Numerical Differentiation

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Overview

Numerical differentiation is a process by which we find the approximate numerical value of the derivative or derivatives of a function at some value of the independent variable when we are given a set of values of that function.

First of all we approximate the function by an interpolation formula and then differentiate it as many times as desired.

In the lecture, we discuss several methods to find derivatives of the function at a point.

Overview

When the values of the argument are **equally spaced**, we represent the function by **Gregory-Newton** formulae.

1. To find the derivative of the function at a point near the beginning of a set of tabular values, Gregory-Newton forward formula is used and backward formula is used if the point is near the end of the tabular values.
2. To find the derivative at a point near the middle of the table, central difference formula should be used.
3. In case the values of argument **are not spaced equally**, Newton's divided difference formula, or, Lagrange's formula should be used to represent the function.

Thus corresponding to each of the formulae discussed in the lecture on "interpolation", we may derive a formula for the derivative.

Introduction

A sheet of corrugated roofing is constructed by pressing a flat sheet of aluminum into one whose cross section has the form of a sine wave.

A corrugated sheet 4 ft long is needed, the height of each wave is 1 in. from the center line, and each wave has a period of approximately 2π in.

Introduction

The problem of finding the length of the initial flat sheet is one of determining the length of the curve given by $f(x) = \sin x$ from $x = 0$ in. and $x = 48$ in. From calculus we know that this length is

$$L = \int_0^{48} \sqrt{1 + [f'(x)]^2} dx = \int_0^{48} \sqrt{1 + \cos^2 x} dx,$$

so the problem reduces to evaluating this integral.

Although the sine function is one of the most common mathematical functions, the calculation of its length involves an elliptic integral of the second kind, which cannot be evaluated by ordinary methods.

Weierstrass Approximation Theorem

One reason for using algebraic polynomials to approximate an arbitrary set of data is that, given any continuous function defined on a closed interval, a polynomial exists that is arbitrarily close to the function at every point in the interval, by the following theorem.

Theorem (Weierstrass Approximation Theorem)

Suppose that f is defined and continuous on $[a, b]$. For each $\varepsilon > 0$, there exists a polynomial $p(x)$, with the property that

$$|f(x) - p(x)| < \varepsilon, \ \textit{for all } x \in [a, b].$$

Also, the derivatives and intervals of polynomials are easily obtained and evaluated. It should not be surprising, then, that most procedures for approximating integrals and derivatives use the polynomials that approximate the function.

Finding Derivatives Using Newton's Forward Difference Formula

We illustrate the derivation with Newton's forward difference formula, the method of derivation being the same with regard to the other formulae.

Consider Newton's forward difference formula

$$y = y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \cdots,$$

where $x = x_0 + ph$. Then

$$\frac{dy}{dx} = \frac{dy}{dp}.\frac{dp}{dx} = \frac{1}{h}\left[\Delta y_0 + \frac{2p-1}{2}\Delta^2 y_0 + \frac{3p^2-6p+2}{6}\Delta^3 y_0 + \cdots\right].$$

This formula can be used for computing the value of $\frac{dy}{dx}$ for **non-tabular values of** x.

Finding Derivatives Using Newton's Forward Difference Formula

For tabular values of x, the formula takes a simpler form, for setting $x = x_0$ $(p = 0)$, wet get

$$\left[\frac{dy}{dx}\right]_{x=x_0} = \frac{1}{h}\left[\Delta y_0 - \frac{1}{2}\Delta^2 y_0 + \frac{1}{3}\Delta^3 y_0 + -\frac{1}{4}\Delta^4 y_0 + \cdots\right].$$

Differentiating once again, we obtain

$$\frac{d^2y}{dx^2} = \frac{1}{h^2}\left[\Delta^2 y_0 + \frac{6p-6}{6}\Delta^3 y_0 + \frac{12p^2 - 36p + 22}{24}\Delta^4 y_0 + \cdots\right].$$

When $x = x_0$, we have

$$\left[\frac{d^2y}{dx^2}\right]_{x=x_0} = \frac{1}{h^2}\left[\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12}\Delta^4 y_0 + \cdots\right].$$

Finding Derivatives Using Newton's Backward Difference Formula

Formulae for computing higher derivatives may be obtained by successive differentiation.

In a similar way, different formulae can be derived by starting with other interpolation formulae. If we consider Newton's backward difference formula,

$$y = y_n + p\nabla y_n + \frac{p(p+1)}{2!}\nabla^2 y_n + \frac{p(p+1)(p+2)}{3!}\nabla^3 y_n + \cdots$$

where $p = (x - x_n)/h$, we get

$$\left[\frac{dy}{dx}\right]_{x=x_n} = \frac{1}{h}\left[\nabla y_n + \frac{1}{2}\nabla^2 y_n + \frac{1}{3}\nabla^3 y_n + \cdots\right]$$

and

$$\left[\frac{d^2y}{dx^2}\right]_{x=x_n} = \frac{1}{h^2}\left[\nabla^2 y_n + \nabla^3 y_n + \frac{11}{12}\nabla^4 y_n + \frac{5}{6}\nabla^5 y_n + \cdots\right].$$

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Finding Derivatives Using Stirling's Formula

Consider Stirling's formula

$$y = y_0 + p\left(\frac{\Delta y_{-1} + \Delta y_0}{2}\right) + \frac{p^2}{2}\Delta^2 y_{-1} + \frac{p(p^2-1)}{3!}\left(\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2}\right) + \cdots,$$

where $x = x_0 + ph$.

$$\left[\frac{dy}{dx}\right]_{x=x_0} = \frac{1}{h}\left[\left(\frac{\Delta y_{-1} + \Delta y_0}{2}\right) - \frac{1}{6}\left(\frac{\Delta^3 y_{-2} + \Delta^5 y_{-2}}{2}\right) + \frac{1}{30}\left(\frac{\Delta^5 y_{-3} + \Delta^5 y_{-2}}{2}\right) + \cdots\right]$$

and

$$\left[\frac{d^2y}{dx^2}\right]_{x=x_0} = \frac{1}{h^2}\left[\Delta^2 y_{-1} - \frac{1}{12}\Delta^4 y_{-2} + \frac{1}{90}\Delta^6 y_{-3} - \cdots\right].$$

Exercises

Exercises

1. Find $\frac{dy}{dx}$ and $\frac{d^2y}{dx^2}$ at $x = 1.2$ and $x = 1.6$, for the following table of values of x and y.

x	1	1.2	1.4	1.6	1.8	2	2.2
y	2.7183	3.3201	4.0552	4.9530	6.0496	7.3891	9.0250

2. Find the first and second derivatives of the funciton $y = f(x)$ tabulated below at the point $x = 1.1$.

x	1	1.2	1.4	1.6	1.8	2
$y = f(x)$	0	0.128	0.5450	1.2960	2.4320	4

3. Using the following data, find $f'(5)$.

x	0	1	2	3	4	5
y	0	0.25	0	2.25	16	56.25

Exercises

4. *Given the values of an empirical function $f(x)$ for certain values of x. Find*
   (a) $f'(93)$
   (b) *the value of $f(x)$ for which $f(x)$ is a maximum,*
   (c) *the maximum value of $f(x)$ in the range of x.*

x	60	75	90	105	120
$f(x)$	28.2	38.2	43.2	40.9	37.7

5. *Compute $f'''(5)$ given*

x	2	4	9	13	16	21
$f(x)$	57	1345	66340	402052	1118209	4287844

Exercises

Exercises

6. *Prove that, the kth derivative of $f(x)$ is*

$$f^{(k)}(x) = \frac{1}{h^k}\frac{d^k}{dp^k}(1+\Delta)^p f_0.$$

Derive

(a) *Newton's forward formula for first derivative (general form) and for $f'(x_0)$.*

(b) *Newton's backward formula for first derivative (general form) and for $f'(x_n)$.*

7. *Compute f' and f'', from the following table, at*

(a) $x = 16$ (b) $x = 15$ (c) $x = 24$ (d) $x = 25$.

x	15	17	19	21	23	25
$f(x) = \sqrt{x}$	3.373	4.123	4.359	4.583	4.796	5

Exercises

Exercises

8. *Given* $u_0 = 5, u_1 = 15, u_2 = 57$, *and* $\frac{du}{dx} = 4$ *at* $x = 0$ *and* 72 *at* $x = 2$. *Find* $\Delta^3 u_0$ *and* $\Delta^4 u_0$.
9. *The population of a certain town is shown in the following table.*

Year (x)	*1931*	*1941*	*1951*	*1961*	*1971*
Population (y)	*40.62*	*60.80*	*79.95*	*103.56*	*132.65*

Find the rate of growth of the population in 1961.

10. *A rod is rotating in a plane. The following table gives the angle* θ *(in radians) through which the rod has turned for various values of time t (in seconds). Calculate the angular velocity* $(\frac{d\theta}{dt})$ *and angular acceleration* $(\frac{d^2\theta}{dt^2})$ *of the rod when* $t = 51$ *seconds.*

t	*50*	*60*	*70*	*80*	*90*
θ	*19.96*	*36.65*	*58.81*	*77.21*	*94.61*

Exercises

Exercises

11. *Find the gradient of the road at the starting point of the elevation above a datum line of 7 points of a road which are given below.*

x	0	300	600	900	1200	1500	1800
y	135	149	157	183	201	205	193

12. *Find the maximum and minimum values of y from the following table.*

x	0	1	2	3	4	5
y	0	1/4	0	9/4	16	225/4

Errors in Numerical Differentiation

We discuss methods with error estimates, to calculate derivatives of the function from a given set of tabular values.

The derivative of the function f at x_0 is

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

This formula gives an obvious way to generate an approximation of $f'(x)$.

That is, we simply compute

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

for small values of h.

First Derivative

To approximate $f'(x_0)$, suppose first that $x_0 \in (a, b)$, where $f \in C^2[a, b]$, and that $x_1 = x_0 + h$ for some $h \neq 0$ that is sufficiently small to ensure that $x_1 \in [a, b]$.

We construct the first Lagrange polynomial

$$p_1(x) = \frac{(x - x_0 - h)}{-h} f(x_0) + \frac{(x - x_0)}{h} f(x_0 + h)$$

for f determined by x_0 and x_1, with its error

$$f(x) = p_1(x) + \frac{(x - x_0)(x - x_0 - h)}{2} f''(\xi)$$

for some ξ in $[a, b]$.

Differentiating gives

$$f'(x) = \frac{f(x_0 + h) - f(x_0)}{h} + D_x \left[\frac{(x - x_0)(x - x_0 - h)}{2} f''(\xi) \right].$$

So

$$f'(x) = \frac{f(x_0+h) - f(x_0)}{h} + \frac{2(x-x_0)-h}{2} f''(\xi) + \frac{(x-x_0)(x-x_0-h)}{2} D_x[f''(\xi)],$$

hence

$$f'(x) = \frac{f(x_0+h) - f(x_0)}{h}.$$

One difficulty with this formula is that we have no information about $D_x[f''(\xi(x))]$, so the truncation error cannot be estimated.

When x is x_0, however, the coefficient of $D_x[f''(\xi(x))]$ is 0, and the formula simplifies to

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

Forward/Backward Difference Formulae for finding First Derivative

For small values of h, the difference quotient $\frac{f(x_0+h)-f(x_0)}{h}$ can be used to approximate $f'(x_0)$ with an error bounded by $\frac{M|h|}{2}$, where M is a bounded on $|f''(x)|$ for $x \in [a, b]$.

This formula is known as the **forward difference formula** if $h > 0$ and the **backward difference formula** if $h < 0$.

To obtain general derivative approximation formulae, suppose that $\{x_0, x_1, \ldots, x_n\}$ are $(n+1)$ distinct numbers in some interval J and that $f \in C^{n+1}(J)$. Then by Lagrange's formula,

$$f(x) = \sum_{k=0}^{n} f(x_k)L_k(x) + \frac{(x-x_0)\cdots(x-x_n)}{(n+1)!}f^{(n+1)}(\xi),$$

for some ξ in J, where $L_k(x)$ denotes the kth **Lagrange coefficient polynomial** for f at $x_0, x_1, \ldots, x_n$.

$(n+1)$-point formula

Differentiating this expression gives

$$f'(x) = \sum_{k=0}^{n} f(x_k)L'_k(x) + D_x\left[\frac{(x-x_0)\cdots(x-x_k)}{(n+1)!}f^{(n+1)}(\xi)\right] + \frac{(x-x_0)\cdots(x-x_k)}{(n+1)!}D_x\left[f^{(n+1)}(\xi)\right].$$

We again have a problem estimating the truncation error unless x is one of the numbers x_j. In this case, the term multiplying $D_x\left[f^{(n+1)}(\xi)\right]$ is 0, and the formula becomes

$$f'(x_j) = \sum_{k=0}^{n} f(x_k)L'_k(x) + \frac{f^{(n+1)}(\xi)}{(n+1)!}\prod(x_j - x_k)$$

which is called an **$(n+1)$-point formula** to approximate $f'(x_j)$.

Three-Point Formulae

In general, using more evaluation points in the above equation produces greater accuracy.

We first derive some useful three-point formulae and consider aspects of their errors. Hence

$$
\begin{aligned}
f'(x_j) \quad = \quad & \left[\frac{2x_j - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)}\right] f(x_0) + \left[\frac{2x_j - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)}\right] f(x_1) \\
& + \left[\frac{2x_j - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)}\right] f(x_2) + \frac{1}{6} f^{(3)}(\xi_j) \prod_{\substack{k=0 \\ k \neq j}}^{2} (x_j - x_k)
\end{aligned}
$$

for each $j = 0, 1, 2$, where the notation ξ_j indicates that this point depends on x_j.

The three formulae the above equation become especially useful if the nodes are equally spaced, that is, when

$$x_1 = x_0 + h \quad \text{and} \quad x_2 = x_0 + 2h, \quad \text{for some} \quad h \neq 0.$$

Three-Point Formulae

Since $x_1 = x_0 + h$ and $x_2 = x_0 + 2h$, these formulae can also be expressed as

$$\begin{aligned} f'(x_0) &= \frac{1}{h}\left[\frac{-3}{2}f(x_0) + 2f(x_0+h) - \frac{1}{2}f(x_0+2h)\right] + \frac{h^2}{3}f^{(3)}(\xi_1), \\ f'(x_0+h) &= \frac{1}{h}\left[\frac{-1}{2}f(x_0) + \frac{1}{2}f(x_0+2h)\right] + \frac{h^2}{6}f^{(3)}(\xi_2), \end{aligned}$$

and

$$f'(x_0+2h) = \frac{1}{h}\left[\frac{1}{2}f(x_0) - 2f(x_0+h) + \frac{3}{2}f(x_0+2h)\right] + \frac{h^2}{3}f^{(3)}(\xi_3),$$

where ξ_1, ξ_2, ξ_3 depend on x_0, x_0+h and x_0+2h.

Three-Point Formulae With Error Term

As a matter of convenience, the variable substitution x_0 for $x_0 + h$ is used in the middle equation to change this formula to an approximation fof $f'(x_0)$.

A similar change, x_0 for $x + 0 + 2h$, is used in the last equation. This gives three formulae for approximating $f'(x_0)$

$$
\begin{aligned}
f'(x_0) &= \frac{1}{2h}\Big[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)\Big] + \frac{h^2}{3} f^{(3)}(\xi_1), \\
f'(x_0) &= \frac{1}{2h}\Big[-f(x_0-h) + f(x_0+h)\Big] + \frac{h^2}{6} f^{(3)}(\xi_2),
\end{aligned}
$$

and

$$
f'(x_0) = \frac{1}{2h}\Big[f(x_0-2h) - 4f(x_0+h) + 3f(x_0)\Big] + \frac{h^2}{3} f^{(3)}(\xi_3).
$$

Finally, note that since the last equation can be obtained from the first by simply replacing h with $-h$, there are actually only two formulae

$$f'(x_0) = \frac{1}{2h}\Big[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)\Big] + \frac{h^2}{3} f^{(3)}(\xi_1), \tag{1}$$

where ξ_1 lies between x_0 and $x_0 + 2h$, and

$$f'(x_0) = \frac{1}{2h}\Big[f(x_0+h) - f(x_0-h)\Big] + \frac{h^2}{6} f^{(3)}(\xi_2), \tag{2}$$

where ξ_2 lies between $x_0 - h$ and $x_0 + h$.

Three-Point Formulae

Although the erros in both equations (1) and (2) are $O(h^2)$, the error in equation (2) is approximately half the error in (1). This is because equation (2) uses data on both sides of x_0 and equation (1) uses data on only one side.

Note also that f needs to be evaluated at only two points in equation (2), whereas in equation (1) three evaluations are needed.

The approximation in equation (1) is useful near the ends of an interval, since information about f outside the interval may not be available.

The methods presented in equations (1) and (2) are called **three-point formulae**.

Five-Point Formulae

Similarly, there are **five-point formulae** that involve evaluating the function at two more points, whose error term is $O(h^4)$.

One is, for some ξ between $x_0 + 2h$ and $x_0 + 2h$,

$$f'(x_0) = \frac{1}{22h}\Big[f(x_0 - 2h) - 8f(x_0 - h) - 8f(x_0 + 2h)\Big] + \frac{h^4}{30} f^{(5)}(\xi).$$

The other five point formula is useful for end point approximations. It is, for some ξ between x_0 and $x_0 + 4h$,

$$\begin{aligned} f'(x_0) \quad &= \quad \frac{1}{22h}\Big[-25f(x_0) - 48f(x_0 + h) - 36f(x_0 + 2h) \\ &\qquad +16f(x_0 + 3h) - 3f(x_0 + 4h)\Big] + \frac{h^4}{5} f^{(5)}(\xi). \end{aligned}$$

Left end point approximations are found using this formula with $h > 0$ and **right end point approximations** with $h < 0$.

Higher Derivatives of a Function

Methods can also be derived to find approximations to higher derivatives of a function using only tabulated values of the function at various points. The derivation is algebraically tedious, however, so only a representative procedure will be presented.

Expand a funtion f in a third Taylor polynomial about a point x_0 and evaluate $x_0 + h$ and $x_0 - h$. Then

$$f(x_0 + h) = f(x_0) + f'(x_0) + \frac{1}{2} f''(x_0)h^2 + \frac{1}{6} f'''(x_0)h^3 + \frac{1}{24} f^{(4)}(\xi_1)h^4$$

and

$$f(x_0 - h) = f(x_0) - f'(x_0) + \frac{1}{2} f''(x_0)h^2 - \frac{1}{6} f'''(x_0)h^3 + \frac{1}{24} f^{(4)}(\xi_{-1})h^4$$

where $x_0 - h < \xi_{-1} < x_0 < \xi_1 < x_0 + h$.

Higher Derivatives of a Function

If we add these equations, the terms involving $f'(x_0)$ and $f''(x_0)$ cancel and so,

$$(x_0+h)+f(x_0-h)=2f(x_0)+f''(x_0)h^2+\frac{1}{24}\left[f^{(4)}(\xi_1)+f^{(4)}(\xi_{-1})\right]h^4.$$

Solving this equation for $f''(x_0)$ gives

$$f''(x_0)=\frac{1}{h^2}\Big[f(x_0-h)-2f(x_0)+f(x_0+h)\Big]-\frac{h^2}{24}\Big[f^{(4)}(\xi_1)+f^{(4)}(\xi_{-1})\Big].$$

Suppose $f^{(4)}$ is continuous on $[x_0-h, x_0+h]$.

Higher Derivatives of a Function

Since

$$\frac{1}{h^2}\left[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})\right]$$

is between $f^{(4)}(\xi_1)$ and $f^{(4)}(\xi_{-1})$, the intermediate value theorem implies that a number ξ exists between ξ and ξ_{-1}, and hence in $(x_0 - h, x_0 + h)$, with

$$f^{(4)}(\xi) = \frac{1}{2}\left[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})\right]. \quad \text{Thus}$$

$$f''(x_0) = \frac{1}{h^2}\Big[f(x_0 - h) - 2f(x_0) + f(x_0 + h)\Big] - \frac{h^2}{12} f^{(4)}(\xi),$$

for some ξ, where $x_0 - h < \xi < x_0 + h$. Since $f^{(4)}$ is continuous on $[x_0 - h, x_0 + h]$ it is also bounded, the approximation is $O(h^2)$.

References

1. **Richard L. Burden and J. Douglas Faires**, *Numerical Analysis - Theory and Applications*, Cengage Learning, Singapore.
2. **Kendall E. Atkinson**, *An Introduction to Numerical Analysis*, Wiley India.
3. **David Kincaid and Ward Cheney**, *Numerical Analysis - Mathematics of Scientific Computing*, American Mathematical Society, Providence, Rhode Island.
4. **S.S. Sastry**, *Introductory Methods of Numerical Analysis*, Fourth Edition, Prentice-Hall, India.