Explicit hierarchy of multistep numerical integration schemes for first order ODEs

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July 15, 2010

Consider the first order differential equation

$$\frac{d}{dt}x_i = v_i(x). \tag{1}$$

The solution to this differential equation is given formally by ξ:

$$x(t+h) = \xi(x(t), h) \tag{2}$$

Define the array

$$\begin{aligned}
y^{(1)}(x,h) &= x + hv(x) \\
y^{(2)}(x,h) &= y^{(1)}(\cdot, \tfrac{1}{2}h) \circ y^{(1)}(x, \tfrac{1}{2}h) \\
y^{(2)}(x,h) &= y^{(1)}(\cdot, \tfrac{1}{3}h) \circ y^{(2)}(x, \tfrac{2}{3}h) \\
&\dots \\
y^{(n)}(x,h) &= y^{(1)}(\cdot, \tfrac{1}{n}h) \circ y^{(n-1)}(x, \tfrac{n-1}{n}h) \\
&\dots
\end{aligned} \tag{3}$$

Construct the formal linear system of equations:

$$\begin{cases}
y^{(1)} = \xi + \epsilon_1 h + \epsilon_2 h^2 + \dots + \epsilon_k h^k + \dots \\
y^{(2)} = \xi + \epsilon_1 \frac{h}{2} + \epsilon_2 (\frac{h}{2})^2 + \dots + \epsilon_k (\frac{h}{2})^k + \dots \\
\qquad \dots \\
y^{(n)} = \xi + \epsilon_1 \frac{h}{n} + \epsilon_2 (\frac{h}{n})^2 + \dots + \epsilon_k (\frac{h}{n})^k + \dots \\
\qquad \dots
\end{cases} \tag{4}$$

Extract n lines from the formal system, and the solution $\xi^{(n)}$ of this new, *finite* equation system will be an approximation of ξ (of the order $n+1$ in h).

Here are the first few approximations:

$$\xi^{(1)} = y^{(1)} \tag{5}$$
$$\xi^{(2)} = 2y^{(2)} - y^{(1)} \tag{6}$$
$$\xi^{(3)} = \frac{1}{2}(9y^{(3)} - 8y^{(2)} + y^{(1)}) \tag{7}$$
$$\xi^{(4)} = -\frac{1}{3!}(-4^3y^{(4)} + 81y^{(3)} - 24y^{(2)} + y^{(1)}) \tag{8}$$
$$\xi^{(5)} = \frac{1}{4!}(5^4y^{(5)} - 1024y^{(4)} + 486y^{(3)} - 64y^{(2)} + y^{(1)}) \tag{9}$$
$$\xi^{(6)} = -\frac{1}{5!}(-6^5y^{(6)} + 15625y^{(5)} - 10240y^{(4)} + 2430y^{(3)} - 160y^{(2)} + y^{(1)}) \tag{10}$$
$$\dots \tag{11}$$

Generally

$$\xi^{(n)} = \frac{\det \mathcal{D}^{(n)}(y^{(1)}, y^{(2)}, \dots, y^{(n)})}{\det \mathcal{D}^{(n)}(1, 1, \dots, 1)} \tag{12}$$

where

$$\mathcal{D}^{(n)}(y_1, y_2, \dots, y_n) = \begin{pmatrix} y_1 & 1 & 1 & \dots & 1 \\ y_2 & \frac{1}{2} & \frac{1}{2^2} & \dots & \frac{1}{2^{n-1}} \\ y_3 & \frac{1}{3} & \frac{1}{3^2} & \dots & \frac{1}{3^{n-1}} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ y_n & \frac{1}{n} & \frac{1}{n^2} & \dots & \frac{1}{n^{n-1}} \end{pmatrix} \tag{13}$$

The denominator is computed as follows:

$$\begin{aligned} \det \mathcal{D}^{(n)}(1, 1, \dots, 1) &= \prod_{1 \le k < j \le n} \left(\frac{1}{j} - \frac{1}{k} \right) = \prod_{1 \le k < j \le n} \frac{k - j}{kj} \\ &= \prod_{2 \le j \le n} \frac{1 - j}{j} \frac{2 - j}{2j} \dots \frac{-1}{(j-1)j} = \prod_{2 \le j \le n} \frac{(-1)^{j-1}(j-1)!}{(j-1)! j^{j-1}} \\ &= \frac{(-1)^{\frac{n(n-1)}{2}}}{2 \times 3^2 \times \dots \times n^{n-1}} \\ &= \frac{(-1)^{\frac{n(n-1)}{2} - \frac{(n-1)(n-2)}{2}}}{n^{n-1}} D^{(n-1)} = \frac{(-1)^{(n-1)}}{n^{n-1}} D^{(n-1)} \end{aligned} \tag{14}$$

(call $\det \mathcal{D}^{(n)}(1, 1, \dots, 1) \equiv D^{(n)}$).

Generally

$$\det \mathcal{D}^{(n)}(y_1, y_2, \dots, y_n) = \sum_{1 \le j < n} (-1)^{j+1} \frac{j}{n!} y_j D_j^{(n)} + (-1)^{n+1} \frac{1}{(n-1)!} y_n D^{(n-1)} \tag{15}$$

where

$$D_j^{(n)} = \begin{vmatrix} 1 & 1 & 1 & \dots & 1 \\ 1 & \frac{1}{2} & \frac{1}{2^2} & \dots & \frac{1}{2^{n-2}} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & \frac{1}{j-1} & \frac{1}{(j-1)^2} & \dots & \frac{1}{(j-1)^{n-2}} \\ 1 & \frac{1}{j+1} & \frac{1}{(j+1)^2} & \dots & \frac{1}{(j+1)^{n-2}} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & \frac{1}{n} & \frac{1}{n^2} & \dots & \frac{1}{n^{n-2}} \end{vmatrix} \tag{16}$$

but we can compute this determinant:

$$D_j^{(n)} = \frac{D^{(n)}}{\prod_{1\le k<j}\left(\frac{1}{j}-\frac{1}{k}\right)\prod_{j<k\le n}\left(\frac{1}{k}-\frac{1}{j}\right)} = \frac{j^{n-1}\, n!}{(-1)^{n-1}(n-j)!\, j!} D^{(n)} \tag{17}$$

because

$$\begin{aligned} \prod_{1\le k<j}\left(\frac{1}{j}-\frac{1}{k}\right) &= \prod_{1\le k<j}\frac{k-j}{jk} = \frac{(-1)^{j-1}(j-1)!}{j^{j-1}(j-1)!} \\ \prod_{j<k\le n}\left(\frac{1}{k}-\frac{1}{j}\right) &= \prod_{j<k\le n}\frac{j-k}{kj} = \frac{(-1)^{n-j}(n-j)!\, j!}{j^{n-j}\, n!} \end{aligned} \tag{18}$$

so

$$\det \mathcal{D}^{(n)}(y_1, y_2, \dots, y_n) = \sum_{1\le j<n} \frac{(-1)^{j-n} j^n}{(n-j)!\, j!} D^{(n)} y_j + \frac{n^n}{n!} y_n D^{(n)} \tag{19}$$

and we have the explicit general solution

$$\xi^{(n)} = \sum_{1\le j\le n} \frac{(-1)^{j-n}\, j^n}{(n-j)!\, j!} y^{(j)} \tag{20}$$

Note[1]: the solution can also be written as

$$\xi^{(n)} = \frac{1}{(n-1)!}\sum_{m=0}^{n-1}(-1)^{n-m-1}\binom{n-1}{m}(m+1)^{n-1} y^{(m)}, \tag{21}$$

which could be easier to deal with.

I call $J = \nabla v$; regarding $\nabla\xi$ we have

$$\nabla\xi^{(n)} = \frac{\det \mathcal{D}^{(n)}(\nabla y^{(1)}, \nabla y^{(2)}, \dots, \nabla y^{(n)})}{\det \mathcal{D}^{(n)}(1, 1, \dots, 1)} \tag{22}$$

so symbolically:

[1] http://www.research.att.com/~njas/sequences/A075513

$$\nabla\xi^{(n)} = \frac{\det \mathcal{D}^{(n)}(1+hJ, (1+\frac{h}{2}J)^2, \ldots, (1+\frac{h}{n}J)^n)}{\det \mathcal{D}^{(n)}(1,1,\ldots,1)} \tag{23}$$

and we obtain (checked up to $n = 20$, no proof for all n):

$$\nabla\xi^{(n)} = 1 + hJ + \frac{1}{2}(hJ)^2 + \cdots + \frac{1}{n!}(hJ)^n \tag{24}$$

It is pretty obvious that an infinity of sequences with ξ as a limit can be built, some of them converging extremely fast. This rapid convergence is probably payed through an increased number of operations to perform (the number of applications of the Euler scheme — $y^{(1)}$). For instance:

$$\begin{aligned}
z^{(1)}(x,h) &= x + hv(x) \\
z^{(2)}(x,h) &= 2z^{(1)}(\cdot, \tfrac{1}{2}h) \circ z^{(1)}(x, \tfrac{1}{2}h) - z^{(1)}(x,h) \\
z^{(3)}(x,h) &= \frac{1}{2^2-1}(2^2 z^{(2)}(\cdot, \tfrac{1}{2}h) \circ z^{(2)}(x, \tfrac{1}{2}h) - z^{(2)}(x,h)) \\
&\ldots \\
z^{(n)}(x,h) &= \frac{1}{2^{n-1}-1}(2^{n-1} z^{(n-1)}(\cdot, \tfrac{1}{2}h) \circ z^{(n-1)}(x, \tfrac{1}{2}h) - z^{(n-1)}(x,h)) \\
&\ldots
\end{aligned} \tag{25}$$

And $\lim z^{(n)} = \xi$, with $z^{(n)}$ an h^{n+1} approximation ($\frac{h}{2}$ for large n?). But for this case an explicit formula would be harder to find.

Back to $\xi^{(n)}$. Symbolically:

$$\begin{aligned}
\nabla\xi^{(n)} &= \sum_{1\le k\le n} \frac{(-1)^{k-n}\, k^n}{(n-k)!\, k!} \left(1 + \frac{h}{k}J\right)^k \\
&= \sum_{1\le k\le n} \frac{(-1)^{k-n}\, k^n}{(n-k)!\, k!} \sum_{0\le i\le k} \frac{k!}{i!\,(k-i)!\,k^i}(hJ)^i \\
&= \sum_{1\le k\le n}\sum_{0\le i\le k} \frac{(hJ)^i}{i!} \frac{(-1)^{k-n}\, k^{n-i}}{(n-k)!\,(k-i)!} \\
&= \sum_{0\le i\le n} \frac{(hJ)^i}{i!} \sum_{i\le k\le n} \frac{(-1)^{k-n}\, k^{n-i}}{(n-k)!\,(k-i)!}
\end{aligned} \tag{26}$$

I need a proof that $\sum_{i\le k\le n} \frac{(-1)^{k-n}\, k^{n-i}}{(n-k)!\,(k-i)!} = 1$.