1 + L_2(x)\, y_2 + L_3(x)\, y_3$$
$$L_1(x) = \frac{(x-x_2)(x-x_3)}{(x_1-x_2)(x_1-x_3)}, \ldots$$
$$f'(x) \approx L'(x) = L_1'(x)\, y_1 + L_2'(x)\, y_2 + L_3'(x)\, y_3$$
$$L_1'(x) = \frac{2\mathrm{x} - x_2 - x_3}{(x_1-x_2)(x_1-x_3)}, \ldots$$

- **Example: Three-point forward difference formula**

$$x_1 = x_0,\ x_2 = x_0 + h,\ x_3 = x_0 + 2\mathrm{h}$$
$$L'(x_1) = \frac{-3\mathrm{f}(x_1) + 4\mathrm{f}(x_1 + h) - f(x_1 + 2\mathrm{h})}{2\mathrm{h}}$$
$$f'(x_0) \approx \frac{-f(x_0 + 2\mathrm{h}) + 4\mathrm{f}(x_0 + h) - 3\mathrm{f}(x_0)}{2\mathrm{h}}$$

- **Other approximations: Spline, etc.**

Richardson‘s Derivative Approximation

- **Richardson extrapolation:**

$$\varphi(h) = \frac{1}{2h}\left[f(x_0+h) - f(x_0-h)\right]$$

$$\varphi(h) = f'(x_0) + a_2 h^2 + a_4 h^4 + a_6 h^6 + \ldots$$

$$f'(x_0) = \frac{4\varphi(\frac{h}{2}) - \varphi(h)}{3} + O(h^4)$$

- **Neville‘s tableaux**

n\m	0	1	2
0	D(0,0)		
1	D(1,0) ←	D(1,1)	
2	D(2,0)	D(2,1)	D(2,2)

$$D(n,0) = \varphi\left(\frac{h}{2^n}\right)$$

$$D(n,m) = \frac{4^m D(n,m-1) - D(n-1,m-1)}{4^m - 1}$$

- **Ridders‘ implementation**

Compute D(n,n) until

$$|D(n+1,n+1) - D(n,n)| \geq |D(n,n) - D(n-1,n-1)|, or$$

$$|D(n+1,n+1) - D(n,n)| \leq tolerance, or$$

$$n+1 > \max number.of.steps$$

Complex-step Derivative Approximation

- **Compex-step derivative**

$$f'(x_0)=\frac{\mathrm{Im}(f(x_0+h\cdot i))}{h}+O(h^2)$$

- **Remark**

  Almost no loss of accuracy (no roundoff error)

- **Proof**
  - Complex Taylor series

- **Assumptions**
  - *f* can be analytically continued into a neighborhood of x_0
  - $f(x_0)$ is real
  - $0 < h << 1$ real
- **Settings**
  - $\varepsilon_{f'}=\varepsilon_f$
  - *h* can be arbitrarily small e.g. take $h=\varepsilon_m$
- **Recent successes (since 2000):**
  - Aerodynamics
  - Wheather forecast
  - Molecular modeling

Other Approaches

- **Automated Differentiation**

  Automated or Automatic Differentiation (AD) is a method for automatically augmenting or wrapping numerical procedures with statements for computing their derivatives.
  Especially useful in combination with complex-step derivative approximation.

- **Symbolic Differentiation**

  Symbolic differentiation is provided by most Computer Algebra Systems (CAS). Such a program finds the derivative of a given formula w.r.t. a specified variable, producing a new formula as output.
  Together with high-precision arithmetic, this approach delivers exact derivatives.

Software and Literature

- **Software**
  - Matlab

    Richardson extrapolation automated differentiation

    (from Mathtools.net)
  - Octave
  - Scilab
  - ***R***

    Richardson extrapolation and in optimization routines
  - Euler, w/ Maxima

    Arbitrary-precision arithmetic symbolic algebra
  - Netlib
    Fortran/C implementations

- **Literature**

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