Hermite integrators and 2-parameter subgroup of Riordan group

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Abstract

- A general form for the family of 2-step Hermite integrators
  - Up to p-th order derivative of the force is calculated directly to obtain $2(p+1)$-th order accuracy
  - Now, a simple and general form for the predictor is available
  - The mathematics was slightly simplified and generalized from the last talk (99% of the proof was invented by Satoko Yamamoto)

Upper triangular Pascal matrix

This following upper triangular Pascal matrix appearers frequently in this story:

(1)
$$\left[U_{\text{pas}}\right]_{ij} = \binom{j}{i}, \quad \left[U_{\text{pas}}^{-1}\right]_{ij} = (-1)^{i+j}\binom{j}{i}.$$

A $(p+1)\times(p+1)$ sized one looks like,

(2)
$$U_{\text{pas}} = \begin{pmatrix} \binom{0}{0} & \binom{1}{0} & \binom{2}{0} & \cdots & \binom{p}{0} \\ 0 & \binom{1}{1} & \binom{2}{1} & \cdots & \binom{p}{1} \\ 0 & 0 & \binom{2}{2} & \cdots & \binom{p}{2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \binom{p}{p} \end{pmatrix}.$$

Polynomial shift

A vector of scaled force

$$F(t) = \begin{pmatrix} f(t) \\ hf^{(1)}(t) \\ h^2 f^{(2)}(t)/2! \\ \vdots \\ h^n f^{(p)}(t)/n! \end{pmatrix}, \tag{3}$$

where $f^{(n)}(t) = \frac{d^n}{dt^n} f(t)$ $(0 \leq n \leq p)$, obeys a transformation

$$F(t+h) = \begin{pmatrix} \binom{0}{0} & \binom{1}{0} & \binom{2}{0} & \cdots & \binom{p}{0} \\ 0 & \binom{1}{1} & \binom{2}{1} & \cdots & \binom{p}{1} \\ 0 & 0 & \binom{2}{2} & \cdots & \binom{p}{2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \binom{p}{p} \end{pmatrix} F(t) = U_{\text{pas}} F(t). \tag{4}$$

Linear equation to solve

For even order polynomial coefficients:

$$
(5) \quad \begin{pmatrix} F_0^+ \\ F_1^- \\ F_2^+ \\ F_3^- \\ \vdots \end{pmatrix} = \begin{pmatrix} \binom{0}{0} & \binom{2}{0} & \binom{4}{0} & \binom{6}{0} & \cdots \\ 0 & \binom{2}{1} & \binom{4}{1} & \binom{6}{1} & \cdots \\ 0 & \binom{2}{2} & \binom{4}{2} & \binom{6}{2} & \cdots \\ 0 & 0 & \binom{4}{3} & \binom{6}{3} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} F_0 \\ F_2 \\ F_4 \\ F_6 \\ \vdots \end{pmatrix}.
$$

For odd order polynomial coefficients:

$$
(6) \quad \begin{pmatrix} F_0^- \\ F_1^+ \\ F_2^- \\ F_3^+ \\ \vdots \end{pmatrix} = \begin{pmatrix} \binom{1}{0} & \binom{3}{0} & \binom{5}{0} & \binom{7}{0} & \cdots \\ \binom{1}{1} & \binom{3}{1} & \binom{5}{1} & \binom{7}{1} & \cdots \\ 0 & \binom{3}{2} & \binom{5}{2} & \binom{7}{2} & \cdots \\ 0 & \binom{3}{3} & \binom{5}{3} & \binom{7}{3} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} F_1 \\ F_3 \\ F_5 \\ F_7 \\ \vdots \end{pmatrix}.
$$

(definitions: $F_i^+ = \frac{1}{2}(F_i^R + F_i^L)$, $F_i^- = \frac{1}{2}(F_i^R - F_i^L)$.)

Generalization

We modify the upper triangular Pascal matrix with 2-parameter (a, b), as in

$$[M_{(a,b)}]_{ij} = \binom{aj+b}{i}. \tag{7}$$

This is no longer an upper triangular matrix.
Our interest is to find the solutions

- $M_{(2,0)}^{-1}$ for the even order terms, and
- $M_{(2,1)}^{-1}$ for the odd order terms.

Unfortunately, explicit forms of their inverses seem to be hardly available.

Matrix inverse (conjecture)

It turned out that, by multiplying (inverse) Pascal matrices, we can write

(8) $$M_{(a,b)}^{-1} = U_{\mathrm{pas}}^{-1}\, M_{(1/a,-b/a)}\, U_{\mathrm{pas}}^{-1},$$

or equivalently,

(9) $$\left(M_{(a,b)}U_{\mathrm{pas}}^{-1}\right)^{-1} = M_{(1/a,-b/a)}U_{\mathrm{pas}}^{-1}.$$

Thus, if we define

(10) $$L_{(a,b)} = M_{(a,b)}U_{\mathrm{pas}}^{-1},$$

then

(11) $$L_{(a,b)}^{-1} = L_{(1/a,-b/a)},$$

(12) $$M_{(a,b)}^{-1} = U_{\mathrm{pas}}^{-1}L_{(1/a,-b/a)}.$$

Interpretation

A 2-parameter dense matrix $M_{(a,b)}$ can be factorized into

$$M_{(a,b)} = L_{(a,b)} U_{\text{pas}} \tag{13}$$

and we will soon see that $L_{(a,b)}$ is upper triangular.
Though explicit matrix elements of $L_{(a,b)}$ in general are hard to obtain (see (3.150) `GouldBK.pdf`, Sprugnoli, 2006), all we need are

$$M^{-1}_{(2,0)} = U^{-1}_{\text{pas}} L_{(1/2,0)}, \tag{14}$$

$$M^{-1}_{(2,1)} = U^{-1}_{\text{pas}} L_{(1/2,-1/2)}. \tag{15}$$

Fortunately, matrix elements of U^{-1}_{pas}, $L_{(1/2,0)}$, and $L_{(1/2,-1/2)}$ are available explicitly.

Example (for $p = 7$, 16th-order) I

$$[L_{1/2,0}]_{nk} = \frac{(-2)^k}{(-4)^n}\frac{k}{n}\binom{2n-k-1}{n-k} \tag{16}$$

$$\begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -\frac{1}{8} & \frac{1}{4} & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{1}{16} & -\frac{1}{8} & \frac{1}{8} & 0 & 0 & 0 & 0 \\
0 & -\frac{5}{128} & \frac{5}{64} & -\frac{3}{32} & \frac{1}{16} & 0 & 0 & 0 \\
0 & \frac{7}{256} & -\frac{7}{128} & \frac{9}{128} & -\frac{1}{16} & \frac{1}{32} & 0 & 0 \\
0 & -\frac{21}{1024} & \frac{21}{512} & -\frac{7}{128} & \frac{7}{128} & -\frac{5}{128} & \frac{1}{64} & 0 \\
0 & \frac{33}{2048} & -\frac{33}{1024} & \frac{45}{1024} & -\frac{3}{64} & \frac{5}{128} & -\frac{3}{128} & \frac{1}{128}
\end{pmatrix}$$

Example (for $p = 7$, 16th-order) II

$$[L_{1/2,-1/2}]_{nk} = \frac{(-2)^k}{(-4)^n}\binom{2n-k}{n-k} \tag{17}$$

$$\begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-\frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{3}{8} & -\frac{3}{8} & \frac{1}{4} & 0 & 0 & 0 & 0 & 0 \\
-\frac{5}{16} & \frac{5}{16} & -\frac{1}{4} & \frac{1}{8} & 0 & 0 & 0 & 0 \\
\frac{35}{128} & -\frac{35}{128} & \frac{15}{64} & -\frac{5}{32} & \frac{1}{16} & 0 & 0 & 0 \\
-\frac{63}{256} & \frac{63}{256} & -\frac{7}{32} & \frac{21}{128} & -\frac{3}{32} & \frac{1}{32} & 0 & 0 \\
\frac{231}{1024} & -\frac{231}{1024} & \frac{105}{512} & -\frac{21}{128} & \frac{7}{64} & -\frac{7}{128} & \frac{1}{64} & 0 \\
-\frac{429}{2048} & \frac{429}{2048} & -\frac{99}{512} & \frac{165}{1024} & -\frac{15}{128} & \frac{9}{128} & -\frac{1}{32} & \frac{1}{128}
\end{pmatrix}$$

$L_{(a,b)}$: 2-parameter lower-triangular matrix

We compute the matrix element from its definition:

$$
\begin{aligned}
(18) \qquad [L_{(a,b)}]_{ij} &= \left[M_{(a,b)}U_{\text{pas}}^{-1}\right]_{ij} \\
&= \sum_{k=0}^{\infty} \binom{ak+b}{i} (-1)^{k+j} \binom{j}{k} \\
&= \sum_{k=0}^{\infty} [y^i](1+y)^{ak+b} \cdot [t^k](-1+t)^j \\
&= \sum_{k=0}^{\infty} [t^k](-1+t)^j \cdot [y^i](1+y)^b \left((1+y)^a\right)^k \\
&= [t^i](1+t)^b \left(-1+(1+t)^a\right)^j \\
&= \left[\mathcal{R}\left((1+t)^b, -1+(1+t)^a\right)\right]_{ij}.
\end{aligned}
$$

$\mathcal{R}(d(t), h(t))$ is a Riordan array of which element is $[t^i]d(t)h(t)^j$.

Composition and convolution

To remove the summation on k, we used a relation

$$
\begin{aligned}
(19)\quad \sum_{k=0}^{\infty}[t^k]f(t)\cdot[y^n]h(y)g(y)^k &= \sum_{m=0}^{\infty}\sum_{k=0}^{\infty}[t^k]f(t)\cdot[y^{n-m}]h_m g(y)^k \\
&= \sum_{m=0}^{\infty} h_m[t^{n-m}]f\left(g(t)\right) \\
&= \sum_{m=0}^{\infty}[y^m]h(y)\cdot[t^{n-m}]f\left(g(t)\right) \\
&= [t^n]h(t)f\left(g(t)\right)
\end{aligned}
$$

with $f(t) = (-1+t)^j$, $g(y) = (1+y)^a$, and $h(t) = (1+t)^b$.

Riordan array

is an infinitesimal lower triangle matrix, taking 2 formal power series. The element at the n-th row and the k-th column is

$$\left[\mathcal{R}\left(d(t), h(t)\right)\right]_{nk} = [t^n]d(t)h(t)^k. \tag{20}$$

Matrix multiplication is given by

$$\mathcal{R}\left(d(t), h(t)\right) \circ \mathcal{R}\left(f(t), g(t)\right) = \mathcal{R}\left(d(t) \cdot f\left(h(t)\right), g\left(h(t)\right)\right). \tag{21}$$

For our 2-parameter matrices

$$\begin{aligned} L_{(a,b)} =& \mathcal{R}\left((1+t)^b, -1 + (1+t)^a\right), \\ L_{(c,d)} =& \mathcal{R}\left((1+t)^d, -1 + (1+t)^c\right), \end{aligned}$$

we have a multiplication

$$L_{(a,b)} L_{(c,d)} = \mathcal{R}\left((1+t)^b (1+t)^{ad}, -1 + (1+t)^{ac}\right) = L_{(ac,ad+b)}. \tag{22}$$

Group structure

$L_{(a,b)}$ forms a subgroup of the Riordan group when $a \neq 0$.

- Multiplication:

$$L_{(a,b)}L_{(c,d)} = L_{(ac,ad+b)}.$$

- Identity:

$$L_{(1,0)}L_{(a,b)} = L_{(a,b)}L_{(1,0)} = L_{(a,b)}$$

- Inverse:

$$L^{-1}_{(a,b)} = L_{(1/a,-b/a)}.$$

The following 2×2 matrix preserves the same structure.

$$\begin{pmatrix} 1 & 0 \\ b & a \end{pmatrix} \begin{pmatrix} 1 & 0 \\ d & c \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ ad+b & ac \end{pmatrix}. \tag{23}$$

Application to the Hermite integrators

Remember:

$$M^{-1}_{(2,0)} = U^{-1}_{\text{pas}} L^{-1}_{(2,0)} = U^{-1}_{\text{pas}} L_{(1/2,0)}, \tag{24}$$

$$M^{-1}_{(2,1)} = U^{-1}_{\text{pas}} L^{-1}_{(2,1)} = U^{-1}_{\text{pas}} L_{(1/2,-1/2)}. \tag{25}$$

All we need is the matrices elements of U^{-1}_{pas}, $L_{(1/2,0)}$, and $L_{(1/2,-1/2)}$.
The first one is very simple: $[U^{-1}_{\text{pas}}]_{ij} = (-1)^{i+j}\binom{j}{i}$.

Implementation ($p = 7$, 16th-order interpolation) I

Even order coefficients are computed in

(26)

$$\begin{pmatrix} F_8 \\ F_{10} \\ F_{12} \\ F_{14} \end{pmatrix} = \begin{pmatrix} 1 & -5 & 15 & -35 \\ 0 & 1 & -6 & 21 \\ 0 & 0 & 1 & -7 \\ 0 & 0 & 0 & 1 \end{pmatrix} \times$$

$$\begin{pmatrix} \frac{5}{64} & -\frac{3}{32} & \frac{1}{16} & 0 & 0 & 0 \\ -\frac{7}{128} & \frac{9}{128} & -\frac{1}{16} & \frac{1}{32} & 0 & 0 \\ \frac{21}{512} & -\frac{7}{128} & \frac{7}{128} & -\frac{5}{128} & \frac{1}{64} & 0 \\ -\frac{33}{1024} & \frac{45}{1024} & -\frac{3}{64} & \frac{5}{128} & -\frac{3}{128} & \frac{1}{128} \end{pmatrix} \begin{pmatrix} F_2^+ - \frac{1}{2} F_1^- \\ F_3^- \\ F_4^+ \\ F_5^- \\ F_6^+ \\ F_7^- \end{pmatrix}.$$

Implementation ($p = 7$, 16th-order interpolation) II

And the odd order ones

(27)

$$\begin{pmatrix} F_9 \\ F_{11} \\ F_{13} \\ F_{15} \end{pmatrix} = \begin{pmatrix} 1 & -5 & 15 & -35 \\ 0 & 1 & -6 & 21 \\ 0 & 0 & 1 & -7 \\ 0 & 0 & 0 & 1 \end{pmatrix} \times$$

$$\begin{pmatrix} -\frac{35}{128} & \frac{15}{64} & -\frac{5}{32} & \frac{1}{16} & 0 & 0 & 0 \\ \frac{63}{256} & -\frac{7}{32} & \frac{21}{128} & -\frac{3}{32} & \frac{1}{32} & 0 & 0 \\ -\frac{231}{1024} & \frac{105}{512} & -\frac{21}{128} & \frac{7}{64} & -\frac{7}{128} & \frac{1}{64} & 0 \\ \frac{429}{2048} & -\frac{99}{512} & \frac{165}{1024} & -\frac{15}{128} & \frac{9}{128} & -\frac{1}{32} & \frac{1}{128} \end{pmatrix} \begin{pmatrix} F_1^+ - F_0^- \\ F_2^- \\ F_3^+ \\ F_4^- \\ F_5^+ \\ F_6^- \\ F_7^+ \end{pmatrix}.$$

Implementation ($p = 7$, 16th-order interpolation) III

Right shift for the next predictor by right-bottom submatrix of U_{pas}:

$$\begin{pmatrix} F_8^R \\ F_9^R \\ F_{10}^R \\ F_{11}^R \\ F_{12}^R \\ F_{13}^R \\ F_{14}^R \\ F_{15}^R \end{pmatrix} = \begin{pmatrix} 1 & 9 & 45 & 165 & 495 & 1287 & 3003 & 6435 \\ 0 & 1 & 10 & 55 & 220 & 715 & 2002 & 5005 \\ 0 & 0 & 1 & 11 & 66 & 286 & 1001 & 3003 \\ 0 & 0 & 0 & 1 & 12 & 78 & 364 & 1365 \\ 0 & 0 & 0 & 0 & 1 & 13 & 91 & 455 \\ 0 & 0 & 0 & 0 & 0 & 1 & 14 & 105 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 15 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} F_8 \\ F_9 \\ F_{10} \\ F_{11} \\ F_{12} \\ F_{13} \\ F_{14} \\ F_{15} \end{pmatrix} \tag{28}$$

Matrix element of $L_{(1/2,0)}$

We use Lagrange inverse formula with $w(t) = -1 + \sqrt{1+t}$. For $t = w(w+2)$, $\phi(t) = 1/(2+t)$ satisfies $w = t\phi(w)$.

$$
\begin{aligned}
[L_{1/2,0}]_{nk} &= [t^n]\left(-1 + (1+t)^{1/2}\right)^k \\
&= [t^n]w^k \\
&= \frac{k}{n}[t^{n-1}]t^{k-1}\phi(t)^n \\
&= \frac{k}{n}[t^{n-k}](2+t)^{-n} \\
&= 2^{k-2n}\frac{k}{n}\binom{-n}{n-k} \\
&= (-1)^{n+k}2^{k-2n}\frac{k}{n}\binom{2n-k-1}{n-k}.
\end{aligned} \tag{29}
$$

In case $n = 0$, it is δ_{k0}.

Matrix element of $L_{(1/2,-1/2)}$

Similarly,

$$
\begin{aligned}
[L_{1/2,-1/2}]_{nk} &= [t^n](1+t)^{-1/2}\left(-1+(1+t)^{1/2}\right)^k \\
&= [t^n]\frac{w^k}{1+w} \\
&= [t^n]\frac{t^k}{1+t}\phi(t)^{n-1}\left(\phi(t)-t\phi'(t)\right) \\
&= [t^n]\frac{t^k}{1+t}\frac{1}{(2+t)^{n-1}}\frac{2(1+t)}{(2+t)^2} \\
&= 2[t^{n-k}](2+t)^{-n-1} \\
&= 2^{k-2n}\binom{-n-1}{n-k} \\
&= (-1)^{n+k}2^{k-2n}\binom{2n-k}{n-k}.
\end{aligned}
\tag{30}
$$

Review

We have concerned with a 2-parameter matrix

$$[M_{(a,b)}]_{ij} = \binom{aj+b}{i}, \tag{31}$$

which has an LU factorized form

$$M_{(a,b)} = L_{(a,b)} U_{\text{pas}} \tag{32}$$

where $U_{\text{pas}} = M_{(1,0)}$ is an upper triangle Pascal matrix and $L_{(a,b)}$ is a lower triangle matrix expressed in a Riordan array form

$$L_{(a,b)} = \mathcal{R}\left((1+t)^b, -1+(1+t)^a\right). \tag{33}$$

Matrix inverse $M^{-1}_{(a,b)}$ is available in

$$M^{-1}_{(a,b)} = U^{-1}_{\text{pas}} L^{-1}_{(a,b)} = U^{-1}_{\text{pas}} L_{(1/a,-b/a)} = U^{-1}_{\text{pas}} M_{(1/a,-b/a)} U^{-1}_{\text{pas}}, \tag{34}$$

Summary

- We have generalized the 2-step Hermite integrators
  - Predictor and corrector
  - General and explicit matrix elements
  - Simple and economical formulation, easy to implement
- Mathematical combinatorics have performed an essential role for the derivation and proof
  - Formal power series, Lagrange inverse formula, Riordan array
  - Implementers only need to know about matrix vector multiplications and binomial coefficients, not the full mathematics