Numerical Simulation of Dynamic Systems: Hw5 - Solution

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[H4.2] Nyström-Milne Predictor-Corrector Techniques

Follow the reasoning of the Adams-Bashforth-Moulton predictor-corrector techniques, and develop similar pairs of algorithms using a Nyström predictor stage followed by a Milne corrector stage.

Plot the stability domains for NyMi3 and NyMi4. What do you conclude?

[H4.2] Nyström-Milne Predictor-Corrector Techniques II

We start with the **NyMi3** algorithm. The formulae are:

predictor:
$$\dot{\mathbf{x}}_k = \mathbf{f}(\mathbf{x}_k, t_k)$$
$$\mathbf{x}^P_{k+1} = \mathbf{x}_{k-1} + \frac{h}{3}(7\dot{\mathbf{x}}_k - 2\dot{\mathbf{x}}_{k-1} + \dot{\mathbf{x}}_{k-2})$$

corrector:
$$\dot{\mathbf{x}}^P_{k+1} = \mathbf{f}(\mathbf{x}^P_{k+1}, t_{k+1})$$
$$\mathbf{x}^C_{k+1} = \mathbf{x}_{k-1} + \frac{h}{3}(\dot{\mathbf{x}}^P_{k+1} + 4\dot{\mathbf{x}}_k + \dot{\mathbf{x}}_{k-1})$$

For the linear system:

$$\mathbf{x}^P_{k+1} = \mathbf{x}_{k-1} + \frac{\mathbf{A}\cdot h}{3}(7\mathbf{x}_k - 2\mathbf{x}_{k-1} + \mathbf{x}_{k-2})$$

$$\begin{aligned}\mathbf{x}^C_{k+1} &= \mathbf{x}_{k-1} + \frac{\mathbf{A}\cdot h}{3}(\mathbf{x}^P_{k+1} + 4\mathbf{x}_k + \mathbf{x}_{k-1}) \\ &= \mathbf{x}_{k-1} + \frac{\mathbf{A}\cdot h}{3}\left[\mathbf{x}_{k-1} + \frac{\mathbf{A}\cdot h}{3}(7\mathbf{x}_k - 2\mathbf{x}_{k-1} + \mathbf{x}_{k-2}) + 4\mathbf{x}_k + \mathbf{x}_{k-1}\right] \\ &= \left[\frac{4(\mathbf{A}\cdot h)}{3} + \frac{7(\mathbf{A}\cdot h)^2}{9}\right]\cdot\mathbf{x}_k + \left[\mathbf{I}^{(n)} + \frac{2(\mathbf{A}\cdot h)}{3} - \frac{2(\mathbf{A}\cdot h)^2}{9}\right]\cdot\mathbf{x}_{k-1} + \frac{(\mathbf{A}\cdot h)^2}{9}\cdot\mathbf{x}_{k-2}\end{aligned}$$

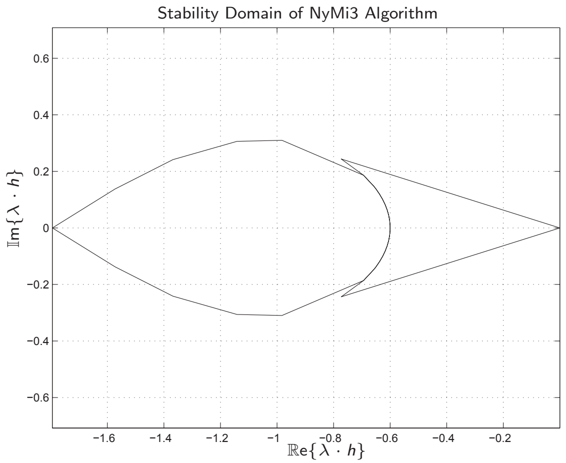
[H4.2] Nyström-Milne Predictor-Corrector Techniques III

Thus:

$$\mathbf{F} = \begin{pmatrix} \mathbf{O}^{(n)} & \mathbf{I}^{(n)} & \mathbf{O}^{(n)} \\ \mathbf{O}^{(n)} & \mathbf{O}^{(n)} & \mathbf{I}^{(n)} \\ \frac{(\mathbf{A}h)^2}{9} & \left[\mathbf{I}^{(n)} + \frac{2(\mathbf{A}h)}{3} - \frac{2(\mathbf{A}h)^2}{9}\right] & \left[\frac{4(\mathbf{A}h)}{3} + \frac{7(\mathbf{A}h)^2}{9}\right] \end{pmatrix}$$

We can now plot the stability domain.

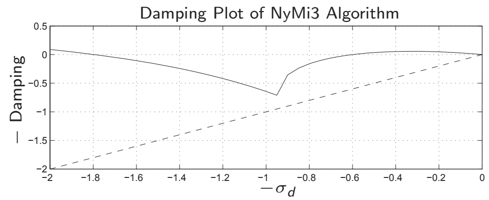
[H4.2] Nyström-Milne Predictor-Corrector Techniques IV



[H4.2] Nyström-Milne Predictor-Corrector Techniques V

This looks funny. It seems our stability domain plotting routine got confused.

Let's look at the damping plot:



- Although both **Ny3** and **Mi3** are totally unstable, the **NyMi3** predictor-corrector method has a stable region in the left-half complex plane. Unfortunately, it doesn't extend all the way to the origin.
- There is no asymptotic region around the origin.
- The method is useless for all practical purposes, because it should never happen that, by reducing the step size, the numerical ODE solution suddenly turns unstable.

[H4.2] Nyström-Milne Predictor-Corrector Techniques VI

Let us now look at **NyMi4**.

predictor:
$$\dot{\mathbf{x}}_\mathbf{k} = \mathbf{f}(\mathbf{x}_\mathbf{k}, t_k)$$
$$\mathbf{x}^\mathbf{P}_{\mathbf{k+1}} = \mathbf{x}_{\mathbf{k-1}} + \frac{h}{3}(8\dot{\mathbf{x}}_\mathbf{k} - 5\dot{\mathbf{x}}_{\mathbf{k-1}} + 4\dot{\mathbf{x}}_{\mathbf{k-2}} - \dot{\mathbf{x}}_{\mathbf{k-3}})$$

corrector:
$$\dot{\mathbf{x}}^\mathbf{P}_{\mathbf{k+1}} = \mathbf{f}(\mathbf{x}^\mathbf{P}_{\mathbf{k+1}}, t_{k+1})$$
$$\mathbf{x}^\mathbf{C}_{\mathbf{k+1}} = \mathbf{x}_{\mathbf{k-1}} + \frac{h}{3}(\dot{\mathbf{x}}^\mathbf{P}_{\mathbf{k+1}} + 4\dot{\mathbf{x}}_\mathbf{k} + \dot{\mathbf{x}}_{\mathbf{k-1}})$$

For the linear system:

$$\mathbf{x}^\mathbf{P}_{\mathbf{k+1}} = \mathbf{x}_{\mathbf{k-1}} + \frac{\mathbf{A}\cdot h}{3}(8\mathbf{x}_\mathbf{k} - 5\mathbf{x}_{\mathbf{k-1}} + 4\mathbf{x}_{\mathbf{k-2}} - \mathbf{x}_{\mathbf{k-3}})$$

$$\mathbf{x}^\mathbf{C}_{\mathbf{k+1}} = \mathbf{x}_{\mathbf{k-1}} + \frac{\mathbf{A}\cdot h}{3}(\mathbf{x}^\mathbf{P}_{\mathbf{k+1}} + 4\mathbf{x}_\mathbf{k} + \mathbf{x}_{\mathbf{k-1}})$$

$$= \mathbf{x}_{\mathbf{k-1}} + \frac{\mathbf{A}\cdot h}{3}\left[\mathbf{x}_{\mathbf{k-1}} + \frac{\mathbf{A}\cdot h}{3}(8\mathbf{x}_\mathbf{k} - 5\mathbf{x}_{\mathbf{k-1}} + 4\mathbf{x}_{\mathbf{k-2}} - \mathbf{x}_{\mathbf{k-3}}) + 4\mathbf{x}_\mathbf{k} + \mathbf{x}_{\mathbf{k-1}}\right]$$

$$= \left[\frac{4(\mathbf{A}h)}{3} + \frac{8(\mathbf{A}h)^2}{9}\right]\mathbf{x}_\mathbf{k} + \left[\mathbf{I}^{(\mathbf{n})} + \frac{2(\mathbf{A}h)}{3} - \frac{5(\mathbf{A}h)^2}{9}\right]\mathbf{x}_{\mathbf{k-1}} + \frac{4(\mathbf{A}h)^2}{9}\mathbf{x}_{\mathbf{k-2}} - \frac{(\mathbf{A}h)^2}{9}\mathbf{x}_{\mathbf{k-3}}$$

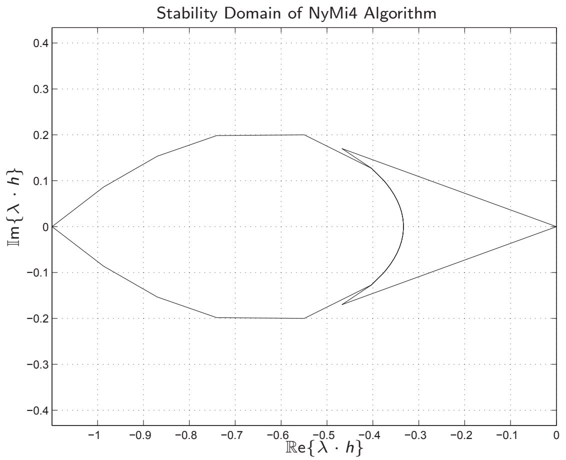
[H4.2] Nyström-Milne Predictor-Corrector Techniques VII

Thus:

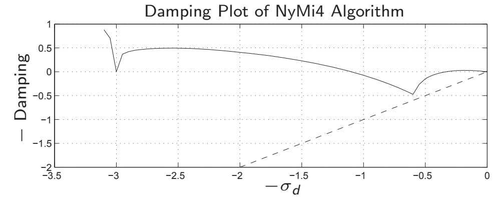
$$\mathbf{F} = \begin{pmatrix} \mathbf{O}^{(\mathbf{n})} & \mathbf{I}^{(\mathbf{n})} & \mathbf{O}^{(\mathbf{n})} & \mathbf{O}^{(\mathbf{n})} \\ \mathbf{O}^{(\mathbf{n})} & \mathbf{O}^{(\mathbf{n})} & \mathbf{I}^{(\mathbf{n})} & \mathbf{O}^{(\mathbf{n})} \\ \mathbf{O}^{(\mathbf{n})} & \mathbf{O}^{(\mathbf{n})} & \mathbf{O}^{(\mathbf{n})} & \mathbf{I}^{(\mathbf{n})} \\ -\frac{(\mathbf{A}h)^2}{9} & \frac{4(\mathbf{A}h)^2}{9} & \left[\mathbf{I}^{(\mathbf{n})} + \frac{2(\mathbf{A}h)}{3} - \frac{5(\mathbf{A}h)^2}{9}\right] & \left[\frac{4(\mathbf{A}h)}{3} + \frac{8(\mathbf{A}h)^2}{9}\right] \end{pmatrix}$$

We can now plot the stability domain.

[H4.2] Nyström-Milne Predictor-Corrector Techniques VIII



[H4.2] Nyström-Milne Predictor-Corrector Techniques IX



- Although both **Ny4** and **Mi4** are totally unstable, also the **NyMi4** predictor-corrector method has a stable region in the left-half complex plane. Unfortunately, it doesn't extend all the way to the origin.
- There is no asymptotic region around the origin.
- The method is useless for all practical purposes.

[H4.4] Milne Integration

Usually, the term "Milne integration algorithm," when used in the literature, denotes a specific predictor-corrector technique, namely:

predictor:
$$\dot{\mathbf{x}}_k = \mathbf{f}(\mathbf{x}_k, t_k)$$
$$\mathbf{x}^P_{k+1} = \mathbf{x}_{k-3} + \frac{h}{3}(8\dot{\mathbf{x}}_k - 4\dot{\mathbf{x}}_{k-1} + 8\dot{\mathbf{x}}_{k-2})$$

corrector:
$$\dot{\mathbf{x}}^P_{k+1} = \mathbf{f}(\mathbf{x}^P_{k+1}, t_{k+1})$$
$$\mathbf{x}^C_{k+1} = \mathbf{x}_{k-1} + \frac{h}{3}(\dot{\mathbf{x}}^P_{k+1} + 4\dot{\mathbf{x}}_k + \dot{\mathbf{x}}_{k-1})$$

The corrector is clearly *Simpson's rule*. However, the predictor is something new that we haven't seen yet.

[H4.4] Milne Integration II

Derive the order of approximation accuracy of the predictor. To this end, use the Newton-Gregory backward polynomial in order to derive a set of formulae with a distance of four steps apart between their two state values.

Plot the stability domain of the predictor-corrector method, and compare it with that of NyMi4. What do you conclude? Why did *William E. Milne* propose to use this particular predictor?

[H4.4] Milne Integration III

We develop the state derivative into a backward Newton-Gregory polynomial around t_k:

$$\dot{\mathbf{x}}(t) = \mathbf{f}_k + \binom{s}{1}\nabla\mathbf{f}_k + \binom{s+1}{2}\nabla^2\mathbf{f}_k + \binom{s+2}{3}\nabla^3\mathbf{f}_k + \dots$$

We integrate from $s = -3$ to $s = +1$:

$$\begin{aligned}\int_{t_{k-3}}^{t_{k+1}} \dot{\mathbf{x}}(t)dt &= \mathbf{x}(t_{k+1}) - \mathbf{x}(t_{k-3}) \\ &= \int_{t_{k-3}}^{t_{k+1}} \left[\mathbf{f}_k + \binom{s}{1}\nabla\mathbf{f}_k + \binom{s+1}{2}\nabla^2\mathbf{f}_k + \binom{s+2}{3}\nabla^3\mathbf{f}_k + \dots\right] dt \\ &= \int_{-3.0}^{1.0} \left[\mathbf{f}_k + \binom{s}{1}\nabla\mathbf{f}_k + \binom{s+1}{2}\nabla^2\mathbf{f}_k + \binom{s+2}{3}\nabla^3\mathbf{f}_k + \dots\right] \cdot \frac{dt}{ds} \cdot ds\end{aligned}$$

[H4.4] Milne Integration IV

$$\begin{aligned}\mathbf{x}(t_{k+1}) &= \mathbf{x}(t_{k-3}) + h\int_{-3}^{1}\left[\mathbf{f}_k + s\nabla\mathbf{f}_k + \left(\frac{s^2}{2} + \frac{s}{2}\right)\nabla^2\mathbf{f}_k\right. \\ &+ \left.\left(\frac{s^3}{6} + \frac{s^2}{2} + \frac{s}{3}\right)\nabla^3\mathbf{f}_k + \dots\right] ds\end{aligned}$$

Thus:

$$\begin{aligned}\mathbf{x}(t_{k+1}) &= \mathbf{x}(t_{k-3}) + h \cdot \left[s \cdot \mathbf{f}_k + \frac{s^2}{2}\nabla\mathbf{f}_k + \left(\frac{s^3}{6} + \frac{s^2}{4}\right)\nabla^2\mathbf{f}_k\right. \\ &+ \left.\left(\frac{s^4}{24} + \frac{s^3}{6} + \frac{s^2}{6}\right)\nabla^3\mathbf{f}_k + \dots\right]_{-3}^{+1}\end{aligned}$$

[H4.4] Milne Integration V

Consequently:

$$\begin{aligned}\mathbf{x}(t_{k+1}) &= \mathbf{x}(t_{k-3}) + h\left(\mathbf{f}_k + \frac{1}{2}\nabla\mathbf{f}_k + \frac{5}{12}\nabla^2\mathbf{f}_k + \frac{3}{8}\nabla^3\mathbf{f}_k + \dots\right) \\ &\quad -h\left(-3\mathbf{f}_k + \frac{9}{2}\nabla\mathbf{f}_k - \frac{9}{4}\nabla^2\mathbf{f}_k - \frac{3}{8}\nabla^3\mathbf{f}_k + \dots\right) \\ &= \mathbf{x}(t_{k-3}) + h\left(4\mathbf{f}_k - 4\nabla\mathbf{f}_k + \frac{8}{3}\nabla^2\mathbf{f}_k + 0\nabla^3\mathbf{f}_k + \dots\right) \\ &= \mathbf{x}(t_{k-3}) + \frac{h}{3}\left(8\mathbf{f}_k - 4\mathbf{f}_{k-1} + 8\mathbf{f}_{k-2} + 0\mathbf{f}_{k-3} + \dots\right)\end{aligned}$$

Hence the method is 4^{th}-order accurate.

[H4.4] Milne Integration VI

predictor:
$$\dot{\mathbf{x}}_\mathbf{k} = \mathbf{f}(\mathbf{x}_\mathbf{k}, t_k)$$
$$\mathbf{x}^\mathbf{P}_\mathbf{k+1} = \mathbf{x}_\mathbf{k-3} + \frac{h}{3}(8\dot{\mathbf{x}}_\mathbf{k} - 4\dot{\mathbf{x}}_\mathbf{k-1} + 8\dot{\mathbf{x}}_\mathbf{k-2})$$

corrector:
$$\dot{\mathbf{x}}^\mathbf{P}_\mathbf{k+1} = \mathbf{f}(\mathbf{x}^\mathbf{P}_\mathbf{k+1}, t_{k+1})$$
$$\mathbf{x}^\mathbf{C}_\mathbf{k+1} = \mathbf{x}_\mathbf{k-1} + \frac{h}{3}(\dot{\mathbf{x}}^\mathbf{P}_\mathbf{k+1} + 4\dot{\mathbf{x}}_\mathbf{k} + \dot{\mathbf{x}}_\mathbf{k-1})$$

For the linear system:

$$\begin{aligned}\mathbf{x}^\mathbf{P}_\mathbf{k+1} &= \mathbf{x}_\mathbf{k-3} + \frac{\mathbf{A}\cdot h}{3}(8\mathbf{x}_\mathbf{k} - 4\mathbf{x}_\mathbf{k-1} + 8\mathbf{x}_\mathbf{k-2}) \\ \mathbf{x}^\mathbf{C}_\mathbf{k+1} &= \mathbf{x}_\mathbf{k-1} + \frac{\mathbf{A}\cdot h}{3}(\mathbf{x}^\mathbf{P}_\mathbf{k+1} + 4\mathbf{x}_\mathbf{k} + \mathbf{x}_\mathbf{k-1}) \\ &= \mathbf{x}_\mathbf{k-1} + \frac{\mathbf{A}\cdot h}{3}\left[\mathbf{x}_\mathbf{k-3} + \frac{\mathbf{A}\cdot h}{3}(8\mathbf{x}_\mathbf{k} - 4\mathbf{x}_\mathbf{k-1} + 8\mathbf{x}_\mathbf{k-2}) + 4\mathbf{x}_\mathbf{k} + \mathbf{x}_\mathbf{k-1}\right] \\ &= \left[\frac{4(\mathbf{A}h)}{3} + \frac{8(\mathbf{A}h)^2}{9}\right]\mathbf{x}_\mathbf{k} + \left[\mathbf{I}^{(\mathbf{n})} + \frac{(\mathbf{A}h)}{3} - \frac{4(\mathbf{A}h)^2}{9}\right]\mathbf{x}_\mathbf{k-1} + \frac{8(\mathbf{A}h)^2}{9}\mathbf{x}_\mathbf{k-2} + \frac{(\mathbf{A}h)}{3}\mathbf{x}_\mathbf{k-3}\end{aligned}$$

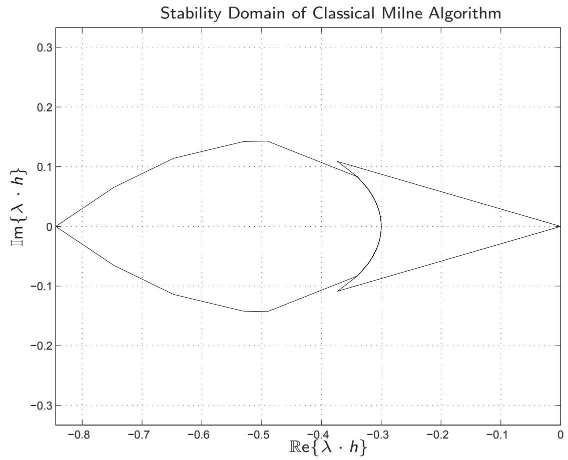
[H4.4] Milne Integration VII

Thus:

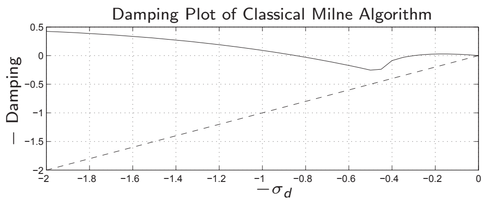
$$\mathbf{F} = \begin{pmatrix} \mathbf{O}^{(n)} & \mathbf{I}^{(n)} & \mathbf{O}^{(n)} & \mathbf{O}^{(n)} \\ \mathbf{O}^{(n)} & \mathbf{O}^{(n)} & \mathbf{I}^{(n)} & \mathbf{O}^{(n)} \\ \mathbf{O}^{(n)} & \mathbf{O}^{(n)} & \mathbf{O}^{(n)} & \mathbf{I}^{(n)} \\ \frac{(\mathbf{A}h)}{3} & \frac{8(\mathbf{A}h)^2}{9} & \left[\mathbf{I}^{(n)} + \frac{(\mathbf{A}h)}{3} - \frac{4(\mathbf{A}h)^2}{9}\right] & \left[\frac{4(\mathbf{A}h)}{3} + \frac{8(\mathbf{A}h)^2}{9}\right] \end{pmatrix}$$

We can now plot the stability domain.

[H4.4] Milne Integration VIII



[H4.4] Milne Integration IX



- The *classical Milne algorithm* is no better than **NyMi4**.
- There is no asymptotic region around the origin.
- The method is complete garbage for all practical purposes.
- When I was a graduate student learning about simulation, the first simulation language I used was the then industry standard, **CSMP-III**, from IBM. CSMP-III offered Milne integration as one of its highlights.

[H4.10] The Nordsieck Form

In the class presentations, I showed the transformation matrix that converts the state history vector into an equivalent *Nordsieck vector*. Since, at the time of conversion, we also have the current state derivative information available, it is more common to drop the oldest state information in the state history vector, and replace it by the current state derivative information. Consequently, we are looking for a transformation matrix $\mathbf{T}$ of the form:

$$\begin{pmatrix} x_k \\ h \cdot \dot{x}_k \\ \frac{h^2}{2} \cdot \ddot{x}_k \\ \frac{h^3}{6} \cdot x_k^{(iii)} \end{pmatrix} = \mathbf{T} \cdot \begin{pmatrix} x_k \\ h \cdot \dot{x}_k \\ x_{k-1} \\ x_{k-2} \end{pmatrix}$$

The matrix $\mathbf{T}$ can easily be found by manipulating the individual equations of the transformation matrix shown in class.

Find corresponding $\mathbf{T}$-matrices of dimensions 3×3 and 5×5.

[H4.10] The Nordsieck Form II

We develop the state vector into a backward Newton-Gregory polynomial around t_k:

$$\mathbf{x}(t) = \mathbf{x}_k + \binom{s}{1}\nabla\mathbf{x}_k + \binom{s+1}{2}\nabla^2\mathbf{x}_k + \binom{s+2}{3}\nabla^3\mathbf{x}_k + \binom{s+3}{4}\nabla^4\mathbf{x}_k + \ldots$$

We differentiate twice, truncating after the quadratic term:

$$\begin{aligned}
\mathbf{x}(t) &= \mathbf{x}_k + s\nabla\mathbf{x}_k + \left(\frac{s^2}{2} + \frac{s}{2}\right)\nabla^2\mathbf{x}_k \\
\dot{\mathbf{x}}(t) &= \frac{1}{h}\left[\nabla\mathbf{x}_k + \left(s + \frac{1}{2}\right)\nabla^2\mathbf{x}_k\right] \\
\ddot{\mathbf{x}}(t) &= \frac{1}{h^2}\left[\nabla^2\mathbf{x}_k\right]
\end{aligned}$$

[H4.10] The Nordsieck Form III

We apply these formulae to the scalar problem and evaluate for $s = 0$:

$$\begin{aligned}
x_k &= x_k \\
h \cdot \dot{x}_k &= \frac{3}{2}x_k - 2x_{k-1} + \frac{1}{2}x_{k-2} \\
\frac{h^2}{2} \cdot \ddot{x}_k &= \frac{1}{2}x_k - x_{k-1} + \frac{1}{2}x_{k-2}
\end{aligned}$$

In matrix-vector form:

$$\begin{pmatrix} x_k \\ h \cdot \dot{x}_k \\ \frac{h^2}{2} \cdot \ddot{x}_k \end{pmatrix} = \frac{1}{2} \cdot \begin{pmatrix} 2 & 0 & 0 \\ 3 & -2 & 1 \\ 1 & -2 & 1 \end{pmatrix} \cdot \begin{pmatrix} x_k \\ x_{k-1} \\ x_{k-2} \end{pmatrix}$$

[H4.10] The Nordsieck Form IV

We need to eliminate x_{k-2}:

$$\begin{aligned}
2h \cdot \dot{x}_k &= 3x_k - 4x_{k-1} + x_{k-2} \\
\Rightarrow x_{k-2} &= -3x_k + 2h \cdot \dot{x}_k + 4x_{k-1}
\end{aligned}$$

Thus:

$$\begin{aligned}
\frac{h^2}{2} \cdot \ddot{x}_k &= \frac{1}{2}x_k - x_{k-1} + \frac{1}{2}x_{k-2} \\
&= -x_k + h \cdot \dot{x}_k + x_{k-1}
\end{aligned}$$

In matrix-vector form:

$$\begin{pmatrix} x_k \\ h \cdot \dot{x}_k \\ \frac{h^2}{2} \cdot \ddot{x}_k \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -1 & 1 & 1 \end{pmatrix} \cdot \begin{pmatrix} x_k \\ h \cdot \dot{x}_k \\ x_{k-1} \end{pmatrix}$$

[H4.10] The Nordsieck Form V

We repeat the analysis, this time differentiating thrice and truncating after the cubic term:

$$\begin{aligned}
\mathbf{x}(t) &= \mathbf{x}_k + s\nabla\mathbf{x}_k + \left(\frac{s^2}{2} + \frac{s}{2}\right)\nabla^2\mathbf{x}_k + \left(\frac{s^3}{6} + \frac{s^2}{2} + \frac{s}{3}\right)\nabla^3\mathbf{x}_k \\
\dot{\mathbf{x}}(t) &= \frac{1}{h}\left[\nabla\mathbf{x}_k + \left(s + \frac{1}{2}\right)\nabla^2\mathbf{x}_k + \left(\frac{s^2}{2} + s + \frac{1}{3}\right)\nabla^3\mathbf{x}_k\right] \\
\ddot{\mathbf{x}}(t) &= \frac{1}{h^2}\left[\nabla^2\mathbf{x}_k + (s+1)\nabla^3\mathbf{x}_k\right] \\
\mathbf{x}^{(iii)}(t) &= \frac{1}{h^3}\left[\nabla^3\mathbf{x}_k\right]
\end{aligned}$$

[H4.10] The Nordsieck Form VI

We apply these formulae to the scalar problem and evaluate for $s = 0$:

$$\begin{aligned} x_k &= x_k \\ h \cdot \dot{x}_k &= \frac{11}{6}x_k - 3x_{k-1} + \frac{3}{2}x_{k-2} - \frac{1}{3}x_{k-3} \\ \frac{h^2}{2} \cdot \ddot{x}_k &= x_k - \frac{5}{2}x_{k-1} + 2x_{k-2} - \frac{1}{2}x_{k-3} \\ \frac{h^3}{6} \cdot x_k^{(\mathrm{iii})} &= \frac{1}{6}x_k - \frac{1}{2}x_{k-1} + \frac{1}{2}x_{k-2} - \frac{1}{6}x_{k-3} \end{aligned}$$

In matrix-vector form:

$$\begin{pmatrix} x_k \\ h \cdot \dot{x}_k \\ \frac{h^2}{2} \cdot \ddot{x}_k \\ \frac{h^3}{6} \cdot x_k^{(\mathrm{iii})} \end{pmatrix} = \frac{1}{6} \cdot \begin{pmatrix} 6 & 0 & 0 & 0 \\ 11 & -18 & 9 & -2 \\ 6 & -15 & 12 & -3 \\ 1 & -3 & 3 & -1 \end{pmatrix} \cdot \begin{pmatrix} x_k \\ x_{k-1} \\ x_{k-2} \\ x_{k-3} \end{pmatrix}$$

[H4.10] The Nordsieck Form VII

We need to eliminate x_{k-3}:

$$\begin{aligned} 6h \cdot \dot{x}_k &= 11x_k - 18x_{k-1} + 9x_{k-2} - 2x_{k-3} \\ \Rightarrow x_{k-3} &= \frac{11}{2}x_k - 3h \cdot \dot{x}_k - 9x_{k-1} + \frac{9}{2}x_{k-2} \end{aligned}$$

Thus:

$$\begin{aligned} \frac{h^2}{2} \cdot \ddot{x}_k &= x_k - \frac{5}{2}x_{k-1} + 2x_{k-2} - \frac{1}{2}x_{k-3} \\ &= -\frac{7}{4}x_k + \frac{3}{2}h \cdot \dot{x}_k + 2x_{k-1} - \frac{1}{4}x_{k-2} \end{aligned}$$

and:

$$\begin{aligned} \frac{h^3}{6} \cdot x_k^{(\mathrm{iii})} &= \frac{1}{6}x_k - \frac{1}{2}x_{k-1} + \frac{1}{2}x_{k-2} - \frac{1}{6}x_{k-3} \\ &= -\frac{3}{4}x_k + \frac{1}{2}h \cdot \dot{x}_k + x_{k-1} - \frac{1}{4}x_{k-2} \end{aligned}$$

[H4.10] The Nordsieck Form VIII

In matrix-vector form:

$$\begin{pmatrix} x_k \\ h \cdot \dot{x}_k \\ \frac{h^2}{2} \cdot \ddot{x}_k \\ \frac{h^3}{6} \cdot x_k^{(\mathrm{iii})} \end{pmatrix} = \frac{1}{4} \cdot \begin{pmatrix} 4 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 \\ -7 & 6 & 8 & -1 \\ -3 & 2 & 4 & -1 \end{pmatrix} \cdot \begin{pmatrix} x_k \\ h \cdot \dot{x}_k \\ x_{k-1} \\ x_{k-2} \end{pmatrix}$$

[H4.10] The Nordsieck Form IX

We repeat the analysis, this time differentiating four times and truncating after the fourth-order term:

$$\begin{aligned} \mathbf{x}(t) &= \mathbf{x}_k + s\nabla\mathbf{x}_k + \left(\frac{s^2}{2} + \frac{s}{2}\right)\nabla^2\mathbf{x}_k + \left(\frac{s^3}{6} + \frac{s^2}{2} + \frac{s}{3}\right)\nabla^3\mathbf{x}_k \\ &\quad + \left(\frac{s^4}{24} + \frac{s^3}{4} + \frac{11s^2}{24} + \frac{s}{4}\right)\nabla^4\mathbf{x}_k \\ \dot{\mathbf{x}}(t) &= \frac{1}{h}\left[\nabla\mathbf{x}_k + \left(s + \frac{1}{2}\right)\nabla^2\mathbf{x}_k + \left(\frac{s^2}{2} + s + \frac{1}{3}\right)\nabla^3\mathbf{x}_k \right. \\ &\quad \left. + \left(\frac{s^3}{6} + \frac{3s^2}{4} + \frac{11s}{12} + \frac{1}{4}\right)\nabla^4\mathbf{x}_k\right] \\ \ddot{\mathbf{x}}(t) &= \frac{1}{h^2}\left[\nabla^2\mathbf{x}_k + (s+1)\nabla^3\mathbf{x}_k + \left(\frac{s^2}{2} + \frac{3s}{2} + \frac{11}{12}\right)\nabla^4\mathbf{x}_k\right] \\ \mathbf{x}^{(\mathrm{iii})}(t) &= \frac{1}{h^3}\left[\nabla^3\mathbf{x}_k + \left(s + \frac{3}{2}\right)\nabla^4\mathbf{x}_k\right] \\ \mathbf{x}^{(\mathrm{iv})}(t) &= \frac{1}{h^4}\left[\nabla^4\mathbf{x}_k\right] \end{aligned}$$

[H4.10] The Nordsieck Form X

We apply these formulae to the scalar problem and evaluate for $s = 0$:

$$\begin{aligned}
x_k &= x_k \\
h \cdot \dot{x}_k &= \frac{25}{12} x_k - 4x_{k-1} + 3x_{k-2} - \frac{4}{3} x_{k-3} + \frac{1}{4} x_{k-4} \\
\frac{h^2}{2} \cdot \ddot{x}_k &= \frac{35}{24} x_k - \frac{13}{3} x_{k-1} + \frac{19}{4} x_{k-2} - \frac{7}{3} x_{k-3} + \frac{11}{24} x_{k-4} \\
\frac{h^3}{6} \cdot x_k^{(\mathrm{iii})} &= \frac{5}{12} x_k - \frac{3}{2} x_{k-1} + 2x_{k-2} - \frac{7}{6} x_{k-3} + \frac{1}{4} x_{k-4} \\
\frac{h^4}{24} \cdot x_k^{(\mathrm{iv})} &= \frac{1}{24} x_k - \frac{1}{6} x_{k-1} + \frac{1}{4} x_{k-2} - \frac{1}{6} x_{k-3} + \frac{1}{24} x_{k-4}
\end{aligned}$$

In matrix-vector form:

$$\begin{pmatrix} x_k \\ h \cdot \dot{x}_k \\ \frac{h^2}{2} \cdot \ddot{x}_k \\ \frac{h^3}{6} \cdot x_k^{(\mathrm{iii})} \\ \frac{h^4}{24} \cdot x_k^{(\mathrm{iv})} \end{pmatrix} = \frac{1}{24} \cdot \begin{pmatrix} 24 & 0 & 0 & 0 & 0 \\ 50 & -96 & 72 & -32 & 6 \\ 35 & -104 & 114 & -56 & 11 \\ 10 & -36 & 48 & -28 & 6 \\ 1 & -4 & 6 & -4 & 1 \end{pmatrix} \cdot \begin{pmatrix} x_k \\ x_{k-1} \\ x_{k-2} \\ x_{k-3} \\ x_{k-4} \end{pmatrix}$$

[H4.10] The Nordsieck Form XI

We need to eliminate x_{k-4}:

$$\begin{aligned}
12h \cdot \dot{x}_k &= 25x_k - 48x_{k-1} + 36x_{k-2} - 16x_{k-3} + 3x_{k-4} \\
\Rightarrow x_{k-4} &= -\frac{25}{3} x_k + 4h \cdot \dot{x}_k + 16x_{k-1} - 12x_{k-2} + \frac{16}{3} x_{k-3}
\end{aligned}$$

Thus:

$$\begin{aligned}
\frac{h^2}{2} \cdot \ddot{x}_k &= \frac{35}{24} x_k - \frac{13}{3} x_{k-1} + \frac{19}{4} x_{k-2} - \frac{7}{3} x_{k-3} + \frac{11}{24} x_{k-4} \\
&= -\frac{85}{36} x_k + \frac{11}{6} h \cdot \dot{x}_k + 3x_{k-1} - \frac{3}{4} x_{k-2} + \frac{1}{9} x_{k-3}
\end{aligned}$$

and:

$$\begin{aligned}
\frac{h^3}{6} \cdot x_k^{(\mathrm{iii})} &= \frac{5}{12} x_k - \frac{3}{2} x_{k-1} + 2x_{k-2} - \frac{7}{6} x_{k-3} + \frac{1}{4} x_{k-4} \\
&= -\frac{5}{3} x_k + h \cdot \dot{x}_k + \frac{5}{2} x_{k-1} - x_{k-2} + \frac{1}{6} x_{k-3}
\end{aligned}$$

and:

$$\begin{aligned}
\frac{h^4}{24} \cdot x_k^{(\mathrm{iv})} &= \frac{1}{24} x_k - \frac{1}{6} x_{k-1} + \frac{1}{4} x_{k-2} - \frac{1}{6} x_{k-3} + \frac{1}{24} x_{k-4} \\
&= -\frac{11}{36} x_k + \frac{1}{6} h \cdot \dot{x}_k + \frac{1}{2} x_{k-1} - \frac{1}{4} x_{k-2} + \frac{1}{18} x_{k-3}
\end{aligned}$$

[H4.10] The Nordsieck Form XII

In matrix-vector form:

$$\begin{pmatrix} x_k \\ h \cdot \dot{x}_k \\ \frac{h^2}{2} \cdot \ddot{x}_k \\ \frac{h^3}{6} \cdot x_k^{(\mathrm{iii})} \\ \frac{h^4}{24} \cdot x_k^{(\mathrm{iv})} \end{pmatrix} = \frac{1}{36} \cdot \begin{pmatrix} 36 & 0 & 0 & 0 & 0 \\ 0 & 36 & 0 & 0 & 0 \\ -85 & 66 & 108 & -27 & 4 \\ -60 & 36 & 90 & -36 & 6 \\ -11 & 6 & 18 & -9 & 2 \end{pmatrix} \cdot \begin{pmatrix} x_k \\ h \cdot \dot{x}_k \\ x_{k-1} \\ x_{k-2} \\ x_{k-3} \end{pmatrix}$$