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 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 formulæ

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. We then derive a corollary based on the second derivative $f''(x)$ that is useful for the following sections.

Lemma. *Given a sufficient regular function $f(x)$ and two integers $m \leq n$, there exists 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 family $\boldsymbol{\alpha} = (\alpha_0, \alpha_1, \ldots, \alpha_N)$ 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.

□

Corollary. *Applying the lemma to the second derivative $f''(x)$ gives the following result when $m \geq 2$:*

$$f^{(m)}(x_0) = \frac{(-1)^m}{h^{m-2}} \sum_{\nu=0}^{n-2} \lambda^{m-2}_{n-2,\nu} f''(x_0 - \nu h) + O(h^{n-m+1}) \tag{5}$$

□

A formula for symmetric linear multistep integrators

In this section we derive a formula suitable for computing the velocity of a body knowing its positions and accelerations at preceding times. This is the formula we use after integration using a symmetry linear multistep integrator.

Proposition. *Given a sufficient regular function $f(x)$ there exists a family of rational numbers $\eta_{n,\nu}$, with $0 \leq \nu \leq n - 2$, such that:*

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

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

$$\begin{aligned} f(x_0 - h) &= \sum_{m=0}^{\infty} \frac{f^{(m)}(x_0)}{m!}(-1)^m h^m \\ &= f(x_0) - hf'(x_0) + \sum_{m=2}^{\infty} \frac{f^{(m)}(x_0)}{m!}(-1)^m h^m \\ &= f(x_0) - hf'(x_0) + \sum_{m=2}^{n} \frac{f^{(m)}(x_0)}{m!}(-1)^m h^m + O(h^{n+1}) \end{aligned} \tag{7}$$

Injecting the expression from corollary (5) into this series we find:

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

The summations are independent and can be exchanged:

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

If we define:

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

the equation (6) follows immediately.

□

The Cohen-Hubbard-Osterwinder formula

In this section we derive the Cohen-Hubbard-Osterwinder formula, equation (1).

Proposition. *Given a sufficient regular function $f(x)$ there exists a family of rational numbers $\beta_{n,\nu}$, with $0 \le \nu \le n-2$, such that:*

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

Proof. We start by writing 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 (7):

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

As we did above, we replace $f^{(m)}(x_0)$ using its expression from corollary (5) 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 exchange the summations and 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 obtain the desired result, which is a reformulation of equation (1) where β_i in [CHO73] is our $\beta_{14,i}$. □

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.
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