Numerical Integration and Differentiation

Computational Economics

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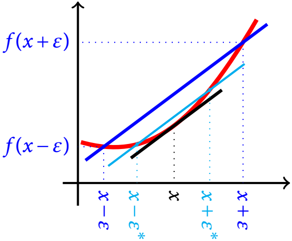
Finite Differences for Numerical Differentiation

basic concepts

- difference quotient: $\frac{\Delta y}{\Delta x} = \frac{f(x_0+\Delta x)-f(x_0)}{\Delta x}$
- derivative: $\frac{\mathrm{d}y}{\mathrm{d}x} \equiv f'(x) \equiv \lim_{\Delta x \to 0} \frac{\Delta y}{\Delta x}$

numerical approximation of f' with central difference

$$f'(x) \approx \frac{f(x+\varepsilon)-f(x-\varepsilon)}{(x+\varepsilon)-(x-\varepsilon)}$$
$$= \frac{f(x+\varepsilon)-f(x-\varepsilon)}{2\varepsilon} \text{ where } \varepsilon \to 0$$



multi-dimensional functions

- gradient: list of all first order derivatives

$$\nabla f = \left[\frac{\partial f}{\partial x_1} \quad \cdots \quad \frac{\partial f}{\partial x_n}\right]$$
$$\approx \left[\frac{f(x_1+\varepsilon,x_2,\ldots,x_n)-f(x_1-\varepsilon,x_2,\ldots,x_n)}{2\varepsilon} \quad \cdots \quad \frac{f(x_1,x_2,\ldots,x_n+\varepsilon)-f(x_1,x_2,\ldots,x_n-\varepsilon)}{2\varepsilon}\right]$$

Finite Differences for Numerical Differentiation

second derivative for one-dimensional functions

- since second derivative = derivative of first derivative, compute by iteratively applying definitions:

$$
\begin{aligned}
f''(x) &\approx \frac{f'(x+\epsilon)-f'(x-\epsilon)}{(x+\epsilon)-(x-\epsilon)} \\
&= \frac{\frac{f(x+\epsilon+\epsilon)-f(x+\epsilon-\epsilon)}{2\epsilon} - \frac{f(x-\epsilon+\epsilon)-f(x-\epsilon-\epsilon)}{2\epsilon}}{(x+\epsilon)-(x-\epsilon)} \\
&= \frac{f(x+2\epsilon)+f(x-2\epsilon)-2f(x)}{(2\epsilon)^2} \\
&= \frac{f(x+\varepsilon)+f(x-\varepsilon)-2f(x)}{\varepsilon^2}
\end{aligned}
$$

  where $\varepsilon = 2\epsilon$
- likewise for higher derivatives

Finite Differences for Numerical Differentiation

second derivative for multi-dimensional functions

- Hessian matrix multi-dimensional functions: matrix of all second order derivatives

$$H = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \vdots & \frac{\partial^2 f}{\partial x_i \partial x_j} & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

- usually, Hessian is symmetric, i.e., $\frac{\partial^2 f}{\partial x_i \partial x_j} = \frac{\partial^2 f}{\partial x_j \partial x_i}$

Finite Differences for Numerical Differentiation

numerical approximation of the Hessian

- vary values in dimensions i and j (leaving all other values unchanged) and evaluate points

$$\begin{array}{c} \\ x_i-\varepsilon \\ x_i \\ x_i+\varepsilon \end{array} \begin{array}{c} \begin{array}{ccc} x_j-\varepsilon & x_j & x_j+\varepsilon \end{array} \\ \begin{pmatrix} f^{--} & f^{-\circ} & f^{-+} \\ f^{\circ-} & f^{\circ\circ} & f^{\circ+} \\ f^{+-} & f^{+\circ} & f^{++} \end{pmatrix} \end{array}$$

- diagonal elements of the Hessian matrix

$$\frac{\partial^2 f}{\partial x_i^2} \approx \begin{cases} \frac{f^{+\circ}+f^{-\circ}-2f^{\circ\circ}}{\varepsilon^2} & \text{alternative 1} \\ \frac{1}{2}\left(\frac{f^{+-}+f^{--}-2f^{\circ-}}{\varepsilon^2}+\frac{f^{++}+f^{-+}-2f^{\circ+}}{\varepsilon^2}\right) & \text{alternative 2} \end{cases}$$

- off-diagonal elements of the Hessian matrix (cross-derivatives)

$$\frac{\partial^2 f}{\partial x_i \partial x_j} \approx \begin{cases} \frac{1}{2}\left(\frac{f^{\circ+}+f^{-\circ}-f^{\circ\circ}-f^{-+}}{\varepsilon^2}+\frac{f^{+\circ}+f^{\circ-}-f^{+-}-f^{\circ\circ}}{\varepsilon^2}\right) & \text{alternative 1} \\ \frac{1}{2}\left(\frac{f^{\circ\circ}+f^{++}-f^{\circ+}-f^{+\circ}}{\varepsilon^2}+\frac{f^{\circ\circ}+f^{--}-f^{\circ-}-f^{-\circ}}{\varepsilon^2}\right) & \text{alternative 2} \\ \frac{1}{4}\left(\frac{f^{++}+f^{--}-f^{-+}-f^{+-}}{\varepsilon^2}\right) & \text{average alt.s 1 and 2} \end{cases}$$

Application Example

local approximation with Taylor Series Approximation

- approximation for region around a given value x_0
- approximate function value at $x = x_0 + \delta$ with a polynomial

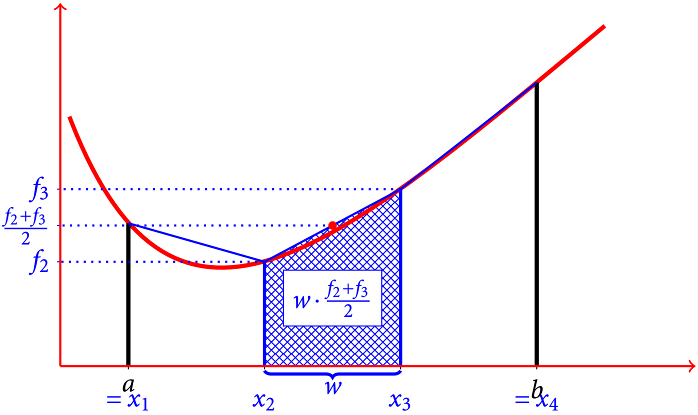
$$f(x) = f(x_0 + \delta) = f(x_0) + \delta f'(x_0) + \frac{\delta^2}{2} f''(x_0) + \frac{\delta^3}{6} f'''(x_0) + \cdots + \cdots + \frac{\delta^n}{n!} f^{(n)}(x_0) + R_n$$

- remainder $R_n < |x - x_0|^{n+1}$

Numerical Integration with Trapezoid Rule

basic idea

- assume function is approximately piecewise linear
- area underneath each line segment is a trapezoid
- integral is the sum of all trapezoids' areas



Numerical Integration with Trapezoid Rule

how solve a problem like $\int_a^b f(x)\mathrm{d}x$

- split range into n segments of equal width $w = (b-a)/n$
- compute borders of segments, $x_i = a + (i-1)w$ for $i = 1..(n+1)$
- approximation for area of one segment: $\int_{x_i}^{x_{i+1}} f(x)\mathrm{d}x \approx w\frac{f(x_i)+f(x_{i+1})}{2}$
- for the entire range (with $f_i = f(x_i)$)

$$\begin{aligned}\int_a^b f(x)\mathrm{d}x &= \sum_{i=1}^{n} \int_{x_i}^{x_{i+1}} f(x)\mathrm{d}x \\ &\approx \sum_{i=1}^{n} w \cdot \frac{f_i + f_{i+1}}{2} = w \cdot \left(\frac{f_1}{2} + f_2 + \cdots + f_n + \frac{f_{n+1}}{2}\right)\end{aligned}$$

- more generally (when segments have different width):

$$\int_a^b f(x)\mathrm{d}x \approx \sum_{i=1}^{n} (x_{i+1} - x_i) \cdot \frac{f_i + f_{i+1}}{2}$$

- extension: Simpson's rule (piecewise quadratic functions)

Numerical Integration with Monte Carlo Simulation

some (very) simple examples

$$f(x) = \frac{1}{2}x \Longrightarrow \int_0^2 f(x)\mathrm{d}x = ? \qquad f(x) = \sin\left(|x|^{\sqrt[5]{|x|}}\right) \Longrightarrow \int_{-1}^3 f(x)\mathrm{d}x = ?$$

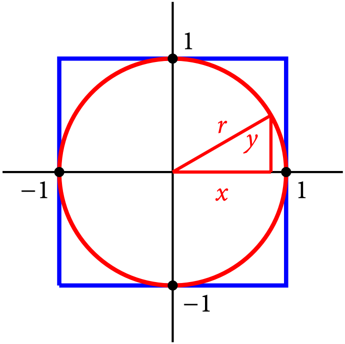
Estimating the Value of π via MCS

$$A_\square = (2r)^2$$

$$A_\circ = r^2\pi$$

$$\frac{A_\circ}{A_\square} = \frac{r^2\pi}{4r^2} = \frac{\pi}{4}$$

$$\Longrightarrow \pi = 4\frac{A_\circ}{A_\square}$$



additional literature

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