FINANČNÍ INŽENÝRSTVÍ
KBP FFÚ & KSTP FIS

6. Numerical evaluation of derivatives

Tento učební text byl podpořen z Operačního programu Praha - Adaptabilita

Hana Hladíková

OPPA
PRAHA PRAGUE PRAGA PRAG
EVROPSKÁ UNIE

Evropský sociální fond Praha & EU: Investujeme do vaší budoucnosti

When evaluating derivatives and definite integrals we substitute the given function $f(x)$ by a function $\varphi(x)$ that will be differentiated or integrated.

Numerical evaluation of derivatives

Estimation of the first derivative

(1)

$f'(x) = D_P(x,h) - \frac{1}{2}hf''(\theta),\ \theta \in (x, x+h)$, where $D_P(x,h) = \frac{f(x+h)-f(x)}{h}$ is **first forward difference**,

$f'(x) = D_L(x,h) - \frac{1}{2}hf''(\theta),\ \theta \in (x-h, x)$, where $D_L(x,h) = \frac{f(x)-f(x-h)}{h}$ is **first backward difference**,

(2)

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

$f'(x) = D_C(x,h) - \frac{1}{6}h^2 f'''(\theta),\ \theta \in (x-h, x+h)$, where $D_C(x,h) = \frac{f(x+h)-f(x-h)}{2h}$ is **first central difference,**

$f'(x) = \frac{3f(x)-4f(x-h)+f(x-2h)}{2h} + \frac{1}{3}h^2 f'''(\theta),\ \theta \in (x-2h, x)$.

Estimation of the second derivative

$$f''(x) = D2_C(x,h) - \frac{1}{12}h^2 f^{(4)}(\theta),\ \theta \in (x-h, x+h),$$

where $D2_C(x,h) = \frac{f(x+h)-2f(x)+f(x-h)}{h^2}$ is **second central difference**.

Example 1: Using forward and central difference estimate the first derivative of the function $f(x) = e^x(x-1)$ at the point $x = 1$ for $h = 0,1$.

First differentiate the function $f(x)$, $f'(x) = e^x(x-1)+e^x = xe^x$ and evaluate $f'(1) = e = 2,7182$.

Forward difference:

$$f'(1) \approx D_P(x,h) = \frac{f(1,1)-f(1)}{0,1} = \frac{e^{1,1}(1,1-1)-e^1(1-1)}{0,1} = e^{1,1} = 3,0041.$$

Error: $0,2859$.

Central difference:

$$f'(1) \approx D_C(x,h) = \frac{f(1,1)-f(0,9)}{0,2} = \frac{e^{1,1}(1,1-1)-e^{0,9}(0,9-1)}{0,2} = \frac{e^{1,1}+e^{0,9}}{2} = 2,7318.$$

Error: $0,0136$.

Bad conditionality of numerical derivative

Numerical evaluation of derivative is badly conditioned. Errors in inputs and rounding errors affect significantly numerical differentiation (more then integration).

Examine *first forward difference*:

Denote $|f'(x_i) - T_1'(x_i)| = R_A = \frac{f''(\theta_i)h}{2}$ We get

$$|f''(x)| \leq M \Rightarrow R_A = \frac{f''(\theta_i)h}{2} \leq \frac{Mh}{2}$$

If instead of $f(x)$ and $f(x+h)$ we use the measured values $f^*(x)$ a $f^*(x+h)$ such that $|f^*(x)-f(x)| \leq \epsilon_1, |f^*(x+h)-f(x+h)| \leq \epsilon_2$, then the error R_Z must be added, $\left|\frac{f(x+h)-f(x)}{h} - \frac{f^*(x+h)-f^*(x)}{h}\right| = R_Z \leq \frac{\epsilon_1+\epsilon_2}{h}$

Total error R when we **(abandon errors in calculations)** is equal to

$$|R| \leq |R_Z| + |R_A| \leq \frac{\epsilon_1+\epsilon_2}{h} + \frac{Mh}{2} \leq \frac{2\epsilon}{h} + \frac{Mh}{2} \equiv g(h)$$

We have h in denominator and h should be small enough. But with small h errors will increase. For $g(h)$ we have $\lim_{h\to 0^+} g(h) = \infty$.

The function $g(h)$ has the unique minimum at $h_{OPT} = \sqrt{\frac{4\epsilon}{M}}$.

Comclusion: numerical derivative is badly conditioned because with decreasing h the error is increasing, but we can find the optimal h_{OPT}.

Richardson extrapolation

For **central difference**.

For an increment h we get: $f_h'(x) = \frac{f(x+h)-f(x-h)}{2h} - \frac{h^2}{6} f'''(\theta_1),\ \theta_1 \in (x-h, x+h)$.

For $2h$ we get: $f_{2h}'(x) = \frac{f(x+2h)-f(x-2h)}{4h} - \frac{(2h)^2}{6} f'''(\theta_2),\ \theta_2 \in (x-2h, x+2h)$.

Suppose $f'''(\theta_1) \approx f'''(\theta_2)$.

We eliminate the error of order h^2. The first equation will be multiplied by 4 and we subtract it from the second equation, and the divide it by 3, a then we get a better approximation of the first derivative:

$$f'(x) \approx F_2(x,h) = \frac{4}{3} f'(x,h) - \frac{1}{3} f'(x,2h)$$

Denote $F_1(x,h) = D_C(x,h)$. Similarly we can eliminate the errors of hiher orders:

$$f'(x) \approx F_{i+1}(x,h) = \frac{2^i F_i(x,h) - F_i(x,2h)}{2^i - 1}.$$

We can find $D_C(x, \frac{h}{2^i})$.

$F_1(x,2h)$
$F_1(x,h)$ $\quad F_2(x,2h)$
$F_1(x,\frac{h}{2})$ $\quad F_2(x,h)$ $\quad F_3(x,2h)$
$F_1(x,\frac{h}{4})$ $\quad F_2(x,\frac{h}{2})$ $\quad F_3(x,h)$ $\quad F_4(x,2h)$
$F_1(x,\frac{h}{8})$ $\quad F_2(x,\frac{h}{4})$ $\quad F_3(x,\frac{h}{2}$ $\quad F_4(x,h)$ $\quad F_5(x,2h)$
::::::
::::::

Example 2: Using Richardson extrapolation evaluate the central difference for $f(x) = \ln(x)$ at $x = 3$ for $h = 0,4$. First evaluate $f'(x) = \frac{1}{x}$, $f'(3) = 0,333333$.

Central difference:

Pro $h = 0,1$: $\ln'(3) \approx D_C(3;0,1) = F_1(3;0,1) = \frac{\ln(3,1)-\ln(2,9)}{0,1} = 0,333456$

Pro $h = 0,2$: $\ln'(3) \approx D_C(3;0,2) = F_1(3;0,2) = \frac{\ln(3,2)-\ln(2,8)}{0,2} = 0,333828$

Pro $h = 0,4$: $\ln'(3) \approx D_C(3;0,4) = F_1(3;0,4) = \frac{\ln(3,4)-\ln(2,6)}{0,4} = 0,335329$

Richardson:

$\ln'(3) \approx\ F_2(3;0,4) = \frac{4}{3}F_1(3,0,2) - \frac{1}{3}F_1(3,0,4) = \frac{4}{3}0,333828 - \frac{1}{3}0,335329 = 0,333327$

$\ln'(3) \approx \ F_2(3;0,2) = \frac{4}{3}F_1(3,0,1) - \frac{1}{3}F_1(3,0,2) = \frac{4}{3}0,333456 - \frac{1}{3}0,333828 = 0,333332$

$\ln'(3) \approx F_3(3;0,4) = \frac{2^3}{2^3-1}F_1(3,0,2) - \frac{1}{2^3-1}F_1(3,0,4) = \frac{8}{7}0,333332 - \frac{1}{7}0,333327 = 0,333333$

MATLAB

```
derivace.m
function dy=derivace(x,y)
% DERIVACE - numerical derivative (with central difference) function given by tablet
% dy=derivace(x,y)
% x ... vector of independetn variable
% y ... vector of function values
% dy ... vector of approximated values of derivatives at [xi,yi]
N = length(x);
h = (x(2)-x(1)); % increment
dy = y;
dy(1) = (-3*y(1)+4*y(2)-y(3))/(2*h); % initial derivative for i=2:N-1
dy(i) = (y(i+1)-y(i-1))/(2*h); % further derivatives
end
dy(N) = (y(N-2)-4*y(N-1)+3*y(N))/(2*h); % end
end
```

In symbolical toolbox: **diff(expression)**.
