Analyse Numérique 2

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Remainder

Nous avons présenté l’approximation numérique de la dérivée d’ordre 1 et de la dérivée d’ordre 2.

Parmi les remarques que nous avons tirées:

1. **La méthode des différences finies progressive (resp. rétrograde) est d’ordre 1, ç-à-d, Erreur=$O(h)$.**
2. **La méthode des différences finies centrée est d’ordre 2, ç-à-d, Erreur=$O(h^2)$.**
3. **La vitesse de convergence des schémas obtenus par la méthode des différences finies dépend de la régularité mise sur la fonction f.**

Key Point

Three approximations to the derivative $f'(a)$ are

1. the one sided (forward) difference $$\frac{f(a+h)-f(a)}{h}$$

2. the one sided (backward) difference $$\frac{f(a)-f(a-h)}{h}$$

3. the central difference $$\frac{f(a+h)-f(a-h)}{2h}$$

In practice, the central difference formula is the most accurate.

Key Point

A central difference approximation to the second derivative $f''(a)$ is

$$f''(a) \approx \frac{f(a+h) - 2f(a) + f(a-h)}{h^2}$$

Raisonnable question

- **Et donc, si on améliore la régularité de notre fonction f, peut on obtenir des approximations [schémas], dont l’erreur converge rapidement par rapport aux schémas déjà établis.**
- **Quelles sont les méthodes qui permettent d’avoir ce résultat ?**

Differentiation Via Interpolation

In this section we demonstrate how to generate differentiation formulas by differentiating an interpolant. The idea is straightforward: the first stage is to construct an interpolating polynomial from the data. An approximation of the derivative at any point can be then obtained by a direct differentiation of the interpolant.

Differentiation Via Interpolation

We follow this procedure and assume that $f(x_0), \ldots, f(x_n)$ are given. The Lagrange form of the interpolation polynomial through these points is

$$Q_n(x) = \sum_{j=0}^{n} f(x_j) l_j(x).$$

Here we simplify the notation and replace $l_i^n(x)$ which is the notation we used in Section ?? by $l_i(x)$. According to the error analysis of Section ?? we know that the interpolation error is

$$f(x) - Q_n(x) = \frac{1}{(n+1)!} f^{(n+1)}(\xi_n) \prod_{j=0}^{n} (x - x_j),$$

Differentiation Via Interpolation

where $\xi_n \in (\min(x, x_0, \ldots, x_n), \max(x, x_0, \ldots, x_n))$. Since here we are assuming that the points $x_0, \ldots, x_n$ are fixed, we would like to emphasize the dependence of ξ_n on x and hence replace the ξ_n notation by ξ_x. We that have:

$$f(x) = \sum_{j=0}^{n} f(x_j) l_j(x) + \frac{1}{(n+1)!} f^{(n+1)}(\xi_x) w(x), \tag{5.7}$$

where

$$w(x) = \prod_{i=0}^{n} (x - x_i).$$

Differentiating the interpolant (5.7):

$$f'(x) = \sum_{j=0}^{n} f(x_j) l_j'(x) + \frac{1}{(n+1)!} f^{(n+1)}(\xi_x) w'(x) + \frac{1}{(n+1)!} w(x) \frac{d}{dx} f^{(n+1)}(\xi_x). \tag{5.8}$$

Differentiation Via Interpolation

We now assume that x is one of the interpolation points, i.e., $x \in \{x_0, \ldots, x_n\}$, say x_k, so that

$$f'(x_k) = \sum_{j=0}^{n} f(x_j) l_j'(x_k) + \frac{1}{(n+1)!} f^{(n+1)}(\xi_{x_k}) w'(x_k). \tag{5.9}$$

Now,

$$w'(x) = \sum_{i=0}^{n} \prod_{\substack{j=0 \\ j \neq i}}^{n} (x - x_j) = \sum_{i=0}^{n} [(x - x_0) \cdot \ldots \cdot (x - x_{i-1})(x - x_{i+1}) \cdot \ldots \cdot (x - x_n)].$$

Hence, when $w'(x)$ is evaluated at an interpolation point x_k, there is only one term in $w'(x)$ that does not vanish, i.e.,

$$w'(x_k) = \prod_{\substack{j=0 \\ j \neq k}}^{n} (x_k - x_j).$$

Differentiation Via Interpolation

The numerical differentiation formula, (5.9), then becomes

$$f'(x_k) = \sum_{j=0}^{n} f(x_j) l_j'(x_k) + \frac{1}{(n+1)!} f^{(n+1)}(\xi_{x_k}) \prod_{\substack{j=0 \\ j \neq k}} (x_k - x_j). \tag{5.10}$$

We refer to the formula (5.10) as a **differentiation by interpolation** algorithm.

Differentiation Via Interpolation

Example 5.1

We demonstrate how to use the differentiation by integration formula (5.10) in the case where $n = 1$ and $k = 0$. This means that we use two interpolation points $(x_0, f(x_0))$ and $(x_1, f(x_1))$, and want to approximate $f'(x_0)$. The Lagrange interpolation polynomial in this case is

$$Q_1(x) = f(x_0)l_0(x) + f(x_1)l_1(x),$$

where

$$l_0(x) = \frac{x - x_1}{x_0 - x_1}, \qquad l_1(x) = \frac{x - x_0}{x_1 - x_0}.$$

Hence

$$l_0'(x) = \frac{1}{x_0 - x_1}, \qquad l_1'(x) = \frac{1}{x_1 - x_0}.$$

Differentiation Via Interpolation

We thus have

$$Q_1'(x_0) = \frac{f(x_0)}{x_0 - x_1} + \frac{f(x_1)}{x_1 - x_0} + \frac{1}{2} f''(\xi)(x_0 - x_1) = \frac{f(x_1) - f(x_0)}{x_1 - x_0} - \frac{1}{2} f''(\xi)(x_1 - x_0).$$

Here, we simplify the notation and assume that $\xi \in (x_0, x_1)$. If we now let $x_1 = x_0 + h$, then

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

which is the (first-order) forward differencing approximation of $f'(x_0)$, (5.3).

Differentiation Via Interpolation

Example 5.2
We repeat the previous example in the case $n = 2$ and $k = 0$. This time

$$Q_2(x) = f(x_0)l_0(x) + f(x_1)l_1(x) + f(x_2)l_2(x),$$

with

$$l_0(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)}, \quad l_1(x) = \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)}, \quad l_2(x) = \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)}.$$

Differentiation Via Interpolation

Hence

$$l_0'(x) = \frac{2x - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)}, \quad l_1'(x) = \frac{2x - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)}, \quad l_2'(x) = \frac{2x - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)}.$$

Evaluating $l_j'(x)$ for $j = 1, 2, 3$ at x_0 we have

$$l_0'(x_0) = \frac{2x_0 - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)}, \quad l_1'(x_0) = \frac{x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)}, \quad l_2'(x_0) = \frac{x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)}$$

Hence

$$\begin{aligned} Q_2'(x_0) &= f(x_0)\frac{2x_0 - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)} + f(x_1)\frac{x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} \\ &\quad + f(x_2)\frac{x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)} + \frac{1}{6}f^{(3)}(\xi)(x_0 - x_1)(x_0 - x_2). \end{aligned} \tag{5.11}$$

Differentiation Via Interpolation

Here, we assume $\xi \in (x_0, x_2)$. For $x_i = x + ih$, $i = 0, 1, 2$, equation (5.11) becomes

$$\begin{aligned} Q_2'(x) &= -f(x)\frac{3}{2h} + f(x+h)\frac{2}{h} + f(x+2h)\left(-\frac{1}{2h}\right) + \frac{f'''(\xi)}{3}h^2 \\ &= \frac{-3f(x) + 4f(x+h) - f(x+2h)}{2h} + \frac{f'''(\xi)}{3}h^2, \end{aligned}$$

which is a one-sided, second-order approximation of the first derivative.

Remark. In a similar way, if we were to repeat the last example with $n = 2$ while approximating the derivative at x_1, the resulting formula would be the second-order centered approximation of the first-derivative (5.5)

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

The Method of Undetermined Coefficients

In this section we present the **method of undetermined coefficients**, which is a very practical way for generating approximations of derivatives (as well as other quantities as we shall see, e.g., when we discuss integration).

Assume, for example, that we are interested in finding an approximation of the second derivative $f''(x)$ that is based on the values of the function at three equally spaced points, $f(x-h), f(x), f(x+h)$, i.e.,

$$f''(x) \approx Af(x+h) + B(x) + Cf(x-h). \tag{5.12}$$

The Method of Undetermined Coefficients

The coefficients A, B, and C are to be determined in such a way that this linear combination is indeed an approximation of the second derivative. The Taylor expansions of the terms $f(x \pm h)$ are

$$f(x \pm h) = f(x) \pm hf'(x) + \frac{h^2}{2}f''(x) \pm \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(\xi_\pm), \tag{5.13}$$

where (assuming that $h > 0$)

$$x - h \leqslant \xi_- \leqslant x \leqslant \xi_+ \leqslant x + h.$$

Using the expansions in (5.13) we can rewrite (5.12) as

$$\begin{aligned} f''(x) &\approx Af(x+h) + Bf(x) + Cf(x-h) \\ &= (A+B+C)f(x) + h(A-C)f'(x) + \frac{h^2}{2}(A+C)f''(x) \\ &+ \frac{h^3}{6}(A-C)f^{(3)}(x) + \frac{h^4}{24}[Af^{(4)}(\xi_+) + Cf^{(4)}(\xi_-)]. \end{aligned} \tag{5.14}$$

The Method of Undetermined Coefficients

Equating the coefficients of $f(x)$, $f'(x)$, and $f''(x)$ on both sides of (5.14) we obtain the linear system

$$\begin{cases} A + B + C = 0, \\ A - C = 0, \\ A + C = \dfrac{2}{h^2}. \end{cases} \tag{5.15}$$

The system (5.15) has the unique solution:

$$A = C = \frac{1}{h^2}, \quad B = -\frac{2}{h^2}.$$

In this particular case, since A and C are equal to each other, the coefficient of $f^{(3)}(x)$ on the right-hand-side of (5.14) also vanishes and we end up with

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

The Method of Undetermined Coefficients

We note that the last two terms can be combined into one using an intermediate values theorem (assuming that $f(x)$ has four continuous derivatives), i.e.,

$$\frac{h^2}{24}[f^{(4)}(\xi_+) + f^{(4)}(\xi_-)] = \frac{h^2}{12} f^{(4)}(\xi), \qquad \xi \in (x-h, x+h).$$

Hence we obtain the familiar second-order approximation of the second derivative:

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

In terms of an algorithm, the method of undetermined coefficients follows what was just demonstrated in the example:

The Method of Undetermined Coefficients

1. Assume that the derivative can be written as a linear combination of the values of the function at certain points.

2. Write the Taylor expansions of the function at the approximation points.

3. Equate the coefficients of the function and its derivatives on both sides.

The only question that remains open is how many terms should we use in the Taylor expansion. This question has, unfortunately, no simple answer. In the example, we have already seen that even though we used data that is taken from three points, we could satisfy four equations. In other words, the coefficient of the third-derivative vanished as well. If we were to stop the Taylor expansions at the third derivative instead of at the fourth derivative, we would have missed on this cancellation, and would have mistakenly concluded that the approximation method is only first-order accurate. The number of terms in the Taylor expansion should be sufficient to rule out additional cancellations. In other words, one should truncate the Taylor series after the leading term in the error has been identified.

Richardson’s Extrapolation

Richardson’s extrapolation can be viewed as a general procedure for improving the accuracy of approximations when the structure of the error is known. While we study it here in the context of numerical differentiation, it is by no means limited only to differentiation and we will get back to it later on when we study methods for numerical integration.

Richardson's Extrapolation

We start with an example in which we show how to turn a second-order approximation of the first derivative into a fourth order approximation of the same quantity. We already know that we can write a second-order approximation of $f'(x)$ given its values in $f(x \pm h)$. In order to improve this approximation we will need some more insight on the internal structure of the error. We therefore start with the Taylor expansions of $f(x \pm h)$ about the point x, i.e.,

$$
\begin{aligned}
f(x+h) &= \sum_{k=0}^{\infty} \frac{f^{(k)}(x)}{k!} h^k, \\
f(x-h) &= \sum_{k=0}^{\infty} \frac{(-1)^k f^{(k)}(x)}{k!} h^k.
\end{aligned}
$$

Richardson's Extrapolation

Hence

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \left[\frac{h^2}{3!} f^{(3)}(x) + \frac{h^4}{5!} f^{(5)}(x) + \dots\right]. \tag{5.16}$$

We rewrite (5.16) as

$$L = D(h) + e_2 h^2 + e_4 h^4 + \dots, \tag{5.17}$$

Richardson's Extrapolation

where L denotes the quantity that we are interested in approximating, i.e.,

$$L = f'(x),$$

and $D(h)$ is the approximation, which in this case is

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

The error is

$$E = e_2 h^2 + e_4 h^4 + \dots$$

Richardson's Extrapolation

where e_i denotes the coefficient of h^i in (5.16). The important property of the coefficients e_i's is that they do not depend on h. We note that the formula

$$L \approx D(h),$$

is a second-order approximation of the first-derivative which is based on the values of $f(x)$ at $x \pm h$. We assume here that in general $e_i \neq 0$. In order to improve the approximation of L our strategy will be to eliminate the term $e_2 h^2$ from the error. How can this be done? one possibility is to write another approximation that is based on the values of the function at different points. For example, we can write

$$L = D(2h) + e_2(2h)^2 + e_4(2h)^4 + \ldots. \tag{5.18}$$

Richardson's Extrapolation

This, of course, is still a second-order approximation of the derivative. However, the idea is to combine (5.17) with (5.18) such that the h^2 term in the error vanishes. Indeed, subtracting the following equations from each other

$$\begin{aligned} 4L &= 4D(h) + 4e_2h^2 + 4e_4h^4 + \dots, \\ L &= D(2h) + 4e_2h^2 + 16e_4h^4 + \dots, \end{aligned}$$

we have

$$L = \frac{4D(h) - D(2h)}{3} - 4e_4h^4 + \dots$$

Richardson’s Extrapolation

In other words, a fourth-order approximation of the derivative is

$$f'(x) = \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h} + O(h^4). \tag{5.19}$$

Note that (5.19) improves the accuracy of the approximation (5.16) by using more points.

Richardson's Extrapolation

This process can be repeated over and over as long as the structure of the error is known. For example, we can write (5.19) as

$$L = S(h) + a_4h^4 + a_6h^6 + \dots \tag{5.20}$$

where

$$S(h) = \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h}.$$

Equation (5.20) can be turned into a sixth-order approximation of the derivative by eliminating the term a_4h^4. We carry out such a procedure by writing

$$L = S(2h) + a_4(2h)^4 + a_6(2h)^6 + \dots \tag{5.21}$$

Combining (5.21) with (5.20) we end up with a sixth-order approximation of the derivative:

$$L = \frac{16S(h) - S(2h)}{15} + O(h^6).$$

Richardson’s Extrapolation

Remarks.

1. In (5.18), instead of using $D(2h)$, it is possible to use other approximations, e.g., $D(h/2)$. If this is what is done, instead of (5.19) we would get a fourth-order approximation of the derivative that is based on the values of f at $x-h, x-h/2, x+h/2, x+h$.

2. Once again we would like to emphasize that Richardson’s extrapolation is a general procedure for improving the accuracy of numerical approximations that can be used when the structure of the error is known. It is not specific for numerical differentiation.

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Exercice

1) Comparer entre la Formule de DF centrée $\frac{f(a+h)-f(a-h)}{2h}$

et l'approximation obtenue par la différentiation polynomiale $\frac{-3f(x)+4f(x+h)-f(x+2h)}{2h}$

(Indication: Utiliser le programme BDF2.sce)

On considère f(x)=ln(x), x_0=3. Faites un tableau contenant la valeur approchée de la dérivée par les 2 méthodes et l'erreur pour

- h=0.1
- h=0.01
- h=0.001
- h=0.0001

Utiliser 8 décimales après la virgule.

2) Conclure.

Exercice

1) Comparer entre l'approximation obtenue par la différentiation polynomiale $\frac{-3f(x)+4f(x+h)-f(x+2h)}{2h}$ et celle obtenue par l'extrapolation de Richardson $\frac{-f(x+2h)+8f(x+h)-8f(x-h)+f(x-2h)}{12h}$

Vous pouvez utilisez la même fonction f(x)=ln(x), x_0=3.
Faites un tableau contenant la valeur approchée de la dérivée par les 2 méthodes et l'erreur pour

- h=0.1
- h=0.01
- h=0.001
- h=0.0001

Bibliographie

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