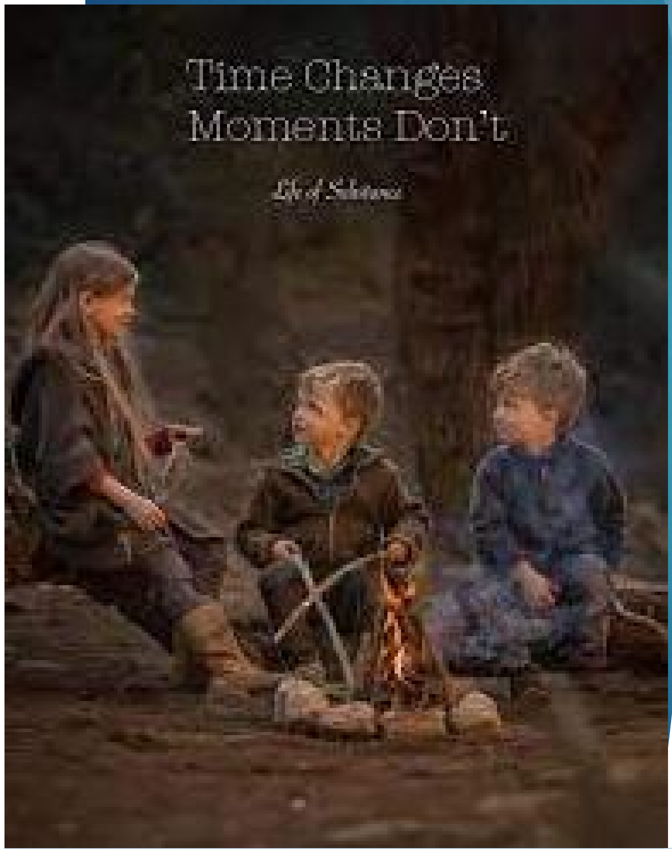
Computational Methods

NUMERICAL DIFFERENTIATION AND NUMERICAL INTEGRATION

QUOTE



Numerical Differentiation

The derivative of the function f at x_0 is

$$f'(x_0) = \lim_{h \to 0} \frac{f(x_0 + h) - f(x_0)}{h}.$$

This formula gives an obvious way to generate an approximation to $f'(x_0)$; simply compute

$$\frac{f(x_0 + h) - f(x_0)}{h}$$

for small values of h. Although this may be obvious, it is not very successful, due to our old nemesis round-off error. But it is certainly a place to start.

Numerical Differentiation

The formula simplifies to

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} - \frac{h}{2} f''(\xi).$$

For small values of h, the difference quotient $[f(x_0 + h) - f(x_0)]/h$ can be used to approximate $f'(x_0)$ with an error bounded by $M|h|/2$, where M is a bound on $|f''(x)|$ for x between x_0 and $x_0 + h$. This formula is known as the **forward-difference formula** if $h > 0$ and the **backward-difference formula** if $h < 0$.

Numerical Differentiation

Use the forward-difference formula to approximate the derivative of $f(x) = \ln x$ at $x_0 = 1.8$ using $h = 0.1$, and determine bounds for the approximation errors.

Solution The forward-difference formula

$$\frac{f(1.8 + h) - f(1.8)}{h}$$

with $h = 0.1$ gives

$$\frac{\ln 1.9 - \ln 1.8}{0.1} = \frac{0.64185389 - 0.58778667}{0.1} = 0.5406722.$$

Because $f''(x) = -1/x^2$ and $1.8 < \xi < 1.9$, a bound for this approximation error is

$$\frac{|hf''(\xi)|}{2} = \frac{|h|}{2\xi^2} < \frac{0.1}{2(1.8)^2} = 0.0154321.$$

Numerical Differentiation

Three-Point Endpoint Formula

- $f'(x_0) = \frac{1}{2h}[-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)] + \frac{h^2}{3} f^{(3)}(\xi_0),$

where ξ_0 lies between x_0 and $x_0 + 2h$.

Three-Point Midpoint Formula

- $f'(x_0) = \frac{1}{2h}[f(x_0 + h) - f(x_0 - h)] - \frac{h^2}{6} f^{(3)}(\xi_1),$

where ξ_1 lies between $x_0 - h$ and $x_0 + h$.

Numerical Differentiation

Values for $f(x) = xe^x$ are given in Table. Use all the applicable three-point formulas to approximate $f'(2.0)$.

x	$f(x)$
1.8	10.889365
1.9	12.703199
2.0	14.778112
2.1	17.148957
2.2	19.855030

Solution The data in the table permit us to find four different three-point approximations. We can use the endpoint formula with $h = 0.1$ or with $h = -0.1$, and we can use the midpoint formula with $h = 0.1$ or with $h = 0.2$.

Numerical Differentiation

Using the endpoint formula with $h = 0.1$ gives

$$\frac{1}{0.2}[-3f(2.0) + 4f(2.1) - f(2.2] = 5[-3(14.778112) + 4(17.148957) \\ - 19.855030)] = 22.032310,$$

and with $h = -0.1$ gives 22.054525.

Using the midpoint formula with $h = 0.1$ gives

$$\frac{1}{0.2}[f(2.1) - f(1.9)] = 5(17.148957 - 12.7703199) = 22.228790,$$

and with $h = 0.2$ gives 22.414163.

Numerical Differentiation

Second Derivative Midpoint Formula

- $$f''(x_0) = \frac{1}{h^2}[f(x_0 - h) - 2f(x_0) + f(x_0 + h)] - \frac{h^2}{12} f^{(4)}(\xi),$$

for some ξ, where $x_0 - h < \xi < x_0 + h$.

In Example we used the data shown in Table to approximate the first derivative of $f(x) = xe^x$ at $x = 2.0$. Use the second derivative formula to approximate $f''(2.0)$.

x	$f(x)$
1.8	10.889365
1.9	12.703199
2.0	14.778112
2.1	17.148957
2.2	19.855030

Numerical Differentiation

Solution The data permits us to determine two approximations for $f''(2.0)$. Using $h = 0.1$ gives

$$\frac{1}{0.01}[f(1.9) - 2f(2.0) + f(2.1)] = 100[12.703199 - 2(14.778112) + 17.148957]$$
$$= 29.593200,$$

and using $h = 0.2$ gives

$$\frac{1}{0.04}[f(1.8) - 2f(2.0) + f(2.2)] = 25[10.889365 - 2(14.778112) + 19.855030]$$
$$= 29.704275.$$

Numerical Integration

Trapezoidal Rule:

$$\int_a^b f(x)\,dx = \frac{h}{2}[f(x_0) + f(x_1)] - \frac{h^3}{12} f''(\xi).$$

Simpson's Rule:

$$\int_{x_0}^{x_2} f(x)\,dx = \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{90} f^{(4)}(\xi).$$

with equally-spaced nodes $x_0 = a$, $x_2 = b$, and $x_1 = a + h$, where $h = (b - a)/2$.

Numerical Integration

Compare the Trapezoidal rule and Simpson's rule approximations to $\int_0^2 f(x)\,dx$ when $f(x)$ is

(a) x^2 **(b)** x^4 **(c)** $(x+1)^{-1}$
(d) $\sqrt{1+x^2}$ **(e)** $\sin x$ **(f)** e^x

Solution On [0, 2] the Trapezoidal and Simpson's rule have the forms

$$\text{Trapezoid: } \int_0^2 f(x)\,dx \approx f(0) + f(2) \quad \text{and}$$

$$\text{Simpson's: } \int_0^2 f(x)\,dx \approx \frac{1}{3}[f(0) + 4f(1) + f(2)].$$

Numerical Integration

When $f(x) = x^2$ they give

$$\text{Trapezoid:} \quad \int_0^2 f(x)\, dx \approx 0^2 + 2^2 = 4 \quad \text{and}$$

$$\text{Simpson's:} \quad \int_0^2 f(x)\, dx \approx \frac{1}{3}[(0^2) + 4 \cdot 1^2 + 2^2] = \frac{8}{3}.$$

The approximation from Simpson's rule is exact because its truncation error involves $f^{(4)}$, which is identically 0 when $f(x) = x^2$.

	(a)	(b)	(c)	(d)	(e)	(f)
$f(x)$	x^2	x^4	$(x+1)^{-1}$	$\sqrt{1+x^2}$	$\sin x$	e^x
Exact value	2.667	6.400	1.099	2.958	1.416	6.389
Trapezoidal	4.000	16.000	1.333	3.326	0.909	8.389
Simpson's	2.667	6.667	1.111	2.964	1.425	6.421

Exercises

Use the forward-difference formulas and backward-difference formulas to determine each missing entry in the following tables.

a.

x	$f(x)$	$f'(x)$
0.5	0.4794	
0.6	0.5646	
0.7	0.6442	

b.

x	$f(x)$	$f'(x)$
0.0	0.00000	
0.2	0.74140	
0.4	1.3718	

Exercises

Use the most accurate three-point formula to determine each missing entry in the following tables.

a.

x	$f(x)$	$f'(x)$
1.1	9.025013	
1.2	11.02318	
1.3	13.46374	
1.4	16.44465	

b.

x	$f(x)$	$f'(x)$
8.1	16.94410	
8.3	17.56492	
8.5	18.19056	
8.7	18.82091	

c.

x	$f(x)$	$f'(x)$
2.9	−4.827866	
3.0	−4.240058	
3.1	−3.496909	
3.2	−2.596792	

d.

x	$f(x)$	$f'(x)$
2.0	3.6887983	
2.1	3.6905701	
2.2	3.6688192	
2.3	3.6245909	

Exercises

Let $f(x) = 3xe^x - \cos x$. Use the following data to approximate $f''(1.3)$ with $h = 0.1$ and with $h = 0.01$.

x	1.20	1.29	1.30	1.31	1.40
$f(x)$	11.59006	13.78176	14.04276	14.30741	16.86187

Compare your results to $f''(1.3)$.

Exercises

Approximate the following integrals using the Trapezoidal rule, and Simpson's rule.

a. $\int_{0.5}^{1} x^4 \, dx$

b. $\int_{0}^{0.5} \frac{2}{x-4} \, dx$

c. $\int_{1}^{1.5} x^2 \ln x \, dx$

d. $\int_{0}^{1} x^2 e^{-x} \, dx$

e. $\int_{1}^{1.6} \frac{2x}{x^2-4} \, dx$

f. $\int_{0}^{0.35} \frac{2}{x^2-4} \, dx$

g. $\int_{0}^{\pi/4} x \sin x \, dx$

h. $\int_{0}^{\pi/4} e^{3x} \sin 2x \, dx$