Numerical Differentiation

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2017

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Numerical differentiation

Formulas for numerical derivatives are important in developing algorithms for solving boundary value problems for ordinary differential equations and partial differential equations. Standard examples of numerical differentiation often use known functions so that the numerical approximation can be compared with the exact answer. For illustration, we use Bessel function $J_1(x)$, whose tabulated values can be found in standard reference books. Eight equally spaced points over $[0, 7]$ are $(0, 0.0000)$, $(1, 0.4400)$, $(2, 0.5767)$, $(3, 0.3391)$, $(4, -0.0660)$,

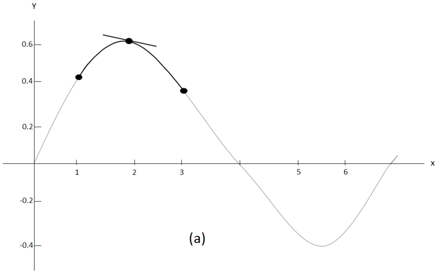


Figure: (a) the tangent to $p_2(x)$ at $(2, 0.5767)$with the slope $p_2'(2) = -0.0505$ (b) the tangent to $p_4(x)$ at $(2, 0.5767)$ with slope $p_4'(2) = -0.0618$

$(5,-0.3276), (6,-0.2767), and (7,-0.004)$. The underlying principle is differentiation of an interpolation polynomial. Let us focus our attention on finding $J_1'(2)$. The interpolation polynomial $p_2(x) = -0.0710 + 0.6982x - 0.1872x^2$ passes trough the three point $(1, 0.4400), (2, 0.5767), and (3, 0.3391)$ and is used to obtain $J_1'(2) \approx P_2'(2) = -0.0505$.this quadratic polynomial $P_2(x)$ and its tangent line at $(2, J_1(2))$ are shown in figure 6.1 (a). If five interpolation points are used, a better approximation can be determined. The polynomial $p_4(x) = 0.4986x + 0.011x^2 - 0.0813x^3 + 0.0116x^4$passes through $(0, 0.0000), (1, 0.4400), (2, 0.5767), (3, 0.3391) and (4, -0.0660)$ and is used to obtain $J_1'(2) \approx P_4'(2) = -0.0618$.

The quadratic polynomial P_4 and its tangent line at $(2, J_1(2))$ are shown in figure 6.1(b). the true value for the derivative is $J_1'(2) = -0.06445$, and the errors in $p_2(x) and P_4(x)$ are -0.0140 and -0.0026, respectively. In this chapter we develop the introductory theory needed to investigate the accuracy of numerical differentiation.

Approximating The Derivative

We now turn our attention to the numerical process for approximating the derivative of $f(x)$:

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

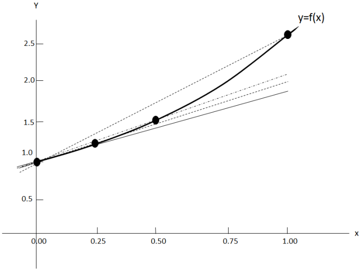
The method seems straightforward; choose a sequence h_k so that $h_k \to 0$ and compute the limit of the sequence:

$$D_k = \frac{f(x+h_k) - f(x)}{h_k} \quad for \;\; k = 1, 2, ..., n, ... \tag{2}$$

The reader may notice that we will only compute a finite number of terms $D_1, D_2, ..., D_N$ in the sequence (2), and it appears that we should use D_N for our answer. The following question is often posed: Why compute $D_1, D_2, ..., D_{N-1}$? Equivalently, we could ask : What value h_N should be chosen so that D_N is a good approximation to the derivative $f'(x)$? To answer this question, we must look at an example to see why there is no simple solution.

For example, consider the function $f(x) = e^x$ and use the step sizes $h = 1, 1/2, 1/4$ to construct the secant lines between point (0,1)and $(h, f(h))$ respectively. As h gets small, the secant line approaches the tangent line as shown in figure 6.2. Although figure 6.2 gives a good visualization of the process described in (1),we must make numerical computation with $h = 0.00001$ to get an acceptable numerical answer, and for this value of h the graphs of the tangent line and secant line would be indistinguishable

figure 6.2 several secant lines for $y = e^x$



Example 6.1 Let $f(x) = e^x$ and $x = 1$. Compute the difference quotients D_k using the step sizes $h_k = 10^{-k}$ for $k = 1, 2, ..., 10$. Carry out nine decimal places in all calculations
. A table of the values $f(1 + h_k)$ and $(f(1 + h_k) - f(1))/h_k$ that are used in the computation of D_k is shown in

h_k	$f_k = f(1 + h_k)$	$f_k - e$	$D_k = (f_k - e)/h_k$
$h_1 = 0.1$	3.004166024	0.285884196	2.858841960
$h_2 = 0.01$	2.745601015	0.027319187	2.731918700
$h_3 = 0.001$	2.721001470	0.002719642	2.719642000
$h_4 = 0.0001$	2.718553670	0.000271842	2.718420000
$h_5 = 0.00004$	2.718309011	0.000027183	2.718300000
$h_6 = 10^{-6}$	2.718284547	0.000002719	2.719000000
$h_7 = 10^{-7}$	2.718282100	0.000000272	2.720000000
$h_8 = 10^{-8}$	2.718281856	0.000000028	2.800000000
$h_9 = 10^{-9}$	2.718281831	0.000000003	3.000000000
$h_10 = 10^{-10}$	2.718281828	0.000000000	0.000000000

table Finding the difference quotients $D_k = (e^{1+h_k} - e)/h_k$

Numerical Differentiation

The largest value $h_1 = 0.1$ does not produce a good approximation $D_1 \approx f'(1)$. Because the step size h_1 is too large and the difference quotient is the slope of the secant line through two points that are not close enough to each other. When formula (2) is used with a fixed precision of nine decimal places, h_9 produced the approximation $D_9 = 3$ and h_10 produced $D_10 = 0$. If h_k is too small, Then the computer function values $f(x+h_k)$ and $f(x)$ are very close together. the difference $f(x+h_k) - f(x)$ can exhibit the problem of loss of significance due to the subtraction of quantities that are nearly equal. The value h_{10}^{-10} is so small that the stored values of $f(x+h_{10})$ and $f(x)$ are the same, and hence the computed difference quotient is zero.

In example 6.1 the mathematical value for the limit is $f'(1) \approx 2.718281828$. observe that the value $h_5 = 10^{-5}$ gives the best approximation, $D_5 = 2.7183$.
Example 6.1 shows that is not easy to find numerically the limit in the equation(2). the sequence start to converge to e, and D_5, is the closest; then the terms move away form e. The terms in the sequence D_k should be computed until $|D_{N+1} - D_N| \geq |D_N - D_{N-1}|$.This is an attempt to determinate the best approximation before the term star to move away from the limit. When this criterion is applied to example 6.1, we have $0.0007 = |D_6 - D_5| > |D_5 - D_4| = 0.00012$;hence$D_5$ is the answer we choose. We now proceed to develop formulas that give a reasonable amount of accuracy for larger values of h.

Central-Difference Formulas

If the function $f(x)$ can be evaluated at values that lie to the left and right of x, then the best two-points formula will involve abscissas that are chosen symmetrically on both sides of x.

theorem 6.1 (centered formula of order $O(h^2)$)

Assume that $f \in C^3[a,b]$ and that $x-h, x+h \in [a,b]$ then

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h} \tag{3}$$

Furthermore, there exist a number $c = c(x) \in [a, bsuchthat]$

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + E_{trunc}(f,h) \tag{4}$$

where $E_{trunc}(f,h) = -\frac{h^2 f^{(3)}(c)}{6} = O(h^2)$

The term $E(f,h)$ is called the truncation error
proof start with the second-degree Taylor expansions $f(x) = p_2(x) + E_2(x)$, about x, for $f(x+h)$ and $f(x-h)$:

$$f(x+h) = f(x) + f'(x)h + \frac{f^{(2)}(x)h^2}{2!} + \frac{f^{(3)}(c_1)h^3}{3!} \quad (5)$$

and

$$f(x-h) = f(x) - f'(x)h + \frac{f^{(2)}(x)h^2}{2!} - \frac{f^{(3)}(c_2)h^3}{3!} \quad (6)$$

after(6) is subtracted from(5), the result is

$$f(x+h) - f(x-h) = 2f'(x)h + \frac{((f^{(3)}(c_1) + f^{(3)}(c_2))h^3}{3!} \quad (7)$$

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since $f^{(3)}(x)$ is continuous, the intermediate value theorem can be used to find a value c son that

$$\frac{f^{(3)}(c_1)+f^{(3)}(c_2)}{2}=f^{(3)}(c) \tag{8}$$

This can be substituted into (7) and the terms rearranged to yield

$$f'(x)=\frac{f(x+h)-f(x-h)}{2h}-\frac{f^{(3)}(c)}{3!} \tag{9}$$

The first term in (9) is the central-difference formula (3),the second term is the truncation error, and the proof is complete.

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suppose that the value of the third derivative $f^{(3)}(c)$ does not change too rapidly; then the truncation error in (4) goes to zero in the same manner as h^2, which is expressed by using the notation $O(h^2)$.when computer calculations are used, it i not desirable to choose h too small. For this reason it is useful to have a formula for approximating $f'(x)$ that has a truncation error term of the order $O(h^4)$.

theorem 6.2 (centered formula of order $O(h^4)$)
Assume that $f \in C^5[a,b]$ and that $x-2h, x-h, x+h, x+2h \in [a,b]$. then

$$f'(x) = \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h} \tag{10}$$

furthermore, there exist a number $c = c(x) \in [a,b]$such that

$$f'(x) = \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h} + E_{trunc}(f,h) \tag{11}$$

where

$$E_{trunc}(f,h) = -\frac{h^4 f^{(5)}(c)}{30} = O(h^4)$$

proof

One way to derive formula (10) is as follows. Start with the difference between the fourth-degree Taylor expansions $f(x) = P_4(x) + E_4(x)$, about x, of $f(x+h)$ and $f(x-h)$:

$$f(x+h) - f(x-h) = 2f'(x)h + \frac{2f^{(3)}(x)h^3}{3!} + \frac{2f^{(5)}(c_1)h^5}{5!} \tag{12}$$

then use the step size 2h, instead of h, and write down the following approximation-.

$$f(x+2h) - f(x-2h) = 4f'(x)h + \frac{16f^{(3)}(x)h^3}{3!} + \frac{64f^{(5)}(c_2)h^5}{5!} \tag{13}$$

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Next multiply the terms in equation (12) by 8 and substract (13) form it. The terms involving $f^3(x)$will be delimited and we get

$$-f(x+2h)+8f(x+h)-8f(x-h)+f(x-2h)= \tag{14}$$

$$12f'(x)h+\frac{(16f^{(5)}(c_1)-64f^{(5)}(c_2))h^5}{120}$$

If $f^{(5)}(x)$ has one sign and if its magnitude does not change rapidly, we can find a value c that lies in $[x-2h,x+2h]$so that

$$16f^{(5)}(c_1)-64^{(5)}(c_2)=-48f^{(5)}(c) \tag{15}$$

After(15) is substituted into (14) and the result is solved for $f'(x)$, we obtain

$$f'(x) = \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h} + \frac{f^{(5)}(c)h^4}{30} \quad (16)$$

The first term on the right side of(16) is the central-difference formula (10) and the second term is the truncation error, the theorem is proved. suppose that $|f^{(5)}(c)|$ is bounded for $c \in [a,b]$;then the truncation error in(11)goes to zero in the same manner as h^4, which is expressed with notation $O(h^4)$. Now we can make a comparison of the two formulas(3) and (10). Suppose that $f(x)$ has five continuous derivatives and that$|f^{(3)}(c)|$ and $|f^{(5)}(c)|$ are about the same. Then the truncation error for the fourth-order formula (10) is $O(h^4)$ and will go to zero faster than the truncation error $O(h^2)$ for the second-order formula(3). This permits the use of larger step size

example 6.2

Let $f(x) = cos(x)$ (a) Use formulas (3) and (10) with step sizes $h = 0.1, 0.01, 0.001$ and $0.0001$and calculate the aproximationsfor $f'(0.8)$. Carry nine decimal placesin all the calculations.

(b) Compare with the true calue $f'(0.8) = -sin(0.8)$.

(a) using th formula (3) with h =0.01, we get

.

$$f'(0.8) \approx \frac{f(0.81) - f(0.79)}{0.02} \approx \frac{0.689498433 - 0.703845316}{0.02} \approx -0.717344150$$

.

using formula (10) with $h = 0.01$

.

$$f'(0.8) \approx \frac{-f(0.82) + 8f(0.81) - 8f(0.79) + f(0.78)}{0.12} \approx -0.717356108$$

(b) The error in approximation formulas (3)and (10) turns out to be -0.000011941 and 0.000000017, respectively. In this example,formula(10) gives a better approximation to$f'(0.8)$ than formula (3) when h=0.01. The error analysis will illuminate this example and show why this happened. the other calculations are summarized in table 6.2

step size	aproximation by formula(3)	error using formula (3)	aproximationby formula(10)	error using formula (10)
0.1	-0.716161095	-0.001194996	-0.717353703	-0.000002389
0.01	-0.717344150	-0.000011941	-0.717353108	-0.000000017
0.001	-0.717356000	-0.000000091	-0.717356167	-0.000000076
0.0001	-0.717360000	-0.000003909	-0.717360833	-0.000004742

table6.2 Numerical differentiation using formular (3) and (10)

Error Analysis and Optimum Step Size

An important topic in the study of numerical differentiation is the effect of the computer's round-off error. Let us examine the formulas more closely. Assume that a computer is used to make numerical computation and that

$f(x_0 - h) = y_{-1} + e_{-1}$ and $f(x_0 + h) = y_1 + e_1$

Where $f(x_0 - h)$ and $f(x_0 + h)$ are aproximated by the numerical values y_{-1} and y_1, and e_{-1} and e_1 are associated roud-off errors, respectively. the following result indicates the complex nature of errors analysis for numerical differentiation.

corollary 6.1 (a)

Assume that f satisfies the hypotheses of theorem 6.1 and use the computational formula

$$f'(x_0) \approx \frac{y_1 - y_{-1}}{2h} \tag{17}$$

The error analysis is explained by the following equations:

$$f'(x_0) = \frac{y_1 - y_{-1}}{2h} + E(f,h) \tag{18}$$

where

$E(f,h) = E_{round}(f,h) + E_{trunc}(f,h)$

$$= \frac{e_1 - e_{-1}}{2h} - \frac{h^2 f^{(3)(c)}}{6} \tag{19}$$

where the total error term E(f,h) has a part due round-off error pplus a part due to truncation error

corollary 6.1 (b)
assumee that f satisfies the hypotheses of theorem 6.1 and that numerical computations are made. If $|e_{-1}| \leq \epsilon, |e_1| \leq \epsilon$, and $M = max_{a \leq x \leq b}|f^{(3)}(x)|$ then

$$|E(f,h)| \leq \frac{\epsilon}{h} + \frac{Mh^2}{6} \tag{20}$$

and the value of h that minimizes the right-hand side of (20)is

$$h = (\frac{3\epsilon}{M})^{1/3} \tag{21}$$

When h is small. the portion of (19) involving $(e_1 - e_{-1})/2h$ can be relatively large. In Example 6,2, when h=0.0001, this difficulty was encountered. The round-off errors

$$f(0.8001) = 0.696634970 + e_1 \text{ where } e_1 = -0.0000000003$$
$$f(0.7999) = 0.696778442 + e_{-1} \text{ where } e_1 = 0.0000000005$$

The truncation error term is

$$\frac{-hf^{(3)}(c)}{6} \approx -(0.0001)^2 (\frac{sin(0.8)}{6}) \approx 0.0000000001$$

The error term $E(f,h)$ in (19) can be estimated:

$$E(f,h) \approx \frac{-0.0000000003 - 0.0000000005}{0.0002} - 0.000000001 = -0.000004001$$

Indeed, the computed numerical approcimation for the derivative using $h = 0.0001$ is found by the calculation

$$f'(0,8) \approx \frac{f(0.8001) - f(0.7999)}{0.0002} = -0.717360000$$

And a loss of about four significant digits is evident. The error is -0.000003909 and this is close to the predicted error -0.000004001. When formula (21) is applied to example 6.2, we can use the bound $|f^{(3)}(x)| < |sin(x)| \leq 1 = M$ and the value $\epsilon = 0.5 * 10^{-9}$ for the magnitude if the round-off. The optimal value for h is easily calculated: $h = (1.5 * 10^{-9}/1)^{1/3} = 0001144714$. The step size h=0.001 was closet to the optimal value 0.001144714 and it give the best approximation to $f'(0.8)$ among the four choices involving formula (3)(see table 6.1 and figure 6.3).

An error analysis of formula (10) is similar. Assume that computer is used to make numerical computations and that $f(x_0 + kh) = y_k + e_k$.

corollary 6.2 (a)

Assume that f satisfies the hypotheses of the theorem 6.2 and use the computational formula

$$f'(x_0) \approx \frac{-y_2 + 8y_1 - 8y_{-1} + y_{-2}}{12h} \tag{22}$$

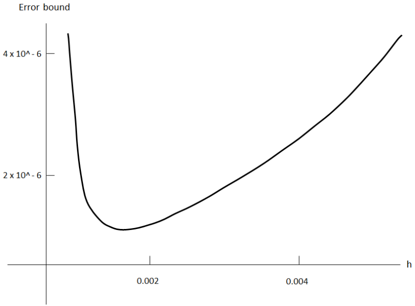

figure 6.3

Finding the optimal step size $h = 0.0011447714$ when formula (21) is applied to $f(x) = cos(x)$ in example 6.2.

The error analysis is explained by the following equations:

$$f'(x_0) = \frac{-y_2 + 8y_1 - 8y_{-1} + y_{-2}}{12h} + E(f,h) \tag{23}$$

where

$E(f,h) = E_{round}(f,h) + E_{trunc}(f,h)$

$$= \frac{ey_2 + 8e_1 - 8e_{-1} + e_{-2}}{12h} + \frac{h^4 f^{(5)}(c)}{30} \tag{24}$$

where the total error term $E(f,h)$, has a part due to round-off error plus a part due to truncation error .

corollary 6.2 (b)

Assume that f satisfies the hypotheses of theorem 6.2 and that numerical computations are made.$|e_k| \leq \epsilon$ and $M = max_{a \leq x \leq b}|f^{(5)}(x)|$

$$|E(f,h)| \leq \frac{3\epsilon}{2h} + \frac{Mh^4}{30} \tag{25}$$

and the value of h that minimizes the right-hand side of (25) is

$$h = (\frac{45\epsilon}{4M})^{1/5} \tag{26}$$

When formula(25) is applied to example 6.2 we can use the bound $f^{(5)}(x) \leq |sin(x)| \leq 1 = M$ and the value $\epsilon = 0.5 * 10^{-9}$ for the magnitude of the round-off error. The optimal value for h us easily calculated : $h = (22.5 * 10^{-9}/4)^{1/5} = 0.022388475$. The step size $h = 0.01$ was closest to the optimal value 0.22388475 and it give the best approximation to $f'(0.8)$ among the four choices involving formula (see table 6.2 and figure 6.4).

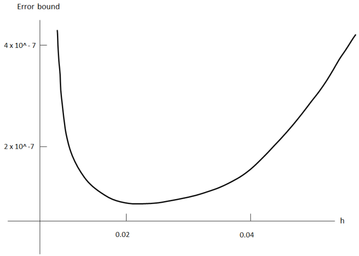

figure 6.4

Finding the optimal step size $h = 0.022388475$ when formula (26) is applied to $f(x) = cos(x)$ in example 6.2.

We should not end the discussion of example 6.2 without mentioning that numerical differentiation formulas can be obtained by an alternative derivation.They can be derived by differentiation of an interpolation polynomial. For example, the Lagrange form of the quadratic polynomial $p_2(x)$ that passe through the three points $(0.7, cos(0.7)), (0.8, cos(0.8)), (0.9, cos(0.9))$ is

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$$p_2 = 38.2421094(x-0.8)(x-0.9) - 69.6706709(x-0.7)(x-0.9) + 31.0804984(x-0.7)(x-0.8).$$

This polynomial can be expanded to obtain the usual form:

$$p_2 = 1.046875165 - 0.159260044x - 0.348063157x^2$$

A similar computation can be used to obtain the quartic polynomial $p_4(x)$ that passes through the points $(0.6, cos(0.6)), (0.7, cos(0.7)), (0.8, cos(0.8)), (0.9, cos(0.9))$ and $(1.0, cos(1.0))$:

$$p_4 = 0.998452927 + 0.009638392x - 0.523291341x^2 + 0.026521229x^3 + 0.028981100x^4$$

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When these polynomials are differentiated, they produce $p_2'(0.8) = -0.716161095$ and $p_4'(0.8) = -0.717353703$,which agree with the values listed under $h = 0.1$ in table 6.2. The graphs of $p_2(x)$ and $p_4(x)$ and their tangent lines at $(0.8, cos(0.8))$ are shown in figure 6.5(a) and (b) respectively

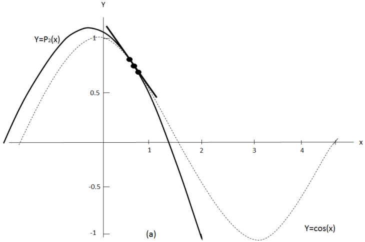

figure 6.5 (a) The graph of $y = cos(x)$ and the interpolating polynomial $p_2(x)$ used to estimate $f'(0.8) \approx p_2'(0.8) = -0.716161095$ (b) The graph of $y = cos(x)$ and the interpolating polynomial $p_4(x)$ used to estimate $f'(0.8) \approx p_4'(0.8) = -0.717353703$

Richardson's Extrapolation
In this section we emphasize the relationship between formulas (3) and (10). Let $f_k = f(x_k) = f(x_0 + kh)$, and use the notation $D_0(h)$ and $D_0(2h)$ to denote the approximations to $f'(x_0)$ that are obtained from (3) with step sizes h and 2h, respectively :

$$f'(x_0) \approx D_0(h) + Ch^2 \tag{27}$$

and

$$f'(x_0) \approx D_0(2h) + 4Ch^2 \tag{28}$$

If we multiply relation (27) by 4 subtract relation (28) from this product, the the terms involving C cancel and the result is

$$3f'(x_0) \approx 4D_0(h) - D_0(2h) = \frac{4(f_1 - f_{-1})}{2h} - \frac{f_2 - f_{-2}}{4h} \tag{29}$$

Next solve for $f'(x_0)$ in (29) and get

$$f'(x_0) \approx \frac{4D_0(h) - D_0(2h)}{3} = \frac{-f_2 + 8f_1 - 8f_{-1} + f_{-2}}{12h} \tag{30}$$

the last expression in (30) is the central-difference formula (10)

Example 6.3

Let $f(x) = cos(x)$.Use (27) and (28) with h=0.01, and show how thelinear combination $(4D_0(h) - D_0(2h))/3$ in (30) can be used to obtain the approximation to $f'(0.8)$ given in (10). Carry nine decimal places in all the calculations.

Use (27) and (28) with $h = 0.01$ to get

$$D_0(h) \approx \frac{f(0.81) - f(0.79)}{0.02} \approx \frac{0.689498433 - 0.703845316}{0.02}$$
$$\approx -0.717344150$$

and

$$D_0(2h) \approx \frac{f(0.82) - f(0.78)}{0.04} \approx \frac{0.682221207 - 0.710913538}{-0.717308275}$$
$$\approx -0.717308275$$

Now the linear combination in (30) is computed:

$$f'(0.8) \approx \frac{4D_0(h) - D_0(2h)}{3} \approx \frac{4(-0.717344150) - (-0.717308275)}{3}$$
$$\approx -0.717356108.$$

This is exactly the same as the solution in Example 6.2 that used (10) directly to approximate $f'(0.8)$.

The method of obtaining a formula for $f'(x_0)$ of higher order from a formula of lower order is called ***extrapolation***. The proof requires that the error term for (3) can be expanded in a series containing only even powers of h. we have already seen how to use step sizes h and $2h$ to remove the term involving h^2. To see how h^4 is removed, let $D_1(h)$ and $D_1(2h)$ denote the approximations to $f'(x_0)$ of order $O(h^4)$ obtained with formula (16) using step sizes h and $2h$, respectively. Then

$$(31) \qquad f'(x_0) = \frac{-f_2 + 8f_1 - 8f_{-1} + f_{-2}}{24h} + \frac{h^4 f^{(5)}(c_1)}{30} \approx D_1(h) + Ch^4$$

and

(32) $$f'(x_0) = \frac{-f_4 + 8f_2 - 8f_{-2} + f_{-4}}{12h} + \frac{16h^4 f^{(5)}(c_2)}{30} \approx D_1(2h) + 16Ch^4.$$

Suppose that $f^{(5)}(x)$ has one sign and does not change too rapidly; then the assumption that $f^{(5)}(c_1) \approx f^{(5)}(c_2)$ can be used to eliminate the terms involving h^4 in (31) and (32), and the result is

(33) $$f'(x_0) \approx \frac{16D_1(h) - D_1(2h)}{15}$$

The general pattern for improving calculations is stated in the next result.

Theorem 6.3 (Richardson's Extrapolation). Suppose that two approximations of order $O(h^{2k})$ for $f'(x_0)$ are $D_{k-1}(h)$ and $D_{k-1}(2h)$ and that they satisfy

(34) $$f'(x_0) = D_{k-1}(h) + c_1 h^{2k} + c_2 h^{2k+2} + \ldots$$

and

(35) $$f'(x_0) = D_{k-1}(2h) + 4^k c_1 h^{2k} + 4^{k+1} c_2 h^{2k+2} + \ldots$$

Then an improved approximation has the form

(36) $$f'(x_0) = D_k(h) + O(h^{2k+2}) = \frac{4^k D_{k-1}(h) - D_{k-1}(2h)}{4^k - 1} + O(h^{2k+2}).$$

More Central-Difference Formulas

The formulas for $f'(x_0)$ in the preceding section required that the function can be computed at abscissas that lie on both sides of x, and they were referred to as central-difference formulas. Taylor series can be used to obtain central-difference formulas for the higher derivatives. The popular choices are those of order $O(h^2)$ and $O(h^4)$ and are given in Tables 6.3 and 6.4. In these tables we use the convention that $f_k = f(x_0 + kh)$ for $k = -3, -2, -1, 0, 1, 2, 3$. For illustration, we will derive the formula for $f''(x)$ of order $0(h^2)$ in Table 6.3. Start with the Taylor expansions

$$(1) \quad f(x+h) = f(x) + hf'(x) + \frac{h^2 f''(x)}{2} + \frac{h^3 f^{(3)}(x)}{6} + \frac{h^4 f^{(4)}(x)}{24} + \ldots$$

Table 6.3 Central-Difference Formulas of Order $O(h^2)$

$$f'(x_0) \approx \frac{f_1 - f_{-1}}{2h}$$

$$f''(x_0) \approx \frac{f_1 - 2f_0 + f_{-1}}{h^2}$$

$$f^{(3)}(x_0) \approx \frac{f_2 - 2f_1 + 2f_{-1} - f_{-2}}{2h^3}$$

$$f^{(4)}(x_0) \approx \frac{f_2 - 4f_1 + 6f_0 - 4f_{-1} + f_{-2}}{h^4}$$

Table 6.4 Central-Difference Formulas of Order $O(h^4)$

$$f'(x_0) \approx \frac{-f_2 + 8f_1 - 8f_{-1} + f_{-2}}{12h}$$

$$f''(x_0) \approx \frac{-f_2 + 16f_1 - 30f_0 + 16f_{-1} - f_{-2}}{12h^2}$$

$$f^{(3)}(x_0) \approx \frac{-f_3 + 8f_2 - 13f_1 + 13f_{-1} - 8f_{-2} + f_{-3}}{8h^3}$$

$$f^{(4)}(x_0) \approx \frac{-f_3 + 12f_2 - 39f_1 + 56f_0 - 39f_{-1} + 12f_{-2} - f_{-3}}{6h^4}$$

$$(2) \quad f(x-h) = f(x) - hf'(x) + \frac{h^2 f''(x)}{2} - \frac{h^3 f^{(3)}(x)}{6} + \frac{h^4 f^{(4)}(x)}{24} - \ldots$$

Adding equations (1) and (2) will eliminate the terms involving the odd derivatives $f'(x), f^3(x), f^5(x), \ldots$

$$(3) \qquad f(x+h) + f(x-h) = 2f(x) + \frac{h^2 f''(x)}{2} + \frac{h^4 f^{(4)}(x)}{24} + \ldots$$

Solving equation (3) for $f''(x)$ yields

$$(4) \qquad f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{2h^2 f^{(4)}(x)}{4!} - \frac{2h^4 f^{(6)}(x)}{6!} - \ldots - \frac{2h^{2k-2} f^{(2k)}(x)}{(2k)!} - \ldots$$

If the series in (4) is truncated at the fourth derivative, there exist a value c that lies in $[x-h, x+h]$, so that

$$(5) \qquad f''(x_0) = \frac{f_1 - 2f_0 + f_{-1}}{h^2} - \frac{h^2 f^{(4)}(c)}{12}$$

This gives us the desired formula for approximating f”(x):

$$(6) \qquad f''(x_0) \approx \frac{f_1 - 2f_0 + f_{-1}}{h^2}$$

Example 6.4. Let $f(x) = cos(x)$.

(a) Use formula (6) with $h = 0.1, 0.01$, and 0.001 and find approximations to $f''(0.8)$. Carry nine decimal place in all calculations.

(b) Compare with the true value $f''(0.8) = -cos(0.8)$.

(a) The calculation for $h = 0.01$ is

$$f''(0.8) \approx \frac{f(0.81) - 2f(0.80) + f(0.79)}{0.0001}$$

$$\approx \frac{0.689498433 - 2(0.696706709) + 0.703845316}{0.0001}$$

$$\approx -0.696690000.$$

(b) The error in this approximation is .0.000016709. the other calculations are summarized in Table 6.5. The error analysis will illuminate this example and show why $h = 0.01$ was best.

Table 6.5 Numerical Approximations to $f''(x)$ for Example 6.4

Step size	Approximation by formula (6)	Error using formula (6)
$h = 0.1$	-0.696126300	-0.000580409
$h = 0.01$	-0.696690000	-0.000016709
$h = 0.001$	-0.696000000	-0.000706709

Error Analysis

Let $f_k = y_k + e_k$, where e_k is the error in computing $f(x_k)$, including noise in measurement and round-off error. Then formula (6) can be written

$$f''(x_0) = \frac{y_1 - 2y_0 + y_{-1}}{h^2} + E(f,h). \tag{7}$$

The error term $E(h,f)$ for the numerical derivative (7) will have a part due to round-off error and a part due to truncation error:

$$E(f,h) = \frac{e_1 - 2e_0 + e_{-1}}{h^2} - \frac{h^2 f^{(4)}(c)}{12} \tag{8}$$

If it is assumed that each error e_k is of the magnitude $\in$, with signs that accumulate errors, and that $\mid f^{(4)}(x) \leq M \mid$, then we get the following error bound:

(9) $$\mid E(f,h) \mid \leq \frac{4 \in}{h^2} + \frac{Mh^2}{12}.$$

If h is small, then the contribution $4 \in /h^2$ due to round-off error is large. When h is large, the contribution $Mh^2/12$ is large. The optimal step size will minimize the quantity

(10) $$g(h) = \frac{4 \in}{h^2} + \frac{Mh^2}{12}.$$

Setting $g'(k) = 0$ results in $-8 \in /h^3 + Mh/6 = 0$, which yields the equation $h^4 = 48 \in /M$, from which we obtain the optimal value:

(11) $$h = \left(\frac{48 \in}{M}\right)^{1/4}.$$

When formula (11) is applied to Example 6.4, use the bound $\mid f^4 \mid \leq \mid cos(x) \mid \leq 1 = M$ and the value $\in = 0.5 \times 10^{-9}$. The optimal step size is $h = (24 \times 10^{-9}/1)^{1/4} = 0.01244666$, and we see that $h = 0.01$ was closest to the optimal value.

Since the portion of the error due to round off is inversely proportional to the square of h, this term grows when h gets small. this is sometimes referred to as the **step-size dilemma**. One partial solution ti this problem is to use a formula of higher order in that a larger value of h will produce the desired accuracy. The formula for $f''(x_0)$ of order $O(h^4)$ in Table 6.4 is

(12) $$f''(x_0) = \frac{-f_2 + 16f_1 - 30f_0 + 16f_{-1} - f_{-2}}{12h^2} + E(f,h)$$

The error term for (12) has the form

(13)
$$E(f,h) = \frac{16 \in}{3h^2} + \frac{h^4 f^{(6)}(c)}{90},$$

where c lies in the interval $[x-2h, x+2h]$. A bound for $\mid E(f,h) \mid$ is

(14)
$$\mid E(f,h) \mid \leq \frac{16 \in}{3h^2} + \frac{h^4 M}{90}.$$

where $\mid f^{(6)}(x) \leq M \mid$. The optimal value for h is given by the formula

(15)
$$h = (\frac{240 \in}{M})^{1/6}.$$

Example 6.5. Let $f(x) = \cos(x)$.

(a) Use formula (12) with $h = 1.0, 0.1$, and 0.01 and find approximations to $f''(0.8)$. Carry nine decimal places in all the calculations.

(b) Compare with the true value $f''(0.8) = -\cos(0.8)$.

(c) Determine the optimal step size.

(a) The calculation for $h = 0.1$ is

$$
\begin{aligned}
&f''(0.8) \\
&\quad\approx \frac{-f(1.0) + 16f(0.9) - 30f(0.8) + 16f(0.7) - f(0.6)}{0.12} \\
&\quad\approx -0.696705958.
\end{aligned}
$$

(b) The error in this approximation is -0.000000751. The other calculations are summarized in Table 6.6.

(c) When formula (15) is applied, we can use the bound $|f^{(6)}(x)| \leq |\cos(x)| \leq 1 = M$ and the value $\in = 0.5 \times 10^{-9}$. These values give the optimal step size $h = (120 \times 10^{-9}/1)^{1/6} = 0.070231219$.

Step size	Approximation by formula (12)	Error using formula (12)
$h = 0.1$	-0.689625413	-0.007081296
$h = 0.01$	-0.696705958	-0.000000751
$h = 0.001$	-0.696690000	-0.000016709

Table 6.7 Forward and Backward-Difference Formulas of Order $O(h^2)$

$$f'(x_0) \approx \frac{-3f_0 + 4f_1 - f_2}{2h} \quad \text{(forward difference)}$$

$$f'(x_0) \approx \frac{3f_0 - 4f_{-1} + f_{-2}}{2h} \quad \text{(backward difference)}$$

$$f''(x_0) \approx \frac{2f_0 - 5f_1 + 4f_2 - f_3}{h^2} \quad \text{(forward difference)}$$

Numerical Differentiation

$$f''(x_0) \approx \frac{2f_0 - 5f_{-1} + 4f_{-2} - f_{-3}}{h^2}$$ (backward difference)

$$f^{(3)}(x_0) \approx \frac{-5f_0 + 18f_1 - 24f_2 + 14f_3 - 3f_4}{2h^3}$$

$$f^{(3)}(x_0) \approx \frac{5f_{-0} - 18f_{-1} + 24f_{-2} - 14f_{-3} + 3f_{-4}}{2h^3}$$

$$f^{(4)}(x_0) \approx \frac{3f_0 - 14f_1 + 26f_2 - 24f_3 + 11f_4 - 2f_5}{h^4}$$

$$f^{(4)}(x_0) \approx \frac{3f_0 - 14f_{-1} + 26f_{-2} - 24f_{-3} + 11f_{-4} - 2f_{-5}}{h^4}$$

Numerical Differentiation

Generally, if numerical differentiation is performed, only about half the accuracy of which the computer is capable is obtained. This severe loss of significant digits will almost always occur unless we are fortunate to find a step size that is optimal. Hence we must always proceed with caution when numerical differentiation is performed. The difficulties are more pronounced when working with experimental data, where the function values have been rounded to only few digits. If a numerical derivative must be obtained form data, we should consider curve fitting, by using least-squares techniques, and differentiate the formula for the curve.

Differentiation of the Lagrange Polynomial

If the function must be evaluated at abscissas that lie on one side of x_0, the central-difference formulas cannot be used. Formulas for equally spaced abscissas that lie to the right (or left) of x_0 are called forward (or backward) -difference formula. These formulas can be derived by differentiation of the Lagrange interpolation polynomial. some of the common forward- and backward-difference formulas are given in Table 6.7.

Example 6.6. Derive the formula

$$f''(x_0) \approx \frac{2f_0 - 5f_1 + 4f_2 - f_3}{h^2}.$$

Start with the Lagrange interpolation polynomial for $f(t)$ based on the four points x_0, x_1, x_2, and x_3.

Numerical Differentiation

$$f(t) \approx f_0 \frac{(t-x_1)(t-x_2)(t-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)} + f_1 \frac{(t-x_0)(t-x_2)(t-x_3)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)}$$

$$+ f_2 \frac{(t-x_0)(t-x_1)(t-x_3)}{(x_2-x_0)(x_2-x_1)(x_0-x_3)} + f_3 \frac{(t-x_0)(t-x_1)(t-x_2)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)}$$

Differentiate the products in the numerators twice and get

$$f''(t) \approx$$

$$f_0 \frac{2((t-x_1)+(t-x_2)+(t-x_3))}{(x_0-x_1)(x_0-x_2)(x_0-x_3)} + f_1 \frac{2((t-x_0)+(t-x_2)+(t-x_3))}{(x_1-x_0)(x_1-x_2)(x_1-x_3)}$$

$$+ f_2 \frac{2((t-x_0)+(t-x_1)+(t-x_3))}{(x_2-x_0)(x_2-x_1)(x_0-x_3)} + f_3 \frac{2((t-x_0)+(t-x_1)+(t-x_2))}{(x_3-x_0)(x_3-x_1)(x_3-x_2)}$$

Numerical Differentiation

Then substitution of $t = x_0$ and the fact that $x_i - x_j = (i-j)h$ produces

$$
\begin{aligned}
f''(t) \approx f_0 & \frac{2((x_0-x_1)+(x_0-x_2)+(x_0-x_3))}{(x_0-x_1)(x_0-x_2)(x_0-x_3)} \\
+f_1 & \frac{2((x_0-x_0)+(x_0-x_2)+(x_0-x_3))}{(x_1-x_0)(x_1-x_2)(x_1-x_3)} \\
+f_2 & \frac{2((x_0-x_0)+(x_0-x_1)+(x_0-x_3))}{(x_2-x_0)(x_2-x_1)(x_0-x_3)} \\
+f_3 & \frac{2((x_0-x_0)+(x_0-x_1)+(x_0-x_2))}{(x_3-x_0)(x_3-x_1)(x_3-x_2)}
\end{aligned}
$$

$$= f_0 \frac{2((-h)+(-2h)+(-3h))}{(-h)(-2h)(-3h)} + f_1 \frac{2((0)+(-2h)+(-3h))}{(h)(-h)(-2h)}$$

$$+ f_2 \frac{2((0)+(-h)+(-3h))}{(2h)(h)(-h)} + f_3 \frac{2((0)+(-h)+(-2h))}{(3h)(2h)(h)}$$

$$= f_0 \frac{-12h}{-6h^3} + f_1 \frac{-10h}{2h^3} + f_2 \frac{-8h}{-2h^3} + f_3 \frac{-6h}{6h^3} = \frac{2f_0 - 5f_1 + 4f_2 - f_3}{h^2}$$

and the formula is established.

Example 6.7. Derive the formula

$$f'''(x_0) \approx \frac{-5f_0 + 18f_1 - 24f_2 + 14f_3 - 3f_4}{2h^3}$$

Start with the Lagrange interpolation polynomial for $f(t)$ based on the five $x_0, x_1, x2, x_3$, and x_4,

$$f(t) \approx f_0 \frac{(t-x_1)(t-x_2)(t-x_3)(t-x_4)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)(x_0-x_4)}$$

$$+f_1 \frac{(t-x_0)(t-x_2)(t-x_3)(t-x_4)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)(x_1-x_4)}$$

$$+f_2 \frac{(t-x_0)(t-x_1)(t-x_3)(t-x_4)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)(x_2-x_4)}$$

$$+f_3 \frac{(t-x_0)(t-x_1)(t-x_2)(t-x_4)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)(x_3-x_4)}$$

$$+f_4 \frac{(t-x_0)(t-x_1)(t-x_2)(t-x_3)}{(x_4-x_0)(x_4-x_1)(x_4-x_2)(x_4-x_3)}$$

Differentiate the numerators three times, then use the substitution $x_i - x_j = (i-j)h$ in the denominators and get

$$
\begin{aligned}
f'''(t) \approx\ & f_0 \frac{6((t-x_1)+(t-x_2)+(t-x_3)+(t-x_4))}{(-h)(-2h)(-3h)(-4h)} \\
& + f_1 \frac{6((t-x_0)+(t-x_2)+(t-x_3)+(t-x_4))}{(h)(-h)(-2h)(-3h)} \\
& + f_2 \frac{6((t-x_0)+(t-x_1)+(t-x_3)+(t-x_4))}{(2h)(h)(-h)(2h)} \\
& + f_3 \frac{6((t-x_0)+(t-x_1)+(t-x_2)+(t-x_4))}{(3h)(2h)(h)(-h)} \\
& + f_4 \frac{6((t-x_0)+(t-x_1)+(t-x_2)+(t-x_3))}{(4h)(3h)(2h)(h)}
\end{aligned}
$$

Then substitution of $t = x_0$ in the form $t - x_j = x_0 - x_j = -jh$ produces

$$f'''(x_0) \approx$$

$$f_0 \frac{6((-h) + (-2h) + (-3h) + (-4h))}{24h^4} + f_1 \frac{6((0) + (-2h) + (-3h) + (-4h))}{-6h^4}$$

$$+ f_2 \frac{6((0) + (-h) + (-3h) + (-4h))}{4h^4} + f_3 \frac{6((0) + (-h) + (-2h) + (-4h))}{-6h^4}$$

$$+ f_4 \frac{6((0) + (-h) + (-2h) + (-3h))}{24h^4}$$

$$= f_0 \frac{-60h}{24h^4} + f_1 \frac{54h}{6h^4} + f_2 \frac{-48h}{4h^4} f_3 \frac{42h}{6h^4} + f_4 \frac{-36h}{24h^4}$$

$$= f_1 \frac{-5f_0 + 18f_1 - 24f_2 + 14f_3 - 3f_4}{2h^3},$$

and the formula is established.

Differentiation of the Newton Polynomial

In this section we show the relationship between the three formulas of order $O(h^2)$ for approximating $f'(x_0)$, and a general algorithm is given for computing the numerical derivative . In section 4.3 we saw that the Newton polynomial $P(t)$ of degree N=2 that approximates $f(t)$ using the nodes t_0, t_1, and t_2 is

(16) $$P(t) = a_0 + a_1(t - t_0) + a_2(t - t_0)(t - t_1),$$

where $a_0 = f(t_0), a_1 = (f(t_1) - f(t_0))/(t_1 - t_0)$, and

$$a_2 = \frac{\dfrac{f(t_2) - f(t_1)}{t_2 - t_1} - \dfrac{f(t_1) - f(t_0)}{t_1 - t_0}}{t_2 - t_0}$$

The derivative of $P(t)$ is

$$P'(t) = a_1 + a_2((t - t_0) + (t - t_1)),$$

and when it is evaluated at $t = t_0$, the result is

$$P'(t_0) = a_1 + a_2((t_0 - t_1) \approx f'(0).$$

Observe that the nodes t_k do not need to be equally spaced for formulas (16) through (18) to hold. Choosing the abscissas in different orders will produce different formulas for approximating $f'(x)$.

Case (i): If $t_0 = x, t_1 = x + h$, and $t_2 = x + 2h$, then

$$a_1 = \frac{f(x+h) - f(x)}{h},$$

$$a_2 = \frac{f(x) - 2f(x+h) + f(x+2h)}{2h^2},$$

When these values are substituted into (18), we get

$$P'(x) = \frac{f(x+h) - f(x)}{h} + \frac{-f(x) + 2f(x+h) - f(x+2h)}{2h}.$$

This is simplified to obtain

(19) $$P'(x) = \frac{-3f(x) + 4f(x+h) - f(x+2h)}{2h} \approx f'(x)$$

which is the second-order forward-difference formula for $f'(x)$.

Case (ii): If $t_0 = x, t_1 = x + h$, and $t_2 = x - h$, then

$$a_1 = \frac{f(x+h) - f(x)}{h},$$

$$a_2 = \frac{f(x+h) - 2f(x) + f(x-h)}{2h^2},$$

When these values are substituted into (18), we get

$$P'(x) = \frac{f(x+h) - f(x)}{h} + \frac{-f(x+h) + 2f(x) - f(x-h)}{2h}.$$

Numerical Differentiation

This is simplified to obtain

$$P'(x) = \frac{f(x+h) - f(x-h)}{2h} \approx f'(x), \tag{20}$$

which is the second-order central-difference formula for $f'(x)$,

Case (iii): If $t_0 = x, t_1 = x - h$, and $t_2 = x - 2h$, then

$$a_1 = \frac{f(x) - f(x-h)}{h},$$

$$a_2 = \frac{f(x) - 2f(x-h) + f(x-2h)}{2h^2},$$

These values are substituted into (18) and simplified to get

$$P'(x) = \frac{3f(x) - 4f(x-h) + f(x-2h)}{2h} \approx f'(x), \tag{21}$$

which is the second-order backward-difference formula for f'(x).

Numerical Differentiation

The newton polynomial $P(t)$ of degree N that approximates $f(t)$ using the nodes $t_0, t_1, ..., t_N$ is

$$P(t) = a_0 + a_1(t - t_0) + a_2(t - t_0)(t - t_1) + a_3(t - t_0)(t - t_1)(t - t_2) + ... + a_N(t - t_0)...(t - t_{N-1}). \tag{22}$$

The derivative of $P(t)$ is

$$\begin{aligned} P'(t) &= a_1 + a_2((t - t_0) + (t - t_1)) \\ &\quad + a_3((t - t_0)(t - t_1) + (t - t_0)(t - t_2) + (t - t_1)(t - t_2)) \\ &\quad + ... + a_N \textstyle\sum_{k=0}^{N-1} \prod_{j=0}^{N-1} (t - t_j), j \neq k \end{aligned} \tag{23}$$

When $P'(t)$ is evaluated at $t = t_0$, several of the terms in the summation are zero, and $P'(t_0)$ has the simpler form

$$\begin{aligned} P'(t_0) &= a_1 + a_2(t_0 - t_1) + a_3(t_0 - t_1)(t_0 - t_2) + ... \\ &\quad + a_N(t_0 - t_1)(t_0 - t_2)(t_0 - t_3)...(t_0 - t_{N-1}) \end{aligned}$$

The kth partial sum on the right side if equation (24) is the derivative of the Newton polynomial of degree k based on the first k nodes. If

$$\mid t_0 - t_1 \mid \leq \mid t_0 - t_2 \mid \leq ... \leq \mid t_0 - t_N \mid \text{, and if } (t_j, 0)_{j=0}^{N}$$

forms a set of $N+1$ equally spaced points on the real axis, the kth partial sum is an approximation to $f'(t_0)$ of order $O(h^{k-1})$.
Suppose that $N = 5$. If the five nodes are $t_k = x + hk$ for $k = 0, 1, 2, 3,$ and 4, then (24) is an equivalent way to compute the forward-difference formula for $f'(x)$ of order $O(h^4)$. If the five nodes $\{t_k\}$ are chosen to be $t_0 = x, t_1 = x + h, t_2 = x - h, t_3 = x + 2h, and t_4 = x - 2h$, then (24) is the central-difference formula for $f'(x)$ of order $O(h^4)$. When the five nodes are $t_k = x - kh$, then (24) is the backward-difference formula for $f'(x)$ of order $O(h^4)$.