Chapter 5
Numerical Differentiation

Dr. Kareem Elgindy

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Lecturer

Mathematics Department, Faculty of Science

Assiut University

Outline

1. Introduction
2. Approximation of the First-Order Derivative of a Function
3. Approximation of the Second-Order Derivative of a Function
4. Round-Off Error Instability

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Introduction

Introduction

Definition 1 (Differentiation)

Differentiation is the process of finding the derivative, or rate of change, of a function.

Definition 2 (Numerical Differentiation)

Numerical differentiation is the process of finding the numerical value of the derivative of a given function.

There are several reasons as of why we still need to approximate derivatives:

1. There are times in which exact formulas are available but they are **very complicated** to the point that an exact computation of the derivative requires a lot of function evaluations.
   - ***It might be significantly simpler to approximate the derivative instead of computing its exact value.***

Introduction

2. Even if there exists an underlying function that we need to differentiate, we might **know its values only at a sampled data set** without knowing the function itself.
   - In particular, if the function values $f(x_0), \ldots, f(x_n)$ are known at some $(n+1)$ distinct points $x_0 < \ldots < x_n$, then the estimated value of $f'(x)$, for a certain value of x, can be obtained by numerical differentiation.

Approximation of the First-Order Derivative of a Function

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First-Order Numerical Differentiation Formulas

Second-Order Numerical Differentiation Formulas

Approximation of the First-Order Derivative of a Function

First-Order Numerical Differentiation Formulas

The derivative of a differentiable function f at a point x_0 is

$$f'(x_0) = \lim_{h \to 0} \frac{f(x_0 + h) - f(x_0)}{h}. \tag{1}$$

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.

Approximation of the First-Order Derivative of a Function

First-Order Numerical Differentiation Formulas

Since the approximation of the derivative at x_0,

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

is based on the values of the function at x_0 and $x_0 + h$, the approximation is called a **forward difference formula** if $h > 0$ and a **backward-difference formula** if $h < 0$.

- Both are called **one-sided differencing formula**.

Approximation of the First-Order Derivative of a Function

First-Order Numerical Differentiation Formulas

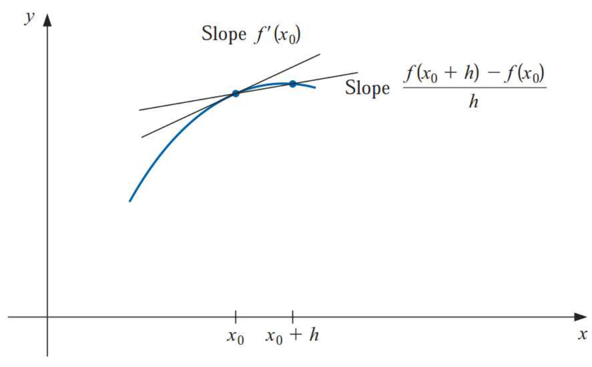

Figure 1: The geometric interpretation of the forward difference formula.

Approximation of the First-Order Derivative of a Function

First-Order Numerical Differentiation Formulas

To compute the approximation error, suppose first that $f \in C^2[a, b]$, and $x_0 \in (a, b)$. We write Taylor's expansion of $f(x_0 + h)$ about x_0, i.e.,

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

where ξ lies between x_0 and $x_0 + h$. Hence,

$$\boxed{f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} - \frac{h}{2} f''(\xi).} \tag{3}$$

The truncation error $-\frac{h}{2} f''(\xi)$, is bounded by $M\,|h|\,/2$, where M is a bound on $|f''(\xi)|$.

Approximation of the First-Order Derivative of a Function

First-Order Numerical Differentiation Formulas

Remark 1.

For constant and linear functions, the one-sided differencing formula is actually an exact expression for the derivative (using exact arithmetic), but ***for almost all other functions, the expression does not yield the exact derivative****.*

Approximation of the First-Order Derivative of a Function

First-Order Numerical Differentiation Formulas

Example 1

Use the forward-difference formula to approximate the derivative of $f(x) = \ln x$ at $x_0 = 1.8$ using $h = 0.1, 0.05$, and 0.01, and determine bounds for the approximation errors.

Solution 1

The forward-difference formula,

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

with $h = 0.1$ *gives*

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

Approximation of the First-Order Derivative of a Function

First-Order Numerical Differentiation Formulas

Solution 1

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

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

The approximation and error bounds when $h = 0.05$ *and* $h = 0.01$ *are found in a similar manner and the results are shown in the table below.*

h	$f(1.8+h)$	$\frac{f(1.8+h)-f(1.8)}{h}$	$\frac{\lvert h\rvert}{2(1.8)^2}$
0.1	0.64185389	0.5406722	0.0154321
0.05	0.61518564	0.5479795	0.0077160
0.01	0.59332685	0.5540180	0.0015432

Approximation of the First-Order Derivative of a Function

First-Order Numerical Differentiation Formulas

Definition 3 (Big O Notation)

Let f and g be two functions defined on some subset of the real numbers. One writes,

$$f(x) = O(g(x)), \text{ as } x \to a, \tag{4}$$

if and only if there exist a positive number M such that,

$$|f(x)| \leq M\, |g(x)|\, , \text{ as } x \to a. \tag{5}$$

The symbol O expresses the **asymptotic behavior of a given function** usually in terms of simpler functions.

Approximation of the First-Order Derivative of a Function

First-Order Numerical Differentiation Formulas

Example 2

Suppose that we want to analyze the asymptotic behavior of $f(x) = 6x^4 - 2x^3 + x$ when $x \to 0$.

Since,

$$\begin{aligned} \left|6x^4 - 2x^3 + x\right| &\leq 6x^4 + 2\left|x^3\right| + |x| \quad \textbf{(triangle inequality)} \\ &< 6|x| + 2|x| + |x|, \quad \text{as } x \to 0, \\ &= 9|x|, \quad \text{as } x \to 0. \end{aligned}$$

Hence, $f(x) = O(x)$, as $x \to 0$.

Approximation of the First-Order Derivative of a Function

First-Order Numerical Differentiation Formulas

Example 3

Suppose that we want to analyze the asymptotic behavior of the same function $f(x) = 6x^4 - 2x^3 + x$ when $x \to 2$.

Since,

$$\begin{aligned} \left|6x^4 - 2x^3 + x\right| &\le 6x^4 + 2x^3 + x \quad \textbf{(triangle inequality)} \\ &< 6x^4 + 2x^4 + x^4, \quad \text{as } x \to 2, \\ &= 9x^4, \quad \text{as } x \to 2. \end{aligned}$$

Hence, $f(x) = O(x^4)$, as $x \to 2$.

Approximation of the First-Order Derivative of a Function

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Infinitesimal Asymptotics

Big O can also be used to **describe the error term in an approximation to a mathematical function**. The most significant terms are written explicitly, and then the least-significant terms are summarized in a single big O term. Consider, for example, the exponential series and two expressions of it that are valid when x is small:

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \dots, \quad \text{for all } x, \tag{6a}$$

$$= 1 + x + \frac{x^2}{2} + O(x^3), \quad \text{as } x \to 0, \tag{6b}$$

$$= 1 + x + O(x^2), \quad \text{as } x \to 0. \tag{6c}$$

The second expression (6b) means that the absolute-value of the error $e^x - (1+x+x^2/2)$ is smaller than some constant times $\left|x^3\right|$ when x is close enough to 0.

Approximation of the First-Order Derivative of a Function

First-Order Numerical Differentiation Formulas

The truncation error of the forward/backward difference formula is of $O(h)$, **as** $h \to 0$, and we say that they are **first-order formulas**; i.e. they give **first-order approximation of the first derivative**.

Approximation of the First-Order Derivative of a Function

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2 Approximation of the First-Order Derivative of a Function

- First-Order Numerical Differentiation Formulas
- Second-Order Numerical Differentiation Formulas

Approximation of the First-Order Derivative of a Function

Second-Order Numerical Differentiation Formulas

- In general, we refer to a numerical differentiation formula by a **pth-order formula** if the truncation error is of $O(h^p)$**, as** $h \to 0$.

It is possible to write more accurate formulas than the forward/backward difference formulas for the first derivative. For example, a more accurate approximation for the first derivative that is based on the values of the function at the points $x - h$ and $x + h$ is the **centered differencing formula** (or **midpoint formula**),

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}. \tag{7}$$

Approximation of the First-Order Derivative of a Function

Second-Order Numerical Differentiation Formulas

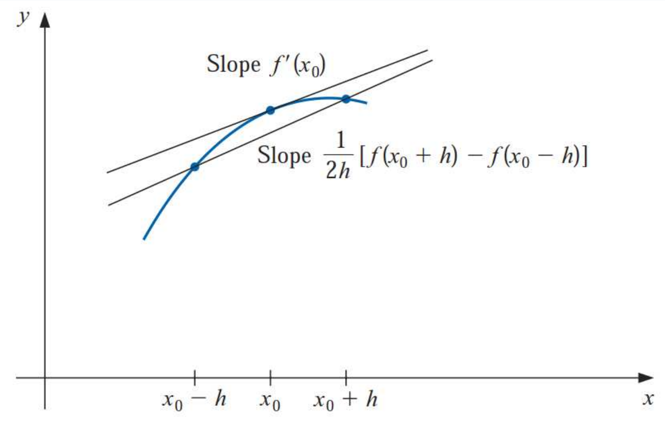

Figure 2: The geometric interpretation of the centered differencing formula.

Approximation of the First-Order Derivative of a Function

Second-Order Numerical Differentiation Formulas

Let us verify that this is indeed a more accurate formula. Suppose that $f \in C^3[a,b], x_0 \in (a,b)$, and $h > 0$. Taylor expansions of the terms of the numerator on the right-hand-side of (7) are

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{6} f'''(\xi_1), \quad \xi_1 \in (x, x+h), \tag{8a}$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2} f''(x) - \frac{h^3}{6} f'''(\xi_2), \quad \xi_2 \in (x-h, x). \tag{8b}$$

Hence,

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{12} \left(f'''(\xi_1) + f'''(\xi_2) \right). \tag{9}$$

Approximation of the First-Order Derivative of a Function

Second-Order Numerical Differentiation Formulas

Since the third-order derivative $f'''(x)$ is a continuous function in the interval $[x - h, x + h]$, then the ***intermediate value theorem*** implies that there exists a point $\xi \in (x - h, x + h)$ such that,

$$f'''(\xi) = \frac{f'''(\xi_1) + f'''(\xi_2)}{2}. \tag{10}$$

Hence,

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{6} f'''(\xi), \tag{11}$$

which means that the centered differencing formula is a **second-order approximation of the first derivative**; i.e. the truncation error is of $\boldsymbol{O(h^2)}$**, as** $\boldsymbol{h \to 0}$.

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Approximation of the Second-Order Derivative of a Function

Second-Order Numerical Differentiation Formulas

In a similar way we can approximate the values of higher-order derivatives. For example, it is easy to verify that the following **centered differencing formula (midpoint formula)** is a **second-order approximation of the second derivative**,

$$f''(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}. \tag{12}$$

Proof.

Suppose that $f \in C^4[a,b], x_0 \in (a,b)$, and $h > 0$. Since,

$$f(x \pm h) = f(x) \pm hf'(x) + \frac{h^2}{2} f''(x) \pm \frac{h^3}{6} f'''(x) + \frac{h^4}{24} f^{(4)}(\xi_\pm), \tag{13}$$

where $\xi_+ \in (x, x+h)$ and $\xi_- \in (x-h, x)$.

Approximation of the Second-Order Derivative of a Function

Second-Order Numerical Differentiation Formulas

Proof.

Since $f \in C^4[x-h, x+h]$, then by the intermediate value theorem, there exists a number $\xi \in (x-h, x+h)$ such that,

$$\frac{f(x+h) - 2f(x) + f(x-h)}{h^2} = f''(x) + \frac{h^2}{24}\left(f^{(4)}(\xi_-) + f^{(4)}(\xi_+)\right) \tag{14}$$

$$= f''(x) + \frac{h^2}{12} f^{(4)}(\xi). \tag{15}$$

Hence, the approximation is indeed a second-order approximation of the second-order derivative with a truncation error $-\frac{h^2}{12} f^{(4)}(\xi)$; that is the truncation error is of $O(h^2)$, as $h \to 0$. □

Approximation of the Second-Order Derivative of a Function

Second-Order Numerical Differentiation Formulas

Example 4

Use the data shown in the table below to approximate the second derivative of $f(x) = x\,e^x$ at $x = 2$ using the centered differencing formula. Calculate also the absolute and relative errors in this approximation.

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

Approximation of the Second-Order Derivative of a Function

Second-Order Numerical Differentiation Formulas

Solution 4

The centered differencing formula of the second derivative is given by

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

Because $f''(x) = (x+2)e^x$*, the exact value is* $f''(2) = 4\,e^2$*. Hence the absolute and relative errors are about* 3.70×10^{-2} *and* 1.3×10^{-3}*, respectively.*

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4 **Round-Off Error Instability**

Round-Off Error Instability

Round-Off Error Instability

It is particularly important to pay attention to **round-off error** when approximating derivatives. To illustrate the situation, let us examine the midpoint formula,

$$f'(x) = \frac{1}{2h}\left(f(x+h) - f(x-h)\right) - \frac{h^2}{6} f'''(\xi),$$

more closely. Suppose that in evaluating $f(x+h)$ and $f(x-h)$ we encounter round-off errors $e(x+h)$ and $e(x-h)$. Then our computations actually use the values $\tilde{f}(x+h)$ and $\tilde{f}(x-h)$, which are related to the true values $f(x+h)$ and $f(x-h)$ by

$$f(x+h) = \tilde{f}(x+h) + e(x+h); \quad \text{(16a)}$$

$$f(x-h) = \tilde{f}(x-h) + e(x-h). \quad \text{(16b)}$$

Round-Off Error Instability

Round-Off Error Instability

The total error in the approximation,

$$f'(x) - \frac{\tilde{f}(x+h) - \tilde{f}(x-h)}{2h} = \underbrace{\frac{e(x+h) - e(x-h)}{2h}}_{\text{round - off error}} \underbrace{- \frac{h^2}{6} f'''(\xi)}_{\text{truncation error}}, \tag{17}$$

is due both to round-off error, the first part, and to truncation error. If we assume that the round-off errors $e(x \pm h)$ are bounded by some number $\varepsilon > 0$ and that the third derivative of f is bounded by a number $M > 0$, then

$$\left| f'(x) - \frac{\tilde{f}(x+h) - \tilde{f}(x-h)}{2h} \right| \leq \underbrace{E(h) = \frac{\varepsilon}{h} + \frac{M\,h^2}{6}}_{\text{total error bound}}. \tag{18}$$

To reduce the truncation error bound, $Mh^2/6$, we need to reduce h. But as h is reduced, the round-off error bound ε/h grows. In practice, then, **it is seldom advantageous to let h be too small, because in that case the round-off error will dominate the calculations**.