NUMERICAL DIFFERENTIATION AND INTEGRATION

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4.1 Numerical Differentiation

The derivative of the function f at x_0 is $f'(x_0) = \lim_{\Delta x \to 0} \dfrac{f(x_0 + \Delta x) - f(x_0)}{\Delta x}$ and if $|\Delta x|$ is sufficiently small, we have $f'(x_0) \approx \dfrac{f(x_0 + \Delta x) - f(x_0)}{\Delta x}$.

Depending on that $\Delta x = h > 0$ or $\Delta x = -h < 0$, we obtain the following formulas to approximate the derivative of f at x_0

Forward-Difference Formula $\quad f'(x_0) \approx \dfrac{f(x_0 + h) - f(x_0)}{h}$

Backward-Difference Formula $\quad f'(x_0) \approx \dfrac{f(x_0) - f(x_0 - h)}{h}$

The other way to approximate the derivative of a function at a point is from Taylor's formula. We have

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2} f''(x_0)(x - x_0)^2 + o((x - x_0)^2) \tag{4.1}$$

Choose $h > 0$ sufficiently small suct that $x_0 \pm h$ are still belonging to any neighbourhood of x_0, and replace them into (4.1), we obtain

$$f(x_0 + h) = f(x_0) + hf'(x_0) + \frac{h^2}{2} f''(x_0) + o(h^2)$$

$$f(x_0 - h) = f(x_0) - hf'(x_0) + \frac{h^2}{2} f''(x_0) + o(h^2)$$

Discarding the last term of these formulas, we obtain the approximation formulas the first and second derivatives at x_0 (these are called *centripetal formulas*):

$$f'(x_0) \approx \frac{f(x_0 + h) - f(x_0 - h)}{2h} \quad \text{and} \quad f''(x_0) \approx \frac{f(x_0 + h) - 2f(x_0) + f(x_0 - h)}{h^2} \tag{4.2}$$

Example 4.1. *Use the formulas* (4.2) *to approximate* $f'(1)$ *and* $f''(1)$ *where* $f(x) = x^2 \ln(x^3 + x + 1)$ *with the value of* h *is* 0.1, 0.05, *and* 0.01, *respectively.*
The results are given in the following table

	$h = 0.1$	$h = 0.05$	$h = 0.01$
$f'(1)$	3.5440	3.5339	3.5307
$f''(1)$	7.7475	7.7515	7.7527

4.2 Numerical Integration

In this part, we will consider the following definite integral:

$$I = \int_a^b f(x)\, dx \tag{4.3}$$

where a, b are finite constants, $a < b$, and $f(x)$ is defined and integrable on $[a, b]$.

We will consider formulas of numerical integration of integral (4.3) produced by using first and second Lagrange polynomials with equally spaced nodes. This give the *Trapezoidal rule* and *Simpson's rule*.

Trapezoidal rule: $\int_a^b f(x)\,dx \approx \frac{b-a}{2}[f(a) + f(b)]$

Simpson's rule: $\int_a^b f(x)\,dx \approx \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$

However, in practice, we can not use these formulas because of the simplicity and large error. First of all, we consider the following equal partition of closed interval $[a, b]$: $a = x_0 < x_1 < \cdots < x_n = b$, where $h = \frac{b-a}{n}$ and $x_k = x_0 + kh,\ k = 0, 1, \ldots, n$. Denote $y_k = f(x_k),\ k = 0, 1, \ldots, n$. We obtain the following composite formulas

Composite Trapezoidal Formula:

$$\int_a^b f(x)\,dx \approx h\left[\frac{y_0}{2} + y_1 + \cdots + y_{n-1} + \frac{y_n}{2}\right]$$

Composite Simpson's Formula: In this case $n = 2m$ is an even integer number.

$$\int_a^b f(x)\,dx \approx \frac{h}{3}\left[y_0 + y_n + 4(y_1 + y_3 + \cdots + y_{2m-1}) + 2(y_2 + y_4 + \cdots + y_{2m-2})\right]$$

4.3 Exercise

Question 1. Given $f(x) = x\,\mathrm{e}^{-2x}\sin x$. Use the centripetal formulas to approximate $f'(0.2)$ and $f''(0.2)$ with the step $h = 0.1$, $h = 0.05$, and $h = 0.01$, respectively.

Question 2. Use the Composite Trapezoidal formula and Composite Simpson's formula to approximate the following integrals with given n.

(a) $\int_0^1 \frac{x}{x^3+1}\,dx \quad (n = 4)$

(b) $\int_{0.2}^{0.8} x \ln x\,dx \quad (n = 6)$

(c) $\int_{1.5}^{2.0} \frac{\sin x\,dx}{2 - \cos^2 x} \quad (n = 8)$

(d) $\int_0^1 \frac{dx}{x^2+1} \quad (n = 10)$

Question 3. Given a function $f(x)$ in the following table

x	1.2	1.4	1.6	1.8	2.0	2.2	2.4
$f(x)$	2.15	2.38	2.65	2.77	3.05	2.81	2.93

Use the Composite Trapezoidal formula and Composite Simpson's formula to approximate

$$(a) \quad \int_{1.2}^{2.4} x^2 f(x)dx \qquad\qquad (b) \quad \int_{1.2}^{2.4} x f^2(x)dx$$
