Journal of Computational Physics: X 2 (2019) 100017

Contents lists available at ScienceDirect

Journal of Computational Physics: X

www.elsevier.com/locate/jcpx

A remark on Richardson's extrapolation process and numerical differentiation formulae

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ARTICLE INFO

Article history:
Received 14 January 2019
Accepted 2 February 2019
Available online 1 March 2019

Keywords:
Numerical differentiation
Richardson's extrapolation process

ABSTRACT

Richardson's extrapolation process is a well known method to improve the order of several approximation processes. Here we observe that for numerical differentiation, Richardson's process can be applied not only to improve the order of a numerical differentiation formula but also to find in fact the original formula.

1. Introduction

Usually Richardson's extrapolation process is used to improve the order of a formula which approximate a given quantity [1,2]. In this paper we observe that the Richardson's extrapolation process can be used in a first phase to find a numerical differentiation formula of low order, and in a second phase to improve this order as usual.

Let us consider an expression

$$T(h) = \sum_{l=0}^{L} a_l h^l + O(h^{L+1}), \tag{1}$$

where $T(h)$ is a given formula. Let $0 \leq n \leq L$, our goal is to extract from (1) a formula for a_n as

$$a_n = A_n(h) + O(h^{L+1-n}). \tag{2}$$

This formula will be obtained in two phases. At the end of a first phase we get a formula of low order, and during the second phase we improve the order using the usual extrapolation process.

2. The process

We initialize the process by setting $T(h) = T_0(h)$, and

$$T_0(h) = \sum_{l=0}^{L} a_{0,l} h^l + O(h^{L+1})$$

where $a_{0,l} = a_l$ for $l = 0, \cdots, L$.

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https://doi.org/10.1016/j.jcpx.2019.100017

2.1. First phase: finding a formula

The goal of the first phase is to eliminate $a_{0,l} = a_l$ for $l = 0, \ldots, n-1$ as follows. Suppose we have already eliminated $a_{0,l} = a_l$ for $l = 0, \cdots, i-1$, and have the formula

$$T_i(h) = \sum_{l=i}^{L} a_{i,l} h^l + O(h^{L+1})$$

where $a_{i,n} = a_n$.

Let $q_i \neq 1$, and let us consider $T_i(h)$ and $T_i(q_i h)$. To eliminate $a_{i,i}$ leaving $a_{i,n} = a_n$ unchanged, we consider

$$q_i^i T_i(h) - T_i(q_i h) = \sum_{l=i+1}^{L} a_{i,l}(q_i^i - q_i^l) h^l + O(h^{L+1}),$$

and

$$\frac{q_i^i T_i(h) - T_i(q_i h)}{q_i^i - q_i^n} = \sum_{l=i+1}^{L} a_{i,l} \frac{(q_i^i - q_i^l)}{(q_i^i - q_i^n)} h^{n_l} + O(h^{L+1}).$$

Let us set

$$T_{i+1}(h) = \frac{q_i^i T_i(h) - T_i(q_i h)}{q_i^i - q_i^n}$$

and

$$a_{i+1,l} = a_{i,l} \frac{(q_i^i - q_i^l)}{(q_i^i - q_i^n)}$$

for $l = i, \cdots, L$. Let us observe that $a_{i+1,i} = 0$ as expected, and $a_{i+1,n} = a_{i,n} = a_n$. At the end of this phase we have

$$T_n(h) = a_n h^n + \sum_{l=n+1}^{L} a_{n,l} h^l + O(h^{L+1}).$$

Since

$$\sum_{l=n+1}^{L} a_{n,l} h^l + O(h^{L+1}) = O(h^{n+1}),$$

we have the approximation

$$a_n h^n = T_n(h) + O(h^{n+1}),$$

or for a_n the formula

$$a_n = \frac{T_n(h)}{h^n} + O(h).$$

2.2. Second phase: improving the formula

Now we can use the standard extrapolation process to improve the order of the formula. Since we skip the elimination of a_n, let us set $T_{n+1}(h) = T_n(h)$, and $a_{n+1,l} = a_{n,l}$ for $l = n+1, \ldots, L$. So we have

$$T_{n+1}(h) = a_n h^n + \sum_{l=n+1}^{L} a_{n+1,l} h^l + O(h^{L+1}),$$

and we would like to eliminate $a_{n+1,l}$ for $l = n+1, \ldots, L$.

Suppose we have already eliminated $a_{n+1,l}$ for $l = n+1, \ldots, n+m-1$. So we have

$$T_{n+m}(h) = a_n h^n + \sum_{l=n+m}^{L} a_{n+m,l} h^l + O(h^{L+1}).$$

We consider

$$T_{n+m}(q_{n+m}h) = a_n(q_{n+m}h)^n + \sum_{l=n+m}^{L} a_{n+m,l}(q_{n+m}h)^l + O(h^{L+1}).$$

To eliminate $a_{n+m,n+m}$ we perform

$$q_{n+m}^{n+m} T_{n+m}(h) - T_{n+m}(q_{n+m}h) = \left(q_{n+m}^{n+m} - q_{n+m}^{n}\right) a_n h^n + \sum_{l=n+m+1}^{L} a_{n+m,l}\left(q_{n+m}^{n+m} - q_{n+m}^{l}\right) h^l + O(h^{L+1}).$$

Let us set

$$T_{n+m+1}(h) = \frac{q_{n+m}^{n+m} T_{n+m}(h) - T_{n+m}(q_{n+m}h)}{\left(q_{n+m}^{n+m} - q_{n+m}^{n}\right)},$$

and

$$a_{n+m+1,l} = a_{n+m,l}\frac{\left(q_{n+m}^{n+m} - q_{n+m}^{l}\right)}{\left(q_{n+m}^{n+m} - q_{n+m}^{n}\right)},$$

for $l = n+m, \ldots, L$. So we have to obtain $a_{n+m+1,n+m} = 0$, and

$$T_{n+m+1}(h) = a_n h^n + \sum_{l=n+m+1}^{L} a_{n+m+1,l} h^l + O(h^{L+1}).$$

Then we have

$$\sum_{l=n+m+1}^{L} a_{n+m+1,l} h^l + O(h^{L+1}) = O(h^{n+m+1}),$$

and we repeat the process to get at the end of this phase

$$T_{L+1}(h) = a_n h^n + O(h^{L+1})$$

It follows that

$$a_n = \frac{T_{L+1}(h)}{h^n} + O(h^{L+1-n})$$

and $A_n(h) = \dfrac{T_{L+1}(h)}{h^n}$ is the formula we look for in (2) to estimate a_n.

3. Towards examples

The process to find derivation formulae with the Richardson's process is based on the Taylor's expansion of $f(x)$ given by

$$f(x+h) = \sum_{j=0}^{L} \frac{f^{(j)}(x)}{j!} h^j + O(h^{L+1}). \tag{3}$$

In the examples we will present, we have chosen $q_i = 2$ for all indices i. Other choices are possible leading to other formulae. Moreover to simplify we have done only one elimination in the second phase of the process.

4. One sided numerical differentiation formulae

We will present some one-sided formulae which use the value of the function at the point we look for the derivative, that is to say $f(x)$, and others that don't use this value $f(x)$.

4.1. Formulae with the point value of the function

For a formula which use $f(x)$, we rewrite (3) as follows

$$f(x+h) - f(x) = \sum_{j=1}^{L} \frac{f^{(j)}(x)}{j!} h^j + O(h^{L+1}),$$

and then use the two phases to find $f^{(n)}(x)$, which correspond to eliminating the derivatives $f^{(j)}(x)$ for $j = 1, \ldots, n-1, n+1, \ldots, L$.

4.1.1. Formulae for the first derivative

In the first phase we have directly

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

In the second phase we eliminate $f''(x)$ to get

$$f'(x) = \frac{-f(x+2h) + 4f(x+h) - 3f(x)}{2h} + O(h^2).$$

4.1.2. Formulae for the second derivative

In the first phase we eliminate $f'(x)$ to get

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

In the second phase we eliminate $f^{(3)}(x)$ to get

$$f''(x) = \frac{-f(x+4h) + 10f(x+2h) - 16f(x+h) + 7f(x)}{4h^2} + O(h^2).$$

4.2. Formulae without the point value of the function

For a formula which does not use $f(x)$ as such we consider directly (3), and then use the two phases to find $f^{(n)}(x)$, which correspond to eliminating the derivatives $f^{(j)}(x)$ for $j = 0, \ldots, n-1, n+1, \ldots, L$.

4.2.1. Formulae for the first derivative

In the first phase we eliminate $f(x)$ and get

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

In the second phase we eliminate $f''(x)$ to get

$$f'(x) = \frac{-f(x+4h) + 5f(x+2h) - 4f(x+h)}{2h} + O(h^2).$$

4.2.2. Formulae for the second derivative

In the first phase we eliminate $f(x)$ and $f'(x)$ to get

$$f''(x) = \frac{f(x+4h) - 3f(x+2h) + 2f(x+h)}{3h^2} + O(h).$$

In the second phase we eliminate $f^{(3)}(x)$ to get

$$f''(x) = \frac{-f(x+8h) + 11f(x+4h) - 26f(x+2h) + 16f(x+h)}{12h^2} + O(h^2).$$

5. Symmetric numerical differentiation formulae

5.1. Odd order derivatives

In this case we use (3), with $L = 2(n + m + 1)$, for $f(x + h)$ and $f(x - h)$, and substract the two series. As a consequence only odd order derivatives remain. We have

$$f(x+h) - f(x-h) = 2\sum_{j=0}^{n+m} \frac{f^{(2j+1)}(x)}{(2j+1)!} h^{2j+1} + O\left(h^{2n+2m+3}\right).$$

Then use the two phases to find $f^{2n+1)}(x)$, which correspond to eliminating the derivatives $f^{(2j+1)}(x)$ for $j = 0, \dots, n-1, n+1, \dots, n+m$.

5.1.1. Formulae for the first derivative

In the first phase there is nothing to do, we get directly

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

In the second phase, we eliminate $f^{(3)}(x)$ to get

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

5.1.2. Formulae for the third derivative

In the first phase we eliminate $f'(x)$ and get

$$f^{(3)}(x) = \frac{f(x+2h) - 2f(x+h) + 2f(x-h) - f(x-2h)}{2h^3} + O(h^2).$$

In the second phase, we eliminate $f^{(5)}(x)$ to get

$$f^{(3)}(x) = \frac{-f(x+4h) + 34f(x+2h) - 64f(x+h) + 64f(x-h) - 34f(x-2h) + f(x-4h)}{48h^3} + O(h^4).$$

5.2. Even order derivatives

In this case we use (3), with $L = 2(n + m) + 1$, for $f(x + h)$ and $f(x - h)$, and add the two series. As a consequence only even order derivatives remain. We have

$$f(x+h) - 2f(x) + f(x-h) = 2\sum_{j=1}^{n+m} \frac{f^{(2j)}(x)}{(2j)!} h^{2j} + O(h^{2n+2m+2}).$$

Then we use the two phases to find $f^{2n+1)}(x)$, in other words to eliminate the derivatives $f^{(2j+1)}(x)$ for $j = 0, \dots, n-1, n+1, \dots, n+m$.

5.2.1. Formulae for the second derivative

In the first phase there is nothing to do, we get directly

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

In the second phase we eliminate $f^{(4)}(x)$ to get

$$f''(x) = \frac{-f(x+2h) + 16f(x+h) - 30f(x) + 16f(x-h) - f(x-2h)}{12h^2} + O(h^4).$$

5.2.2. Formulae for the fourth derivative

In the first phase we eliminate $f''(x)$ and get

$$f^{(4)}(x) = \frac{f(x+2h) - 4f(x+h) + 6f(x) - 4f(x-h) + f(x-2h)}{h^4} + O(h^2).$$

In the second phase, we eliminate $f^{(6)}(x)$ to get

$$f^{(4)}(x) = \frac{-f(x+4h) + 68f(x+2h) - 256f(x+h) + 378f(x) - 256f(x-h) + 68f(x-2h) - f(x+4h)}{48h^4} + O(h^4).$$

6. Conclusion

In this short paper we have pointed out that Richardson's extrapolation process can be used not only to improve the order of a given numerical differentiation formula but also to find in fact the given basic numerical differentiation formula of low order. This process could be included in any computer code which already use the Richardson process.

Conflict of interest statement

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgement

This work has been financially supported by an individual discovery grant (RGPIN-2016-05572) from NSERC (Natural Sciences and Engineering Research Council) of Canada.

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