CS5016: Computational Methods and Applications

Numerical Differentiation and Integration

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Differentiation

Consider the following function

$$f(x) = \sin(e^{x^2})$$

What the derivative of the above function?

An application of chain rule gives us

$$f^{'}(x) = \cos(e^{x^2}) \cdot e^{x^2} \cdot 2x$$

We can do it easily; what about a computer?

Numerical differentiation

Consider a function $f : [a, b] \to \mathbb{R}$ that is continuously differentiable in the internal $[a, b]$. We would like to approximate the first derivative at any point $x \in [a, b]$.

By definition,

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

For a small value of $h > 0$; good approximations are

$$\delta_h^+(x) = \frac{f(x+h) - f(x)}{h} \qquad \delta_h^-(x) = \frac{f(x) - f(x-h)}{h}$$

Above approximations are known as forward finite difference and backward finite difference.

Error of approximation

Assume that f is twice differntiable in $[a, b]$. Then, from Taylor series expansion, we get

$$f(x+h) = f(x) + hf^{'}(x) + \frac{h^2}{2} f^{''}(\zeta)$$

where $\zeta \in [x, x+h]$.

Thus, we have

$$|\delta_h^{+}(x) - f^{'}(x)| = \frac{h}{2} f^{''}(\zeta)$$

For a good approximation, how should h be chosen when $f(x) = x^2$ and $f(x) = x^3$?

Centered finite difference

For a small value of $h > 0$, consider the following approximations

$$\delta_h^c(x) = \frac{f(x+h) - f(x-h)}{2h}$$

Can you figure out the error due to this approximation?
Hint: Taylor series expansion

Numerical integration

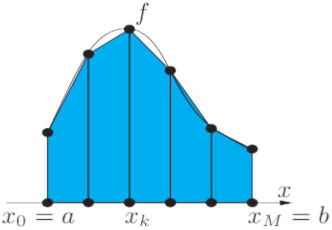
We want to evaluate the following

$$I(f) = \int_a^b f(x)dx$$

where f is a an arbitrary continuous function in $[a, b]$.

Trapezoidal formula

Divide the interval $[a, b]$ into M equal-length intervals. Let $x_k = a + kM$ for $k \in \{0, 1, \ldots, M\}$ and $h = (b - a)/M$. Then, the approximate integral is given as



$$I_M(f) = \frac{(b-a)}{2M} \sum_{k=1}^{M} [f(x_k) + f(x_{k-1})]$$

Figure: Visualization of composite trapezoidal formula[2]

Can you figure out the approximation error?

Hint: Taylor series for each interval

[2] "Scientific Computing with MATLAB and Octave", Alfio Quateroni and Fausto Saleri

Python's scipy.integrate module

This sub-package provides several integration techniques including an ordinary differential equation integrator

To know more, visit `https://docs.scipy.org/doc/scipy/reference/tutorial/integrate.html`

Thank You