On a Formula by Cohen, Hubbard and Oesterwinter

Robin Leroy (eggrobin) & Pascal Leroy (phl)

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This document proves and generalizes a formula given in [CHO73] to compute the velocity of a body in the context of 12th-order numerical integration of n-body systems.

Statement

[CHO73] states that

> the formula for a velocity component [is] of the form:

$$\dot{x}_{n+1} = \frac{1}{h}\left(x_n - x_{n-1} + h^2 \sum_{i=0}^{12} \beta_i \ddot{x}_{n-i}\right) \tag{1}$$

They then proceed to tabulate explicit values for the (rational) coefficients β_i without explaining how they are computed. This makes it impossible to use this formula for integrators of a different order or to construct similar formulæ for slightly different purposes.

Finite difference formula

In this section we prove a backward difference formula that makes it possible to compute an approximation of any derivative of a function on an equally-spaced grid at any desired order.

Lemma. *Given a sufficient regular function $f(x)$ and two integers $m \leq n$, there exist a family of rational numbers $\lambda^m_{n,\nu}$, with $0 \leq \nu \leq n$ such that:*

$$f^{(m)}(x_0) = \frac{(-1)^m}{h^m} \sum_{\nu=0}^{n} \lambda^m_{n,\nu} f(x_0 - \nu h) + O(h^{n-m+1}) \tag{2}$$

Furthermore, the $\lambda^m_{n,\nu}$ are independent from x_0 and h.

Proof. [For88] gives finite difference formulæ for any order and for kernels of arbitrary size. Given a sufficient regular function $f(x)$ and a family $\boldsymbol{\alpha} = (\alpha_0, \alpha_1, ..., \alpha_N)$ of points (which may not be equidistant), the m-th derivative at any point x_0 may be approximated to order $n - m + 1$ as:

$$f^{(m)}(x_0) \cong \sum_{\nu=0}^{n} \delta^m_{n,\nu}(\boldsymbol{\alpha}) f(\alpha_\nu)$$

where $m \leq n$ and the coefficients $\delta^m_{n,\nu}$ are dependent on $\boldsymbol{\alpha}$ but independent of f.

If the $\boldsymbol{\alpha}$ are equally spaced with step $-h$ (i.e., $\alpha_\nu = x_0 - \nu h$) then we can write a backward formula as follows:

$$f^{(m)}(x_0) = \sum_{\nu=0}^{n} \delta^m_{n,\nu}(\boldsymbol{\alpha}) f(x_0 - \nu h) + O(h^{n-m+1}) \tag{3}$$

In this case equation (3.8) from [For88] may be rewritten as follows, restoring x_0:

$$\begin{aligned}\delta^m_{n,\nu} &= \frac{1}{\alpha_n - \alpha_\nu}((\alpha_n - x_0)\delta^m_{n-1,\nu} - m\delta^{m-1}_{n-1,\nu}) \\ &= \frac{1}{(\nu - n)h}(-nh\delta^m_{n-1,\nu} - m\delta^{m-1}_{n-1,\nu})\end{aligned} \tag{4}$$

It is possible to extract the powers of h from the coefficients by defining, for $\nu < n$:

$$\lambda^m_{n,\nu} \coloneqq \delta^m_{n,\nu}(\boldsymbol{\alpha})(-1)^m h^m$$

Substituting into equation (4) we obtain:

$$\lambda^m_{n,\nu} = \frac{1}{n-\nu}(n\lambda^m_{n-1,\nu} - m\lambda^{m-1}_{n-1,\nu})$$

and we see that $\lambda^m_{n,\nu}$ is independent from x_0 and h and therefore that $\delta^m_{n,\nu}$ is independent from x_0.

Note that the definition of $\lambda^m_{n,\nu}$ extends immediately to $n = \nu$, that is to $\lambda^m_{n,n}$, using equation (3.10) of [For88].

Now knowing that:

$$\delta^m_{n,\nu}(\boldsymbol{\alpha}) = (-1)^m \frac{\lambda^m_{n,\nu}}{h^m}$$

it is straightforward to rewrite equation (3) to obtain equation (2), thus demonstrating the lemma.

□

Derivation

In this section we derive equation (1) and obtain an explicit expression for the coefficients appearing in the sum, using equation (2) from the preceding lemma.

We start by writing the Taylor series of $f(x_0 - h)$ for h close to 0, extracting the leading terms:

$$\begin{aligned}f(x_0 - h) &= \sum_{m=0}^{\infty} \frac{f^{(m)}(x_0)}{m!}(-1)^m h^m \\ &= f(x_0) - hf'(x_0) + \sum_{m=2}^{\infty} \frac{f^{(m)}(x_0)}{m!}(-1)^m h^m \\ &= f(x_0) - hf'(x_0) + \sum_{m=2}^{n} \frac{f^{(m)}(x_0)}{m!}(-1)^m h^m + O(h^{n+1})\end{aligned} \tag{5}$$

Equation (2) can be applied to the second derivative $f''(x_0)$ to yield an approximation of $f^{(m)}(x_0)$ of order $n - m + 1$ when $m \geq 2$:

$$f^{(m)}(x_0) = \frac{(-1)^m}{h^{m-2}} \sum_{\nu=0}^{n-2} \lambda^{m-2}_{n-2,\nu} f''(x_0 - \nu h) + O(h^{n-m+1}) \tag{6}$$

Injecting this expression into equation (5) we find:

$$f(x_0 - h) = f(x_0) - hf'(x_0) + h^2 \sum_{m=2}^{n} \sum_{\nu=0}^{n-2} \frac{\lambda^{m-2}_{n-2,\nu}}{m!} f''(x_0 - \nu h) + O(h^{n+1})$$

The summations are independent and can be exchanged:

$$f(x_0 - h) = f(x_0) - hf'(x_0) + h^2 \sum_{\nu=0}^{n-2} \left(\sum_{m=2}^{n} \frac{\lambda^{m-2}_{n-2,\nu}}{m!} \right) f''(x_0 - \nu h) + O(h^{n+1})$$

We can then define:

$$\eta_{n,\nu} \coloneqq \sum_{m=2}^{n} \frac{\lambda_{n-2,\nu}^{m-2}}{m!}$$

and we finally obtain:

$$f'(x_0) = \frac{1}{h}\left(f(x_0) - f(x_0 - h) + h^2 \sum_{\nu=0}^{n-2} \eta_{n,\nu} f''(x_0 - \nu h)\right) + \mathcal{O}(h^n) \tag{7}$$

This is the formula we use, after integration using a symmetry linear multistep integrator, to compute the velocity of a body knowing its positions and accelerations are preceding times.

The alert reader will notice that equation (7) is similar, but not identical, to equation (1). To derive the latter, we write the Taylor series of $f'(x_0 + h)$ for h close to 0:

$$\begin{aligned} f'(x_0 + h) &= f'(x_0) + \sum_{m=2}^{\infty} \frac{h^{m-1}}{(m-1)!} f^{(m)}(x_0) \\ &= f'(x_0) + \sum_{m=2}^{n} \frac{h^{m-1}}{(m-1)!} f^{(m)}(x_0) + \mathcal{O}(h^n) \end{aligned}$$

and we replace $f'(x_0)$ with its value from equation (5):

$$f'(x_0 + h) = \frac{1}{h}(f(x_0) - f(x_0 - h)) + \sum_{m=2}^{n} \frac{h^{m-1}}{(m-1)!}\left(1 + \frac{(-1)^m}{m}\right) f^{(m)}(x_0) + \mathcal{O}(h^n)$$

As we did above, we replace $f^{(m)}(x_0)$ using its expression from equation (6) to obtain:

$$f'(x_0 + h) = \frac{1}{h}(f(x_0) - f(x_0 - h)) + h \sum_{m=2}^{n}\left(\frac{1}{(m-1)!}\left((-1)^m + \frac{1}{m}\right) \sum_{\nu=0}^{n-2} \lambda_{n-2,\nu}^{m-2} f''(x_0 - \nu h)\right) + \mathcal{O}(h^n)$$

If we define:

$$\beta_{n,\nu} = \sum_{m=2}^{n} \frac{\lambda_{n-2,\nu}^{m-2}}{(m-1)!}\left((-1)^m + \frac{1}{m}\right)$$

we finally find an expression equivalent to equation (1):

$$f'(x_0 + h) = \frac{1}{h}(f(x_0) - f(x_0 - h)) + h \sum_{\nu=0}^{n-2} \beta_{n,\nu} f''(x_0 - \nu h) + \mathcal{O}(h^n)$$

Conclusion

References

[CHO73] C. J. Cohen, E. C. Hubbard and C. Oesterwinter. *Astronomical Papers Prepared for the Use of the American Ephemeris and Nautical Almanac – Elements of the Outer Planets for One Million Years.* Vol. XXII. I. United States Government Printing Office, 1973.

[For88] B. Fornberg. “Generation of Finite Difference Formulas on Arbitrarily Spaced Grids”. In: *Mathematics of Computation* 51 (Oct. 1988), pp. 699–706. DOI: `10.1090/S0025-5718-1988-0935077-0`.