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 [**CohenHubbardOesterwinter1973**] to compute the velocity of a body in the context of 12th-order numerical integration of n-body systems.

Statement

[**CohenHubbardOesterwinter1973**] 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.

Lemma

[**Fornberg1987**] gives finite difference formulæ for any order and for kernels of arbitrary size. Given a sufficient regular function $f(x)$ and a family $\boldsymbol{\alpha} = (\alpha_0, \alpha_1, \ldots, \alpha_N)$ 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 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:

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

In this case equation (3.8) from [**Fornberg1987**] may be rewritten as follows, restoring x_0:

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

It is convenient to extract the powers of h from the coefficients:

$$\delta^m_{n,\nu}(x_0, h) = \frac{\lambda^m_{n,\nu}}{h^m}$$

where $\lambda_{n,\nu}^m$ is independent from x_0 and h. We can check that equation (3.8) is still verified by multiplying both sides by h^m:

$$\lambda_{n,\nu}^m = \frac{1}{\nu - n}(-n\lambda_{n-1,\nu}^m - m\lambda_{n-1,\nu}^{m-1})$$

and rewrite equation (2) as:

$$f^{(m)}(x_0) = \frac{1}{h^m}\sum_{\nu=0}^{n} \lambda_{n,\nu}^m f(x_0 - \nu h) + \mathcal{O}(h^{n-m+1}) \tag{3}$$

Derivation

In this section we derive equation (1) and obtain an explicit expression for the coefficients appearing in the sum, using equation (3) 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:

$$\begin{aligned} f(x_0 - h) &= \sum_{m=0}^{\infty} \frac{f^{(m)}(x_0)}{m!}(-1)^m h^m \\ &= f(x_0) - hf'(x_0) + \sum_{m=2}^{\infty} \frac{f^{(m)}(x_0)}{m!}(-1)^m h^m \\ &= f(x_0) - hf'(x_0) + \sum_{m=2}^{n} \frac{f^{(m)}(x_0)}{m!}(-1)^m h^m + \mathcal{O}(h^{n+1}) \end{aligned} \tag{4}$$

Equation (3) can be applied to the second derivative $f''(x_0)$ to yield an approximation which is still of order $n - m + 1$:

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

Injecting this expression into equation (4) we find:

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

The summations are independent and can be exchanged:

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

We can then define:

$$\eta_{n,\nu} \coloneqq \sum_{m=2}^{n} \frac{(-1)^m \lambda_{n-2,\nu}^{m-2}}{m!}$$

and we finally obtain:

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

Conclusion