Numerical Analysis (10th ed)

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Chapter 4

Numerical Differentiation and Integration

Chapter 4.1: Numerical Differentiation*

Although various techniques to find the derivative of a function were learned in beginning calculus, sometimes a function is so complicated that an explicit form for the derivative is not evident with the techniques we have learned in the past. Further, in reality, from discussions we have had in previous sections, we may not know the function. That is, all we have available are function values at specific points. We might also only have values of the derivative at these points. In situations such as these, numerical differentiation is key.

From calculus, the derivative of f at x_0 was defined as $f'(x_0) = \lim_{h \to 0} \frac{f(x_0 + h) - f(x_0)}{h}$. Certainly, for small enough values of h, the derivative can be approximated by the difference quotient. Thus, our first attempt at an approximation formula for the derivative of f at x_0 is

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

where the last term represents the computational truncation error. Although we cannot compute this error, we can find a bound on it by maximizing the error term on $[x_0, x_0 + h]$.

The formula for $f'(x_0)$ is called a **forward-difference formula** if $h > 0$ and a **backward-difference formula** if $h < 0$.

If we increase the number of evaluation points, we obtain other numerical differentiation formulas, each with their own unique error term.

THREE-POINT ENDPOINT FORMULA:

$f'(x_0) = \frac{1}{2h}\left[-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)\right] + \frac{h^2}{3} f^{(3)}(\xi_0)$; ξ_0 between x_0 and $x_0 + 2h$

THREE-POINT MIDPOINT FORMULA:

$f'(x_0) = \frac{1}{2h}\left[f(x_0 + h) - f(x_0 - h)\right] + \frac{h^2}{6} f^{(3)}(\xi_1)$; ξ_1 between x_0 and $x_0 + h$

FIVE-POINT MIDPOINT FORMULA:

$$f'(x_0) = \frac{1}{12\,h}\left[f(x_0 - 2\,h) - 8\,f(x_0 - h) + 8\,f(x_0 + h) - f(x_0 + 2\,h)\right] + \frac{h^4}{30}f^{(5)}(\xi);$$
ξ between x_0 and $x_0 + 2\,h$

THREE-POINT ENDPOINT FORMULA:

$$f'(x_0) = \frac{1}{12\,h}\left[-25\,f(x_0) + 48\,f(x_0 + h) - 36\,f(x_0 + 2\,h) + 16\,f(x_0 + 3\,h) - 3\,f(x_0 + 4\,h)\right]$$
$$+ \frac{h^4}{5}f^{(5)}(\xi);\ \xi \text{ between } x_0 \text{ and } x_0 + 4\,h$$

The second order derivative can be derived using Taylor polynomial expansions.
SECOND DERIVATIVE MIDPOINT FORMULA:

$$f''(x_0) = \frac{1}{h^2}\left[f(x_0 - h) - 2\,f(x_0) + f(x_0 + h)\right] - \frac{h^2}{12}f^{(4)}(\xi);\ \xi \text{ between } x_0 - h \text{ and } x_0 + h.$$

Not only do we need to be cognizant of the truncation error in each of the above formulas, we must also be aware of the round-off error that is produced by the computations (as was pointed out in Chapter 2). Interestingly, as h decreases, truncation error also decreases, but round-off error increases. So it is important that we find a suitably sized h that will reduce both types of error.

Chapter 4.2: Richardson's Extrapolation*

The goal of extrapolation is to find an easy way to combine approximations where the truncation error is on the order of $O(h)$ in such a way that the result is an approximation whose truncation error is of higher order. Richardson's extrapolation makes this possible. Basically, we can take ANY method whose truncation error can be expressed as a summation of higher powers of h and generate new columns of approximations that have higher order truncation error. Given a stepsize, h, and either the function, $f(x)$, or values of the function at specific x values, we can use Richardson's extrapolation to approximate the derivative $f'(x)$ as follows, where H_1 is the approximation obtained from any $O(h)$ method :

	$O(h)$	$O(h^2)$	$O(h^4)$	$O(h^6)$
h	$H_1(h) = f'(x_0)$			
h	$H_1\left(\frac{h}{2}\right) = f'(x_0)$	$H_2(h) = H_1\left(\frac{h}{2}\right) + \left[H_1\left(\frac{h}{2}\right) - H_1(h)\right]$		
h	$H_1\left(\frac{h}{4}\right) = f'(x_0)$	$H_2\left(\frac{h}{2}\right) = H_1\left(\frac{h}{4}\right) + \left[H_1\left(\frac{h}{4}\right) - H_1\left(\frac{h}{2}\right)\right]$	$H_3(h) = H_2\left(\frac{h}{2}\right) + \frac{\left[H_2\left(\frac{h}{2}\right) - H_2(h)\right]}{3}$	

h	$H_1\left(\frac{h}{8}\right) = f'(x_0)$	$H_2\left(\frac{h}{4}\right) = H_1\left(\frac{h}{8}\right) + \left[H_1\left(\frac{h}{8}\right) - H_1\left(\frac{h}{2}\right)\right]$	$H_3\left(\frac{h}{2}\right) = H_2\left(\frac{h}{4}\right) + \frac{1}{3}\left[H_2\left(\frac{h}{4}\right) - H_2\left(\frac{h}{2}\right)\right]$	$H_4(h) = H_3\left(\frac{h}{2}\right) + \frac{\left[H_3\left(\frac{h}{2}\right) - H_3(h)\right]}{15}$

Chapter 4.3: Elements of Numerical Integration*

Just like we found that we might need approximations to derivatives, we may also find that we need to evaluate a definite integral that has no explicit antiderivative or whose antiderivative is not easily obtained. The basic methods to approximate these definite integrals are called numerical quadrature. The methods discussed in this section are rooted in the interpolation polynomials from Chapter 3 of your text. Methods of this type are called Newton-Cotes Quadrature rules because they involve evaluating the integrand at equally spaced points. There are two types of Newton-Cotes Quadrature rules: open and closed.

This section opens with the development of two closed quadrature formulas (rules), the Trapezoidal rule and Simpson's rule. These formulas were derived by integrating the first and second Lagrange interpolating polynomials respectively using distinct nodes $\{x_0, x_1, \ldots, x_n\}$in the interval [a,b].

When reading the derivation in the text, remember that $f(x_i)$ is a constant and can therefore, be pulled out of the integral as a coefficient a_i.

Since the derivation is developed extensively in the text, we will only provide the rules here and some additional comments.

COMMON CLOSED NEWTON-COTES FORMULAS:

n **= 1: TRAPEZOIDAL RULE:**

$$\int_a^b f(x)\,\mathrm{d}x = \frac{h}{2}\left[f(x_0) + f(x_1)\right] - \frac{h^3}{12} f''(\xi) \quad \text{where } x_0 < \xi < x_1$$

n **= 2: SIMPSON'S RULE:**

$$\int_{a=x_0}^{b=x_2} f(x)\,\mathrm{d}x = \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right] - \frac{h^5}{90} f^{(4)}(\xi) \quad \text{where } x_0 < \xi < x_2$$

n **= 3: SIMPSON'S THREE-EIGHTS RULE:**

$$\int_{a=x_0}^{b=x_3} f(x)\,\mathrm{d}x = \frac{3h}{8}\left[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)\right] - \frac{h^5}{80} f^{(4)}(\xi) \quad \text{where } x_0 < \xi < x_3$$

n **= 4:**

$$\int_{a=x_0}^{b=x_4} f(x)\,dx = \frac{2h}{45}\left[7f(x_0) + 32f(x_1) + 12f(x_2) + 32f(x_3) + 7f(x_4)\right]$$
$$- \frac{8h^7}{945} f^{(6)}(\xi) \quad \text{where } x_0 < \xi < x_4$$

To measure the precision of a quadrature method, we simply look for the largest positive integer n such that the formula is exact for x^k, for each $k = 0, 1, \ldots, n$.

For example, suppose we have a quadrature formula that is given by

$$\int_{-1}^{1} f(x)\,dx = f\left(-\frac{2}{3}\right) + f\left(\frac{2}{3}\right)$$ we compare as follows

$f(x)$	Integral result	Quadrature result
$x^0 = 1$	$\int_{-1}^{1} 1\,dx = 2$	$f\left(-\frac{2}{3}\right) + f\left(\frac{2}{3}\right) = 1 - (-1) = 2$
x^1	$\int_{-1}^{1} x\,dx = 0$	$f\left(-\frac{2}{3}\right) + f\left(\frac{2}{3}\right) = -\frac{2}{3} + \left(\frac{2}{3}\right) = 0$
x^2	$\int_{-1}^{1} x^2\,dx = \frac{2}{3}$	$f\left(-\frac{2}{3}\right) + f\left(\frac{2}{3}\right) = \left(-\frac{2}{3}\right)^2 + \left(\frac{2}{3}\right)^2 = \frac{8}{9}$

Since the last function at which the integral result equals the quadrature result is x^1 the precision of this quadrature method is one.

COMMON OPEN NEWTON-COTES FORMULA: (these do not include the endpoints o [a,b] as nodes).

***n* = 0: MIDPOINT RULE:**

$$\int_{a=x_{-1}}^{b=x_1} f(x)\,dx = 2hf(x_0) + \frac{h^3}{3} f''(\xi), \quad \text{where } x_{-1} < \xi < x_1$$

***n* = 1:**

$$\int_{a=x_{-1}}^{b=x_2} f(x)\,\mathrm{d}x = \frac{3h}{2}\left[f(x_0)+f(x_1)\right] + \frac{3h^3}{4}f''(\xi), \quad \text{where } x_{-1} < \xi < x_2$$

***n* = 2:**

$$\int_{a=x_{-1}}^{b=x_3} f(x)\,\mathrm{d}x = \frac{4h}{3}\left[2f(x_0)-f(x_1)+2f(x_2)\right] + \frac{14h^5}{45}f^{(4)}(\xi), \text{ where } x_{-1} < \xi < x_3$$

***n* = 3:**

$$\int_{a=x_{-1}}^{b=x_4} f(x)\,\mathrm{d}x = \frac{5h}{24}\left[11f(x_0)+f(x_1)+f(x_2)+11f(x_3)\right] + \frac{95h^5}{144}f^{(4)}(\xi), \text{ where}$$

$x_{-1} < \xi < x_4$

Chapter 4.4: Composite Numerical Integration*

The Newton-Cotes formulas that were discussed in the last section are not suitable for use over large intervals of integration for the reasons specified in the text. This brings us to a *piecewise* approach to numerical integration that uses the low-order Newton-Cotes formulas.

As an example, for an approximation to $\int_0^4 e^x\,\mathrm{d}x$, the text compares the following:

- Simpson's rule on [0,4]
- Simpson's rule on each of the intervals [0,2] and [2,4]
- Simpson's rule on each of the four intervals [0,1], [1,2], [2,3], and [3,4]

What we found was as the number of subintervals increased, the accuracy in our approximation increased as well. Thus, the procedure was generalized as follows: subdivide the interval [a, b] into n subintervals, and apply Simpson's rule on each consecutive pair of subintervals. We also found that the same process could be used with the Trapezoidal rule and the Midpoint rule forming Simpson's Composite rule, Composite Trapezoidal rule, and the Composite Midpoint rule.

In each case, the error formula for the corrsponding rule can be used to find a bound on the error. An important property shared by all composite integrations techniques is a stability with respect to round-off error.

Chapter 4.5: Romberg Integration*

This section illustrates how Richardson's extrapolation (discussed in Chapter 4.2) can be used on the results of the Composite Trapezoidal rule to obtain high accuracy approximation with little computational cost. Table 4.10 shows the process in notation form. The second column of values are the approximations to the integral using the Composite Trapezoidal rule. Since the Composite Trapezoidal rule is $O(h^2)$, Richardson's extrapolation $O(h^4)$ formulas from the Section 4.2 table above are applied to that column to generate the third column. Richardson's extrapolation is then applied to the third column to generate the fourth column, and so on.

All computations are shown in the example so we will not go into greater detail here.

Chapter 4.6: Adaptive Quadrature Methods

Chapter 4.7: Gaussian Quadrature

Chapter 4.8: Multiple Integrals

Chapter 4.9: Improper Integrals*

Improper integrals are definite integrals where one or both limits are infinite or where the integrand approaches infinity (**singularity**) at one or more points over the interval of integration. We often encounter improper integrals in physics or probability & statistics applications so it is important to know how to numerically deal with them. In Calculus, you took a limit from the left or right of the offending *x* value to see what happened to the function values as you approached the offending *x* value. In numerical integration, the rules of integral approximation for these integrals must be modified in a way that deal with the situation.

LEFT ENDPOINT SINGULARITY:

- Given: $f(x) = \dfrac{g(x)}{(x-a)^p}$ where $0 < p < 1$ and g is continuous on [a,b].
- Construct the fourth degree Taylor Polynomial, P_4, for g about $x = a$ (assuming that $g \in C^5[a, b]$.
- Evaluate $\displaystyle\int_a^b \frac{P_4}{(x-a)^p}\,dx$.
- Use Composite Simpson's rule to approximate $\displaystyle\int_a^b G(x)\,dx$ where the function values of $G(x)$ are determined

by $G(x) = \begin{cases} \dfrac{g(x) - P_4(x)}{(x-a)^p}, & a < x \le b \\ 0, & x = a \end{cases}$

- Find $\displaystyle\int_a^b \frac{P_4}{(x-a)^p}\,\mathrm{d}x + \int_a^b G(x)\,\mathrm{d}x$

RIGHT ENDPOINT SINGULARITY:

- Proceed as in the left endpoint singularity but expand in terms of the right endpoint b instead of the left endpoint a.
- OR make the substitution $z = -x, \quad dz = -dx$
- Evaluate $\displaystyle\int_a^b f(x)\,\mathrm{d}x = \int_{-b}^{-a} f(-z)\,\mathrm{d}z$ which has a singularity at the left endpoint and proceed as in the left endpoint singularity.

INFINITE SINGULARITY:

- Given: $\displaystyle\int_a^{\infty} \frac{1}{x^p}\,\mathrm{d}x$ where $p > 1$
- $t = x^{-1}, \ dt = -x^{-2}\,dx$
- Use the quadrature formula to approximate $\displaystyle\int_a^{\infty} \frac{f(x)}{x^p}\,\mathrm{d}x = \int_0^{\frac{1}{a}} t^{-2} f\left(\frac{1}{t}\right)\mathrm{d}t$