Hermite integrators and Riordan arrays

When one feels tired in round-off error

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Today I talk about

- A general form of the correctors 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
  - A mathematical proof in elementary algebra is presented
- In my last talk in MODEST 15-S, a simple and beautiful proof made by Satoko Yamamoto were mostly omitted, but today I would like you to see the full story.

References

I appreciate for many useful online documents:

1. R. Sprugnoli (2006). An Introduction to Mathematical Methods in Combinatorics.
   `http://www.dsi.unifi.it/~resp/Handbook.pdf`
2. R. Sprugnoli (2006). Riordan Array Proofs of Identities in Gould's Book.
   `http://www.dsi.unifi.it/~resp/GouldBK.pdf`
3. D. Merlini (2011). A survey on Riordan arrays.
   `https://lipn.univ-paris13.fr/~banderier/Seminaires/Slides/merlini.pdf`
4. P. Barry (2005) A Catalan Transform and Related Transformations on Integer Sequences. *Journal of Integer Sequences* **8**. `https://cs.uwaterloo.ca/journals/JIS/VOL8/Barry/barry84.html`

Polynomial shift by Pascal matrix I

We consider to shift a finite order polynomial $f(t)$, of which up to the p-th derivatives are $f^{(n)}(t) = \frac{d^n}{dt^n} f(t)$ $(0 \leq n \leq p)$. Adjusting the dimension of the derivatives by a step size h, a vector

$$\boldsymbol{F}(t) = \begin{pmatrix} f(t) \\ hf^{(1)}(t) \\ h^2 f^{(2)}(t)/2! \\ \vdots \\ h^n f^{(p)}(t)/n! \end{pmatrix}. \quad (1)$$

obeys a differential equation

$$\frac{d}{dt}\boldsymbol{F}(t) = \frac{1}{h} \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 2 & \cdots & 0 \\ 0 & 0 & 0 & \ddots & \vdots \\ \vdots & \vdots & \vdots & \ddots & p \\ 0 & 0 & 0 & \cdots & 0 \end{pmatrix} \boldsymbol{F}(t). \quad (2)$$

Polynomial shift by Pascal matrix II

A formal solution at $t + h$ is,

$$\boldsymbol{F}(t+h) = \exp\left[\begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 2 & \cdots & 0 \\ 0 & 0 & 0 & \ddots & \vdots \\ \vdots & \vdots & \vdots & \ddots & p \\ 0 & 0 & 0 & \cdots & 0 \end{pmatrix}\right]\boldsymbol{F}(t)$$

$$= \begin{pmatrix} \binom{0}{0} & \binom{1}{0} & \binom{2}{0} & \cdots & \binom{p}{0} \\ 0 & \binom{1}{1} & \binom{2}{1} & \cdots & \binom{p}{1} \\ 0 & 0 & \binom{2}{2} & \cdots & \binom{p}{2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \binom{p}{p} \end{pmatrix}\boldsymbol{F}(t). \quad (3)$$

This matrix is referred to as *upper triangle Pascal matrix*.

Polynomial shift by Pascal matrix III

Example

For $p = 9$,

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \\ 0 & 0 & 1 & 3 & 6 & 10 & 15 & 21 & 28 & 36 \\ 0 & 0 & 0 & 1 & 4 & 10 & 20 & 35 & 56 & 84 \\ 0 & 0 & 0 & 0 & 1 & 5 & 15 & 35 & 70 & 126 \\ 0 & 0 & 0 & 0 & 0 & 1 & 6 & 21 & 56 & 126 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 7 & 28 & 84 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 8 & 36 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 9 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

Construction of the Hermite integrators I

For simplicity, we integrate from $t = -h$ to $t = h$, thus a timestep becomes $\Delta t = 2h$ (not h).

The inputs are additions and subtractions

$$F_n^+ = \frac{1}{2}\frac{h^n}{n!}\left(f^{(n)}(h) + f^{(n)}(-h)\right), \tag{4}$$

$$F_n^- = \frac{1}{2}\frac{h^n}{n!}\left(f^{(n)}(h) - f^{(n)}(-h)\right), \tag{5}$$

for $0 \le n \le p$. The outputs are fitting polynomial at $t = 0$,

$$F_n = \frac{h^n}{n!} f^{(n)}(0), \tag{6}$$

for $0 \le n \le 2p + 1$.

The integral includes only the even order terms:

$$\Delta v = \int_{-h}^{h} f(t)dt = F_0 + \frac{1}{3}F_2 + \frac{1}{5}F_4 + \cdots + \frac{1}{2p+1}F_{2p}, \tag{7}$$

for a $2(p + 1)$-th order integrator.

Construction of the Hermite integrators II

A linear equation we want to solve is

$$\begin{pmatrix} F_0^+ \\ F_1^- \\ F_2^+ \\ F_3^- \\ \vdots \end{pmatrix} = \begin{pmatrix} \binom{0}{0} & \binom{2}{0} & \binom{4}{0} & \binom{6}{0} & \cdots \\ 0 & \binom{2}{1} & \binom{4}{1} & \binom{6}{1} & \cdots \\ 0 & \binom{2}{2} & \binom{4}{2} & \binom{6}{2} & \cdots \\ 0 & 0 & \binom{4}{3} & \binom{6}{3} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} F_0 \\ F_2 \\ F_4 \\ F_6 \\ \vdots \end{pmatrix}, \tag{8}$$

of size $(p+1)$. The element of matrix is $\binom{2j}{i}$ (counted from $(0,0)$), which means we have picked up the even number columns from the Pascal matrix.

Construction of the Hermite integrators III

Example

By solving

$$\begin{pmatrix} F_0^+ \\ F_1^- \\ F_2^+ \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 \\ 0 & 2 & 4 \\ 0 & 1 & 6 \end{pmatrix} \begin{pmatrix} F_0 \\ F_2 \\ F_4 \end{pmatrix}, \tag{9}$$

we have

$$\begin{pmatrix} F_0 \\ F_2 \\ F_4 \end{pmatrix} = \frac{1}{8} \begin{pmatrix} 8 & -5 & 2 \\ 0 & 6 & -4 \\ 0 & -1 & 2 \end{pmatrix} \begin{pmatrix} F_0^+ \\ F_1^- \\ F_2^+ \end{pmatrix}. \tag{10}$$

The sixth-order integrator is thus

$$\begin{aligned} \varDelta v =& 2 \left(F_0 + \frac{1}{3} F_2 + \frac{1}{5} F_4 \right) h \\ =& \left(F_0^+ - \frac{2}{5} F_1^- + \frac{2}{15} F_2^+ \right) \varDelta t \end{aligned} \tag{11}$$

Coefficients table

	F_0^+	F_1^-	F_2^+	F_3^-	F_4^+	F_5^-	F_6^+	F_7^-
A2	1							
H4	1	$-\frac{1}{3}$						
H6	1	$-\frac{2}{5}$	$\frac{2}{15}$					
H8	1	$-\frac{3}{7}$	$\frac{4}{21}$	$-\frac{2}{35}$				
H10	1	$-\frac{4}{9}$	$\frac{6}{27}$	$-\frac{2}{21}$	$\frac{8}{315}$			
H12	1	$-\frac{5}{11}$	$\frac{8}{33}$	$-\frac{4}{33}$	$\frac{8}{165}$	$-\frac{8}{693}$		
H14	1	$-\frac{6}{13}$	$\frac{10}{39}$	$-\frac{20}{143}$	$\frac{48}{715}$	$-\frac{32}{1287}$	$\frac{16}{3003}$	
H16	1	$-\frac{7}{15}$	$\frac{12}{45}$	$-\frac{2}{13}$	$\frac{16}{195}$	$-\frac{16}{429}$	$\frac{64}{5005}$	$-\frac{16}{6435}$

Table: Coefficients for up to the 16th-order Hermite integrator

General form

For the $2(p+1)$-th order integrator ($p \geq 0$), the k-th term ($0 \leq k \leq p$) is,

$$c^{(p)}{}_k = \frac{1}{(-2)^k} \frac{(2k)!!}{(2k+1)!!} \binom{p-k+m}{p-k} \frac{(2k+1)!!}{(2k+1-2m)!!} \frac{(2p+1-2m)!!}{(2p+1)!!}, \tag{12}$$

with $m = \lfloor (k+1)/2 \rfloor$. A recurrent form starting from the diagonal element to the bottom is

$$c^{(p)}{}_k = \begin{cases} \dfrac{1}{(-2)^p} \dfrac{(2p)!!}{(2p+1)!!} & (p = k) \\ \dfrac{p-k+m}{p-k} \dfrac{2p+1-2m}{2p+1} c^{(p-1)}{}_k & (p > k) \end{cases} . \tag{13}$$

It is a rational recurrent form, however, we still seek for a differential recurrent form in $c^{(p)}{}_k - c^{(p-1)}{}_k$ for our proof.

Coffee break (double factorial)

Definition:

$$n!! = n \cdot (n-2)!! \text{ (for } n \geq 2\text{)}, \quad 1!! = 0!! = 1. \tag{14}$$

(There are products of odd numbers, and even numbers)
Properties:

$$(2n)!! = 2^n n!, \tag{15}$$

$$(2n+1)!!(2n)!! = (2n+1)!, \tag{16}$$

$$(2n+1)!! = \frac{(2n+1)!}{2^n n!} = \frac{(n+1)!}{2^n}\binom{2n+1}{n}, \tag{17}$$

$$(2n)!!(2n-1)!! = (2n)!, \tag{18}$$

$$(2n-1)!! = \frac{(2n)!}{2^n n!} = \frac{n!}{2^n}\binom{2n}{n} = \frac{n!}{2^n}\frac{2n}{n}\binom{2n-1}{n-1}, \tag{19}$$

etc.

Outline of the proof

1. We wrote an expected form of the coefficients, ${c^{(p)}}_k$
2. Then calculate a differential recurrence, ${c^{(p)}}_k - {c^{(p-1)}}_k$
3. We set a linear equation $A\boldsymbol{x} = \boldsymbol{b}$, of which solution $\boldsymbol{x}$ should correspond to the expected coefficients
4. LU decomposition, $A = LU$
5. The proof for the form of inverse matrices L^{-1} and U^{-1} will be shown later, by using of a modern tool *Riordan arrays*
6. Calculate $L^{-1}\boldsymbol{b}$
7. Finally we see that the solution $\boldsymbol{x} = U^{-1}L^{-1}\boldsymbol{b}$ obeys the same recursion to ${c^{(p)}}_k$, given a matrix size $(p + 1)$

Differential recurrence I

This is a hand exercise (remember $m = \lfloor (k+1)/2 \rfloor$):

$$\begin{aligned} {c^{(p)}}_k - {c^{(p-1)}}_k &= {c^{(p)}}_k \left(1 - \frac{p-k+m}{p-k}\frac{2p+1-2m}{2p+1}\right) \\ &= {c^{(p)}}_k \frac{m(2k+1-2m)}{(p-k+m)(2p+1-2m)} \end{aligned} \tag{20}$$

Now, the difference is simplified as in

$$\begin{aligned} & \frac{1}{(-2)^k}\frac{(2k)!!}{(2k+1)!!}\binom{p-k+m}{m}\frac{(2k+1)!!}{(2k+1-2m)!!}\frac{(2p+1-2m)!!}{(2p+1)!!} \\ & \times \frac{m(2k+1-2m)}{(p-k+m)(2p+1-2m)} \\ = & \frac{(-1)^k k!}{(2p+1)!!}\binom{p-k+m-1}{m-1}\frac{(2p-1-2m)!!}{(2k-1-2m)!!} \\ = & \frac{(-1)^k k!}{(2p+1)!!}\frac{(p-k+m-1)!}{(p-k)!(m-1)!}\frac{2^{k-m}}{2^{p-m}}\frac{(k-m)!}{(p-m)!}\frac{(2p-2m)!}{(2k-2m)!} \end{aligned} \tag{21}$$

Differential recurrence II

Let us now introduce $b = k \mod 2 \in \{0, 1\}$, and $\bar{b} = 1 - b$, hence $k = 2m - b$. Some useful properties are:

$$\frac{(n+b)!}{n!} = (n+1)^b, \quad \frac{(n-b)!}{(n-1)!} = n^{\bar{b}}, \quad (n-1)^b a^{\bar{b}} = n - b,$$

$$\begin{aligned}
&\frac{(-1)^k}{2^{p-k}} \frac{(2m-b)!}{(2p+1)!!} \frac{(p-m-1+b)!}{(p-2m+b)!(m-1)!} \frac{(m-b)!}{(p-m)!} \frac{(2p-2m)!}{(2m-2b)!} \\
=&\frac{(-1)^k}{2^{p-k}} \frac{(2m-1)^b}{(2p+1)!!} \frac{(2p-2m)!}{(p-2m+b)!} \frac{m^{\bar{b}}}{(p-m)^{\bar{b}}} \times \frac{2^{\bar{b}}}{2^{\bar{b}}} \\
=&\frac{(-1)^k}{2^{p-k}(2p+1)!!} \frac{(2m-1)^b (2m)^{\bar{b}}}{(p-2m+b)!} \frac{(2p-2m)!}{(2p-2m)^{\bar{b}}} \\
=&\frac{(-1)^k}{2^{p-k}(2p+1)!!} \frac{2m-b}{(p-2m+b)!} (2p-2m+b-1)! \times \frac{(2p)!!}{2^p p(p-1)!} \\
=&\frac{(-1)^k}{2^{2p-k}} \frac{(2p)!!}{(2p+1)!!} \frac{k}{p} \frac{(2p-k-1)!}{(p-k)!(p-1)!}
\end{aligned} \tag{22}$$

Differential recurrence III

Finally, we have

$$c^{(p)}{}_k = \begin{cases} \dfrac{1}{(-2)^p} \dfrac{(2p)!!}{(2p+1)!!} & (p = k) \\[2ex] c^{(p-1)}{}_k + \dfrac{(-1)^k}{2^{2p-k}} \dfrac{(2p)!!}{(2p+1)!!} \dfrac{k}{p} \dbinom{2p-k-1}{p-k} & (p > k) \end{cases} . \tag{23}$$

for which we are going to make the proof. Note that this form does not include $m = \lfloor (k+1)/2 \rfloor$.

Differential recurrence (old version) I

When k is even ($k = 2m$),

$$
\begin{aligned}
&\frac{(2m)!}{(2p+1)!!}\binom{p-m-1}{m-1}\frac{(2p-2m-1)!!}{(2m-1)!!} \\
&= \frac{(2m)!!}{(2p+1)!!}\frac{(p-m-1)!}{(p-2m)!(m-1)!}\frac{(2p-2m-1)!}{(2p-2m-2)!!} \\
&= \frac{1}{2^{p-m-1}}\frac{2^m m!}{(2p+1)!!}\frac{(2p-2m-1)!}{(p-2m)!(m-1)!}\quad\left(\times\frac{m!}{m!}\right) \\
&= \frac{k}{2^{p-k}}\frac{1}{(2p+1)!!}\frac{(2p-2m-1)!}{(p-2m)!}\quad\left(\times\frac{(p-1)!}{(p-1)!}\right) \\
&= \frac{k}{2^{p-k}}\frac{(p-1)!}{(2p+1)!!}\binom{2p-k-1}{p-k}\quad\left(\times\frac{p}{p}\frac{(2p)!!}{(2p)!!}\right) \\
&= \frac{k}{2^{p-k}}\frac{(2p)!!}{(2p+1)!!}\frac{(p-1)!}{2^p p!}\binom{2p-k-1}{p-k} \\
&= \frac{1}{2^{2p-k}}\frac{(2p)!!}{(2p+1)!!}\frac{k}{p}\binom{2p-k-1}{p-k}.
\end{aligned}
\tag{24}
$$

Differential recurrence (old version) II

When k is odd ($k = 2m - 1$),

$$
\begin{aligned}
& -\frac{(2m-1)!}{(2p+1)!!}\binom{p-m}{m-1}\frac{(2p-2m-1)!!}{(2m-3)!!} \\
&= -\frac{(2m-1)(2m-2)!!}{(2p+1)!!}\frac{(p-m)(p-m-1)!}{(p-2m+1)!(m-1)!}\frac{(2p-2m-1)!}{(2p-2m-2)!!} \\
&= -\frac{2^{m-1}}{2^{p-m-1}}\frac{(2m-1)(p-m)}{(2p+1)!!}\frac{(2p-2m-1)!}{(p-2m+1)!}\left(\times\frac{2p-2m}{2p-2m}\right) \\
&= -\frac{1}{2^{p-k-1}}\frac{k}{(2p+1)!!}\frac{p-m}{2p-2m}\frac{(2p-2m)!}{(p-2m+1)!}\left(\times\frac{(p-1)!}{(p-1)!}\right) \\
&= -\frac{k}{2^{p-k}}\frac{(p-1)!}{(2p+1)!!}\binom{2p-k-1}{p-k}\left(\times\frac{p}{p}\frac{(2p)!!}{(2p)!!}\right) \\
&= -\frac{1}{2^{2p-k}}\frac{(2p)!!}{(2p+1)!!}\frac{k}{p}\binom{2p-k-1}{p-k}. \qquad (25)
\end{aligned}
$$

Linear equation to solve

What we want to solve is

$$Ax = b, \quad (A \in \mathbb{N}_0^{(p+1)\times(p+1)},\ x, b \in \mathbb{Q}^{p+1}) \tag{26}$$

where

$$A_{ij} = \binom{2i}{j} \quad \text{and} \quad b_j = \frac{1}{2j+1}, \quad (0 \le i, j \le p) \tag{27}$$

For example when $p = 5$,

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 2 & 1 & 0 & 0 & 0 \\ 1 & 4 & 6 & 4 & 1 & 0 \\ 1 & 6 & 15 & 20 & 15 & 6 \\ 1 & 8 & 28 & 56 & 70 & 56 \\ 1 & 10 & 45 & 120 & 210 & 252 \end{pmatrix} \begin{pmatrix} 1 \\ -5/11 \\ 8/33 \\ -4/33 \\ 8/165 \\ -8/693 \end{pmatrix} = \begin{pmatrix} 1 \\ 1/3 \\ 1/5 \\ 1/7 \\ 1/9 \\ 1/11 \end{pmatrix}. \tag{28}$$

gives the coefficients of the 12th-order integrator

LU decomposition

An LU decomposition $A = LU$ is available in,

$$A_{ij} = \binom{2i}{j}, \quad L_{ij} = \binom{i}{j}, \quad U_{ij} = 2^{2i-j}\binom{i}{j-i}, \tag{29}$$

irrespective to the matrix size $(p+1)$. Thus, $LU\boldsymbol{x} = \boldsymbol{b}$ can be solved as $\boldsymbol{x} = U^{-1}L^{-1}\boldsymbol{b}$.

Example

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 2 & 1 & 0 & 0 & 0 \\ 1 & 4 & 6 & 4 & 1 & 0 \\ 1 & 6 & 15 & 20 & 15 & 6 \\ 1 & 8 & 28 & 56 & 70 & 56 \\ 1 & 10 & 45 & 120 & 210 & 252 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 2 & 1 & 0 & 0 & 0 \\ 1 & 3 & 3 & 1 & 0 & 0 \\ 1 & 4 & 6 & 4 & 1 & 0 \\ 1 & 5 & 10 & 10 & 5 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 1 & 0 & 0 & 0 \\ 0 & 0 & 4 & 4 & 1 & 0 \\ 0 & 0 & 0 & 8 & 12 & 6 \\ 0 & 0 & 0 & 0 & 16 & 32 \\ 0 & 0 & 0 & 0 & 0 & 32 \end{pmatrix} \tag{30}$$

For the proof, we prepare the tools in mathematical combinatorics.

Formal power series, and coefficient extraction

- Formal power series

$$f(t) = \sum_{k=0}^{\infty} t^k f_k$$

  $f(t)$ is referred to as a *generating function* of a sequence $(f_0, f_1, f_2, \ldots)$.
- Coefficient extraction

$$[t^n]f(t) = f_n$$

  This is an operator but with a weak associativity.
- Shifting

$$[t^n]t^k f(t) = [t^{n-k}]f(t)$$

- Newton's binomial theorem

$$[t^k](1+t)^n = \binom{n}{k}$$

Proof for $A = LU$

$$\begin{aligned}\binom{2i}{j} &= [t^j](1+t)^{2i} \\ &= [t^j]\left(1+t(t+2)\right)^i \\ &= [t^j]\sum_{k=0}^{\infty}\binom{i}{k}t^k(t+2)^k \\ &= [t^{j-k}]\sum_{k=0}^{\infty}\binom{i}{k}\sum_{\ell=0}^{\infty}\binom{k}{\ell}t^{\ell}2^{k-\ell} \\ &= \sum_{k=0}^{\infty}\binom{i}{k}\binom{k}{j-k}2^{2k-j}. \quad \square \end{aligned} \tag{31}$$

This discussion is valid for finite matrices, for k iterates from 0 to $\min(i, j)$, touching only the non-zero elements of the upper and lower triangular matrices.

Inverse triangle matrices, L^{-1} and U^{-1}

For the lower triangle $L_{ij} = \binom{i}{j}$,

$$\left[L^{-1}\right]_{ij} = (-1)^{i+j}\binom{i}{j}, \tag{32}$$

and for the upper triangle $U_{ij} = 2^{2i-j}\binom{i}{j-i}$,

$$[U^{-1}]_{ij} = \begin{cases} \dfrac{(-1)^{i+j}}{2^{2j-i}}\dfrac{i}{j}\dbinom{2j-i-1}{j-i} & (1 \le i \le j) \\ 1 & (i = j = 0) \\ 0 & (\text{otherwise}) \end{cases}. \tag{33}$$

The both do not depend on the matrix size $0 \le i, j \le p$. The proof is a little bit technical and we put them later.

$Ux = L^{-1}\boldsymbol{b}$

$$
\begin{aligned}
\left[L^{-1}\boldsymbol{b}\right]_i &= \sum_{j=0}^{\infty}(-1)^{i+j}\binom{i}{j}\frac{1}{2j+1} \\
&= \sum_{j=0}^{\infty}(-1)^{i+j}\binom{i}{j}\int_0^1 x^{2j}\,dx \\
&=(-1)^i \int_0^1 \left(1-x^2\right)^i dx \\
&=(-1)^i \frac{(2i)!!}{(2i+1)!!}. \qquad (34)
\end{aligned}
$$

This vector does not depend on the vector length p. A proof of the fourth identity (an integral to double factorials) is in the next slide.

Integral and double factorial

We apply the integration by parts:

$$
\begin{aligned}
I_n &= \int_0^1 \left(1 + x^2\right)^n dx \\
&= \int_0^1 (x') \left(1 + x^2\right)^n dx \\
&= \left[x \left(1 - x^2\right)^n\right]_0^1 - \int_0^1 x \left(\left(1 - x^2\right)^n\right)' dx \\
&= -2n \int_0^1 \left(-x^2\right) \left(1 + x^2\right)^{n-1} dx \\
&= -2n \int_0^1 \left[\left(1 - x^2\right) \left(1 + x^2\right)^{n-1} - \left(1 + x^2\right)^{n-1}\right] dx \\
&= -2n \left(I_n - I_{n-1}\right).
\end{aligned} \tag{35}
$$

For $I_n = \frac{2n}{2n+1} I_{n-1}$ and $I_0 = 1$, we have $I_n = \frac{(2n)!!}{(2n+1)!!}$.

The solution, $\boldsymbol{x} = U^{-1}L^{-1}\boldsymbol{b}$

The last element of unknown vector $\boldsymbol{x}^{(p)}$ is now available in

$$x^{(p)}{}_p = \left[L^{-1}\boldsymbol{b}\right]_p / \left[U\right]_{pp} = \frac{1}{(-2)^p}\frac{(2p)!!}{(2p+1)!!}. \tag{36}$$

In a general case,

$$x^{(p)}{}_k = \sum_{j=k}^{p}\left[U^{-1}\right]_{kj}\left[L^{-1}\boldsymbol{b}\right]_j. \tag{37}$$

From the p-dependency of the solution vector $\boldsymbol{x}^{(p)}$, we have a recursion

$$x^{(p)}{}_k - x^{(p-1)}{}_k = \left[U^{-1}\right]_{kp}\left[L^{-1}\boldsymbol{b}\right]_p = \frac{(-1)^k}{2^{2p-k}}\frac{k}{p}\frac{(2p)!!}{(2p+1)!!}\binom{2p-k-1}{p-k}. \tag{38}$$

This is (23), exactly what we wanted!!

Riordan array

For the proof of our matrix form L^{-1} and U^{-1}, we make a brief review of *Riordan arrays*.
A Riordan array is an infinite lower triangular matrix taking a pair of formal power series $d(t)$ ($d_0 \neq 0$) and $h(t)$ ($h_0 = 0, h_1 \neq 0$) [1], of which element in the n-th row k-th column (counted from $(0, 0)$) is

$$\mathcal{R}\left(d(t), h(t)\right)_{n,k} = [t^n]d(t)\,(h(t))^k \tag{39}$$

They make a *group*, providing explicit forms of
matrix multiplication, *identity*, and *inverse*.
In this study, we exploit the Riordan arrays to find matrix inverses of which coefficients are expressed in binomials.

[1] Notice that `Handbook.pdf` by Sprugnoli takes a slightly different notation $\mathcal{R}(d(t), th(t))$ with $d_0, h_0 \neq 0$, which does not make a practical difference.

Matrix multiplication

By definition, the product of two Riordan arrays is

$$\begin{aligned}
&\left[\mathcal{R}\left(d(t), h(t)\right)\ \mathcal{R}\left(a(t), b(t)\right)\right]_{n,k} \\
&= \sum_{j=0}^{\infty} [t^n] d(t)\, (h(t))^j \cdot [y^j] a(y)\, (b(y))^k \\
&= [t^n] d(t) \sum_{j=0}^{\infty} (h(t))^j \cdot [y^j] a(y)\, (b(y))^k \\
&= [t^n] d(t) \cdot a\left(h(t)\right) \left(b\left(h(t)\right)\right)^k \\
&= \left[\mathcal{R}\left(d(t) \cdot a(h(t)),\ b(h(t))\right)\right]_{n,k} .
\end{aligned} \tag{40}$$

In the third equality, we used a relation

$$\sum_{j=0}^{\infty} x^j \cdot [y^j] f(y) = f(x), \tag{41}$$

with $x = (h(t))^j$ and $f(y) = a(y)(b(y))^k$.

Riordan group

Identity:

$$\mathcal{R}\left(1, t\right)_{n,k} = [t^n]t^k = \delta_{nk} \tag{42}$$

Inverse:

$$\mathcal{R}\left(d(t), h(t)\right)^{-1} = \mathcal{R}\left(\frac{1}{d(\bar{h}(t))}, \bar{h}(t)\right) \tag{43}$$

where $\bar{h}(t)$ is an inverse function of $h(t)$ such that $\bar{h}(h(t)) = h(\bar{h}(t)) = t$.

Proof.

Just substitute $a(t) = 1/d(\bar{h}(t))$ and $b(t) = \bar{h}(t)$ for the matrix multiplication to obtain an identity $\mathcal{R}(1, t)$ as a product. □

Maxima script

Since I am not a mathematician but rather a programmer as you know, I need concrete examples and numeric dumps to study the arrays. Maxima is a nice free software for such purposes.

```
RAelem(d, h, n, k)
  := coeff(taylor(d*h^k, t, 0, n), t^n);
genRA(d, h, nmax)
  := genmatrix(
       lambda([i,j], RAelem(d, h, i-1, j-1)),
       nmax,
       nmax);
```

Today, these software are not clever enough to find a general form or a proof automatically, but they help us greatly.

Pascal matrix (the matrix L) I

We consider $d(t) = 1/(1-t)$ and $h(t) = t/(1-t)$,

$$L = \mathcal{R}\left(\frac{1}{1-t}, \frac{t}{1-t}\right) \tag{44}$$

The elements are binomial coefficients:

$$\begin{aligned} L_{n,k} = [t^n]\frac{1}{1-t}\left(\frac{t}{1-t}\right)^k =& [t^{n-k}](1-t)^{-k-1} \\ =& [t^{n-k}]\sum_{\ell=0}^{\infty}\binom{-k-1}{\ell}1^{-k-1-\ell}(-t)^{\ell} \\ =& (-1)^{n-k}\binom{-k-1}{n-k} \\ =& \binom{n}{k}. \end{aligned} \tag{45}$$

Here, we used $\binom{-n}{k} = (-1)^k\binom{n+k-1}{k}$.

Pascal matrix (the matrix L) II

Now we seek for its inverse.

$$h = \frac{t}{1-t} \iff t = \frac{h}{1+h} \iff \bar{h}(t) = \frac{t}{1+t} \tag{46}$$

Thus,

$$L^{-1} = \mathcal{R}\left(\frac{1}{1+t}, \frac{t}{1+t}\right) \tag{47}$$

$$\begin{aligned}\left[L^{-1}\right]_{n,k} [t^n]\frac{1}{1+t}\left(\frac{t}{1+t}\right)^k =& [t^{n-k}](1+t)^{-k-1} \\ =& \binom{-k-1}{n-k} \\ =& (-1)^{n-k}\binom{n}{k}\end{aligned} \tag{48}$$

Pascal matrix (the matrix L) III

The inverse relation to the infinite triangle matrices is valid for the finite ones, thus, for example:

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 2 & 1 & 0 & 0 & 0 \\ 1 & 3 & 3 & 1 & 0 & 0 \\ 1 & 4 & 6 & 4 & 1 & 0 \\ 1 & 5 & 10 & 10 & 5 & 1 \end{pmatrix}^{-1} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 \\ -1 & 3 & -3 & 1 & 0 & 0 \\ 1 & -4 & 6 & -4 & 1 & 0 \\ -1 & 5 & -10 & 10 & -5 & 1 \end{pmatrix}$$

This confirms the relation $L_{ij} = \binom{i}{j}$ and $[L^{-1}]_{ij} = (-1)^{i+j}\binom{i}{j}$ in the main story.

Catalan's triangle (the matrix U) I

Let us consider special case that $d(t) = 1$, and set $h(t) = t(1 - t)$.

$$B = \mathcal{R}\left(1, t(1-t)\right) \tag{49}$$

$$\begin{aligned} B_{n,k} &= [t^n](t(1-t))^k \\ &= [t^{n-k}](1-t)^k \\ &= (-1)^{n-k}\binom{k}{n-k} \end{aligned} \tag{50}$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -3 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & -4 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 6 & -5 & 1 & 0 \\ 0 & 0 & 0 & 0 & -4 & 10 & -6 & 1 \end{pmatrix}$$

Catalan's triangle (the matrix U) II

Now, let us find the inverse.

$$h = t(1-t) \iff t = \frac{1 \pm \sqrt{1-4h}}{2}, \quad \text{but} \quad \bar{h}(t) = \frac{1-\sqrt{1-4t}}{2}$$

$$B^{-1} = \mathcal{R}\left(1, \frac{1-\sqrt{1-4t}}{2}\right) \tag{51}$$

$$\left[B^{-1}\right]_{n,k} = [t^n]\left(\frac{1-\sqrt{1-4t}}{2}\right)^k = \frac{k}{n}\binom{2n-k-1}{n-k} \tag{52}$$

for $1 \le k \le n$, otherwise δ_{nk}.

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 5 & 5 & 3 & 1 & 0 & 0 & 0 \\ 0 & 14 & 14 & 9 & 4 & 1 & 0 & 0 \\ 0 & 42 & 42 & 28 & 14 & 5 & 1 & 0 \\ 0 & 132 & 132 & 90 & 48 & 20 & 6 & 1 \end{pmatrix}$$

Catalan's triangle (the matrix U) III

Proof. If we put

$$w(t) = \frac{1-\sqrt{1-4t}}{2} \tag{53}$$

Then, $t = \dfrac{w}{1-w}$ or $w = \dfrac{t}{1-w}$. What we want is $[B^{-1}]_{n,k} = [t^n](w(t))^k$ and we can apply the following *Lagrange inverse theorem*:

$$[t^n]\left[F(w)\middle| w = t\phi(w)\right] = \frac{1}{n}[t^{n-1}]F'(t)\left(\phi(t)\right)^n \tag{54}$$

In our case, $F(w) = w^k$ and $\phi(t) = (1-t)^{-1}$.

Catalan's triangle (the matrix U) IV

$$
\begin{aligned}
[t^n]\left[w^k \,\middle|\, w = \frac{t}{1-w}\right] &= \frac{1}{n}[t^{n-1}]kt^{k-1}(1-t)^{-n} \\
&= \frac{k}{n}[t^{n-k}](1-t)^{-n} \\
&= \frac{k}{n}(-1)^{n-k}\binom{-n}{n-k} \\
&= \frac{k}{n}\binom{2n-k-1}{n-k}
\end{aligned}
\tag{55}
$$

for $1 \leq k \leq n$. For other cases $n = 0$, $k = 0$, or $k > n$, we have trivial elements $[B^{-1}]_{n,k} = \delta_{nk}$. □

Catalan's triangle (the matrix U) V

Just transposing and multiplying diagonal matrices from our result $(\{a^i b^j M_{ij}\}^{-1} = \{a^{-j} b^{-i} [M^{-1}]_{ij}\})$

$$B_{ij} = (-1)^{i+j} \binom{j}{i-j},$$
$$\left[B^{-1}\right]_{ij} = \frac{j}{i} \binom{2i-j-1}{i-j}$$
$$\text{for } 1 \leq j \leq i \text{ otherwise } \delta_{ij},$$

we have the last piece needed in our study:

$$U_{ij} = (-1)^{i+j} 2^{2i-j} B_{ji} = 2^{2i-j} \binom{i}{j-i}$$
$$[U^{-1}]_{ij} = \frac{(-1)^{i+j}}{2^{2j-i}} \left[B^{-1}\right]_{ji} = \frac{(-1)^{i+j}}{2^{2j-i}} \frac{i}{j} \binom{2j-i-1}{j-i}$$
$$\text{for } 1 \leq i \leq j \text{ otherwise } \delta_{ij},$$

except that *Lagrange inverse theorem* is used without proof.

Lagrange inverse theorem I

From "Handbook of Mathematical Functions"
If $y = f(x)$, $y_0 = f(x_0)$, $f'(x_0) \neq 0$, then
3.6.6

$$x = x_0 + \sum_{k=1}^{\infty} \frac{(y - y_0)^k}{k!} \left[\frac{d^{k-1}}{dx^{k-1}} \left\{ \frac{x - x_0}{f(x) - y_0} \right\}^k \right]_{x=x_0}$$

3.6.7

$$g(x) = g(x_0) + \sum_{k=1}^{\infty} \frac{(y - y_0)^k}{k!} \left[\frac{d^{k-1}}{dx^{k-1}} \left(g'(x) \left\{ \frac{x - x_0}{f(x) - y_0} \right\}^k \right) \right]_{x=x_0}$$

where $g(x)$ is any function indefinitely differentiable.

In formal power series,

$$[t^n] \left[w(t) \middle| w = t\phi(w) \right] = \frac{1}{n} [t^{n-1}] \left(\phi(t) \right)^n, \tag{56}$$

$$[t^n] \left[F(w) \middle| w = t\phi(w) \right] = \frac{1}{n} [t^{n-1}] F'(t) \left(\phi(t) \right)^n. \tag{57}$$

Lagrange inverse theorem II

This is the last one piece for which we need to see a proof.
As an inverse of a Riordan array $\mathcal{R}(1, h(t))$, that is $\mathcal{R}(1, \bar{h}(t))$ for $d(t) = 1$, we assume the following form:

$$d_{n,k} = \left[\mathcal{R}\left(1, \bar{h}(t)\right)\right]_{n,k} = \frac{k}{n}[t^{n-k}]\left(\frac{t}{h(t)}\right)^n . \tag{58}$$

If the following relation

$$v_{n,k} = \sum_{j=0}^{\infty} d_{n,j}[y^j]\,(h(y))^k = \delta_{nk}, \tag{59}$$

if satisfied, it is equivalent to

$$[t^n]\left(\bar{h}(t)\right)^k = \left[\mathcal{R}\left(1, h(t)\right)^{-1}\right]_{n,k} = \left[\mathcal{R}\left(1, \bar{h}(t)\right)\right]_{n,k} = \frac{k}{n}[t^{n-k}]\left(\frac{t}{h(t)}\right)^n . \tag{60}$$

Lagrange inverse theorem III

We start the multiplication

$$v_{n,k} = \sum_{j=0}^{\infty} \frac{j}{n}[t^{n-j}] \left(\frac{t}{h(t)}\right)^{n} [y^j] \, (h(y))^k \, , \tag{61}$$

and by applying a differentiation rule

$$j[y^j] \, (h(y))^k = [y^{j-1}] \left((h(y))^k\right)' = [y^j] y \, h'(y) \, k \, (h(y))^{k-1} \, , \tag{62}$$

we continue the calculation, as in

$$\begin{aligned} v_{n,k} =& \frac{k}{n} \sum_{j=0}^{\infty} [t^{n-j}] \left(\frac{t}{h(t)}\right)^{n} [y^j] y h'(y) \, (h(y))^{k-1} \\ =& \frac{k}{n} [t^n] \left(\frac{t}{h(t)}\right)^{n} t h'(t) \, (h(t))^{k-1} \, . \end{aligned} \tag{63}$$

Here, we used a convolution rule:

$$[t^n] f(t) g(t) = \sum_{j=0}^{\infty} [t^j] f(t) \cdot [y^{n-j}] g(y). \tag{64}$$

Lagrange inverse theorem IV

When $k = n$,

$$v_{n,n} = [t^n]t^n t\left(\frac{h'(t)}{h(t)}\right) = [t^0]\left(\frac{h'(t)}{h(t)/t}\right) = [t^0]\frac{h_1 + 2h_2t + 3h_3t^2 + \cdots}{h_1 + h_2t + h_3t^2 + \cdots} = 1 \quad (65)$$

When $k \neq n$,

$$v_{n,k} = \frac{k}{n}[t^n]t^{n+1}\left(h(t)\right)^{k-n-1}h'(t) = \frac{k}{n}[t^{-1}]\frac{1}{k-n}\left(\left(h(t)\right)^{k-n}\right)' = 0 \quad (66)$$

Here, $(h(t))^{k-n}$ is a *formal Laurent series* of which derivative cannot contain a non-zero coefficient for t^{-1}.

Lagrange inverse theorem V

Let us set $\phi(t) = t/h(t)$ and $w = \bar{h}(t)$. Then $w(t)$ is an implicit function of t such that $w = t\phi(w)$.

For a special case $k = 1$, we have

$$[t^n]\left[w(t)\,\middle|\,w = t\phi(w)\right] = d_{n,1} = \frac{1}{n}[t^{n-1}]\left(\phi(t)\right)^n.$$

In more general cases, for a formal power series $F(w)$, we have

$$\begin{aligned}
[t^n]\left[F(w)\,\middle|\,w = t\phi(w)\right] =& [t^n]\sum_{k=0}^{\infty} F_k w^k = \sum_{k=0}^{\infty} F_k d_{n,k} \\
=& \sum_{k=0}^{\infty} F_k \frac{k}{n}[t^{n-k}]\left(\phi(t)\right)^n \\
=& \frac{1}{n}[t^{n-1}]\left(\sum_{k=0}^{\infty} kF_k t^{k-1}\right)\left(\phi(t)\right)^n \\
=& \frac{1}{n}[t^{n-1}]F'(t)\left(\phi(t)\right)^n. \qquad \square
\end{aligned}$$

Summary

- Combinatorics, a branch of mathematics, turned out to be a powerful tool to study numerical integrators for the N-body problem. Especially the *formal power series*, *Lagrange inverse theorem* and modern *Riordan arrays* are practical tools for even non-mathematicians.
- LU decomposition is not only for Top500/Green500, but a general tool for studying integers.
- Mathematics is useful.
- Satoko Yamamoto did a great work.