Numerical Simulation of Dynamic Systems VI

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Introduction

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Maybe this way of solving the problem is inefficient. At the end of each step, we have available a lot of valuable information that could be used during the next step. Until now, we simply threw that information away and started from scratch.

There exist other classes of higher-order numerical ODE solvers that preserve some of the information gathered during previous steps. As a consequence, they manage to get away with a single function evaluation in each step. These algorithms are called *linear multi-step integration algorithms*.

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Given a function $f(t)$ equidistantly sampled over time, t_0, $t_1 > t_0$, $t_2 > t_1$, $\ldots$. The function assumes the values f_0, f_1, f_2, $\ldots$ at the sampling points.

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We introduce the *forward difference operator*, Δ:

$$\begin{aligned}
\Delta f_0 &= f_1 - f_0 \\
\Delta^2 f_0 &= \Delta(\Delta f_0) = \Delta(f_1 - f_0) = \Delta f_1 - \Delta f_0 = f_2 - 2f_1 + f_0 \\
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\end{aligned}$$

In general:

$$\begin{aligned}
\Delta^n f_i &= f_{i+n} - n \cdot f_{i+n-1} + \frac{n(n-1)}{2!} \cdot f_{i+n-2} - \frac{n(n-1)(n-2)}{3!} \cdot f_{i+n-3} + \ldots \\
&= \binom{n}{0} f_{i+n} - \binom{n}{1} f_{i+n-1} + \binom{n}{2} f_{i+n-2} - \binom{n}{3} f_{i+n-3} + \cdots \pm \binom{n}{n} f_i
\end{aligned}$$

The Newton-Gregory Polynomials II

As we assumed *equidistant sampling*, we can write: $t_1 = t_0 + h$, $t_2 = t_0 + 2h$, $\ldots$, $t_n = t_0 + n \cdot h$.

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We now introduce a *normalized time variable*, s:

$$s = \frac{t - t_0}{h}$$

Consequently:

$$t = t_0 \;\Leftrightarrow\; s = 0.0, t = t_1 \;\Leftrightarrow\; s = 1.0, \dots$$

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It is possible to define an *interpolation polynomial* of order n that passes through the $n+1$ points f_0, f_1, $\dots$, f_n:

$$f(s) \approx \binom{s}{0} f_0 + \binom{s}{1} \Delta f_0 + \binom{s}{2} \Delta^2 f_0 + \dots + \binom{s}{n} \Delta^n f_0$$

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This polynomial is called *forward Newton-Gregory interpolation polynomial*. It is trivial to show that this polynomial of order n passes through the $n+1$ points f_0, f_1, $\ldots$, f_n.

The Newton-Gregory Polynomials III

It is important to mention that the variable s is allowed to assume also *non-integer values*. For example:

$$\binom{s}{3}_{s=1.5} \equiv \left[\frac{s(s-1)(s-2)}{3!}\right]_{s=1.5} = -\frac{1}{16}$$

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Sometimes it is more useful to work with a different interpolation polynomial:

$$f(s) \approx f_0 + \binom{s}{1}\Delta f_{-1} + \binom{s+1}{2}\Delta^2 f_{-2} + \binom{s+2}{3}\Delta^3 f_{-3} + \cdots + \binom{s+n-1}{n}\Delta^n f_{-n}$$

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This polynomial is called *backward Newton-Gregory interpolation polynomial*. It is equally easy to demonstrate that this polynomial of order n passes through the $n+1$ points f_0, f_{-1}, ..., f_{-n}.

The Newton-Gregory Polynomials IV

We introduce now a second operator, the *backward difference operator*, ∇:

$$\nabla f_i = f_i - f_{i-1}$$
$$\nabla^2 f_i = \nabla(\nabla f_i) = \nabla(f_i - f_{i-1}) = \nabla f_i - \nabla f_{i-1} = f_i - 2\ f_{i-1} + f_{i-2}$$
$$\nabla^3 f_i = \nabla(\nabla^2 f_i) = f_i - 3f_{i-1} + 3f_{i-2} - f_{i-3}$$

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In general:

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The *backward Newton-Gregory interpolation polynomial* can also be written in terms of the ∇ operator:

$$f(s) \approx f_0 + \binom{s}{1} \nabla f_0 + \binom{s+1}{2} \nabla^2 f_0 + \binom{s+2}{3} \nabla^3 f_0 + \cdots + \binom{s+n-1}{n} \nabla^n f_0$$

The Newton-Gregory Polynomials V

Another operator is also sometimes useful, namely the *displacement operator*, $\mathcal{E}$:

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Evidently:

$$\begin{aligned} \Delta f_i &= \mathcal{E}f_i - f_i = (\mathcal{E} - 1)f_i \\ \nabla f_i &= f_i - \mathcal{E}^{-1}f_i = (1 - \mathcal{E}^{-1})f_i \\ \mathcal{E}(\nabla f_i) &= \mathcal{E}(f_i - f_{i-1}) = f_{i+1} - f_i = \Delta f_i \end{aligned}$$

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By abstraction (a bit dangerous!):

$$\begin{aligned}
\Delta &= \mathcal{E} - 1 \\
\nabla &= 1 - \mathcal{E}^{-1} \\
\Delta &= \mathcal{E} \nabla
\end{aligned}$$

The Newton-Gregory Polynomials VI

The three operators Δ, ∇, and $\mathcal{E}$ are *linear operators*. Hence they can be used in algebraic expressions.

In particular:

$$\Delta^n = (\mathcal{E} - 1)^n = \mathcal{E}^n - n\mathcal{E}^{n-1} + \binom{n}{2}\mathcal{E}^{n-2} - + \cdots \pm \binom{n}{n-1}\mathcal{E} \mp 1$$

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Making use of operator calculus, the derivation of the Newton-Gregory polynomials is much simplified:

$$f(s) \approx \mathcal{E}^s f_0 = (1 + \Delta)^s f_0 = \left[1 + \binom{s}{1}\Delta + \binom{s}{2}\Delta^2 + \binom{s}{3}\Delta^3 + \dots\right] f_0$$

and:

$$f(s) \approx (1 - \nabla)^{-s} f_0 = \left[1 + \binom{s}{1}\nabla + \binom{s+1}{2}\nabla^2 + \binom{s+2}{3}\nabla^3 + \dots\right] f_0$$

The Newton-Gregory Polynomials VII

Also *differentiation* is a *linear operation*. Therefore:

$$\begin{aligned}\dot{f}(t) &= \frac{d}{dt}f(t) = \frac{\partial}{\partial s}f(s) \cdot \frac{ds}{dt} \\ &\approx \frac{1}{h} \cdot \frac{\partial}{\partial s}\left(f_0 + s\Delta f_0 + \frac{s(s-1)}{2!}\Delta^2 f_0 + \ldots \right)\end{aligned}$$

In particular:

$$\dot{f}(t_0) \approx \frac{1}{h} \cdot \left(\Delta f_0 - \frac{1}{2}\Delta^2 f_0 + \frac{1}{3}\Delta^3 f_0 - \cdots \pm \frac{1}{n}\Delta^n f_0 \right)$$

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It makes sense to introduce yet another operator, the *differentiation operator*, $\mathcal{D}$:

$$\mathcal{D} = \frac{1}{h}\cdot\left(\Delta - \frac{1}{2}\Delta^2 + \frac{1}{3}\Delta^3 - \dots \pm \frac{1}{n}\Delta^n\right)$$

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Thus, the second derivative can be obtained in the following manner:

$$\begin{aligned}\mathcal{D}^2 &= \frac{1}{h^2}\cdot\left(\Delta - \frac{1}{2}\Delta^2 + \frac{1}{3}\Delta^3 - \dots \pm \frac{1}{n}\Delta^n\right)^2 \\ &= \frac{1}{h^2}\cdot\left(\Delta^2 - \Delta^3 + \frac{11}{12}\Delta^4 - \frac{5}{6}\Delta^5 + \dots\right)\end{aligned}$$

Linear Multi-step Integration Methods

All families of numerical linear multi-step integration methods used for the simulation of dynamic systems can be elegantly derived by means of Newton-Gregory polynomials.

To this end, we either approximate the function itself by a Newton-Gregory polynomial and differentiate this polynomial with respect to time, or alternatively, we approximate the first time derivative by a Newton-Gregory polynomial and integrate this polynomial with respect to time.

The Explicit Adams-Bashforth Formulae

Let us formulate a *backward Newton-Gregory polynomial* of the first time derivative $\dot{\mathbf{x}}$ around the time instant t_k:

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

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We integrate this polynomial over the time interval $t \in [t_k, t_{k+1}]$:

$$\begin{aligned}
\int_{t_k}^{t_{k+1}} \dot{\mathbf{x}}(t)dt &= \mathbf{x}(t_{k+1}) - \mathbf{x}(t_k) \\
&= \int_{t_k}^{t_{k+1}} \left[\mathbf{f}_k + \binom{s}{1}\nabla\mathbf{f}_k + \binom{s+1}{2}\nabla^2\mathbf{f}_k + \binom{s+2}{3}\nabla^3\mathbf{f}_k + \dots\right] dt \\
&= \int_{0.0}^{1.0} \left[\mathbf{f}_k + \binom{s}{1}\nabla\mathbf{f}_k + \binom{s+1}{2}\nabla^2\mathbf{f}_k + \binom{s+2}{3}\nabla^3\mathbf{f}_k + \dots\right] \cdot \frac{dt}{ds} \cdot ds
\end{aligned}$$

The Explicit Adams-Bashforth Formulae II

Therefore:

$$\mathbf{x}(t_{k+1}) = \mathbf{x}(t_k) + h \int_0^1 \left[\mathbf{f}_k + s\nabla\mathbf{f}_k + \left(\frac{s^2}{2} + \frac{s}{2} \right) \nabla^2\mathbf{f}_k \right.$$
$$\left. + \left(\frac{s^3}{6} + \frac{s^2}{2} + \frac{s}{3} \right) \nabla^3\mathbf{f}_k + \ldots \right] ds$$

and consequently:

$$\mathbf{x}(t_{k+1}) = \mathbf{x}(t_k) + h \left(\mathbf{f}_k + \frac{1}{2}\nabla\mathbf{f}_k + \frac{5}{12}\nabla^2\mathbf{f}_k + \frac{3}{8}\nabla^3\mathbf{f}_k + \ldots \right)$$

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If we truncate this infinite series after the quadratic term, we obtain:

$$\mathbf{x}(t_{k+1}) = \mathbf{x}(t_k) + \frac{h}{12} (23\mathbf{f}_k - 16\mathbf{f}_{k-1} + 5\mathbf{f}_{k-2})$$

which is the well-known *Adams-Bashforth third order algorithm (AB3)*.

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If we truncate the series only after the cubic term, we obtain:

$$\mathbf{x}(t_{k+1}) = \mathbf{x}(t_k) + \frac{h}{24}\left(55\mathbf{f}_k - 59\mathbf{f}_{k-1} + 37\mathbf{f}_{k-2} - 9\mathbf{f}_{k-3}\right)$$

which is the *Adams-Bashforth fourth order algorithm (AB4)*.

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- The *step-size control* is complicated by the need to use information of the past. You may remember that the Newton-Gregory polynomials were developed on the basis of *equidistant sampling*.
- The AB formulae were derived under the *linearity assumption*. It is therefore not guaranteed that AB3 is a third-order accurate algorithm also when used in the simulation of non-linear systems.

The Explicit Adams-Bashforth Formulae IV

The AB algorithms can be characterized by a vector α specifying the factor associated with the time step h and by a matrix β that lists the weights of the derivative values:

$$\alpha = \begin{pmatrix} 1 \\ 2 \\ 12 \\ 24 \\ 720 \\ 1440 \end{pmatrix} \quad , \quad \beta = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 3 & -1 & 0 & 0 & 0 & 0 \\ 23 & -16 & 5 & 0 & 0 & 0 \\ 55 & -59 & 37 & -9 & 0 & 0 \\ 1901 & -2774 & 2616 & -1274 & 251 & 0 \\ 4277 & -7923 & 9982 & -7298 & 2877 & -475 \end{pmatrix}$$

Every row specifies the coefficients of one of these algorithms.

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$$\alpha = \begin{pmatrix} 1 \\ 2 \\ 12 \\ 24 \\ 720 \\ 1440 \end{pmatrix} \quad , \quad \beta = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 3 & -1 & 0 & 0 & 0 & 0 \\ 23 & -16 & 5 & 0 & 0 & 0 \\ 55 & -59 & 37 & -9 & 0 & 0 \\ 1901 & -2774 & 2616 & -1274 & 251 & 0 \\ 4277 & -7923 & 9982 & -7298 & 2877 & -475 \end{pmatrix}$$

Every row specifies the coefficients of one of these algorithms.

The *algorithm AB1* is the algorithm:

$$\mathbf{x}(t_{k+1}) = \mathbf{x}(t_k) + \frac{h}{1}\,(1\mathbf{f}_k)$$

i.e., *AB1* $=$ *FE*.

The Stability Domain

We would like to draw the *stability domain of the AB3 algorithm*:

$$\mathbf{x}(t_{k+1}) = \mathbf{x}(t_k) + \frac{h}{12}\left(23\mathbf{f}_k - 16\mathbf{f}_{k-1} + 5\mathbf{f}_{k-2}\right)$$

We apply this algorithm to our standard linear system:

$$\mathbf{x}(t_{k+1}) = \left[\mathbf{I}^{(\mathbf{n})} + \frac{23}{12}\mathbf{A}h\right] \cdot \mathbf{x}(t_k) - \frac{4}{3}\mathbf{A}h \cdot \mathbf{x}(t_{k-1}) + \frac{5}{12}\mathbf{A}h \cdot \mathbf{x}(t_{k-2})$$

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By substitution:

$$\mathbf{z_1}(t_k) = \mathbf{x}(t_{k-2})$$
$$\mathbf{z_2}(t_k) = \mathbf{x}(t_{k-1})$$
$$\mathbf{z_3}(t_k) = \mathbf{x}(t_k)$$

Therefore:

$$\mathbf{z_1}(t_{k+1}) = \mathbf{z_2}(t_k)$$
$$\mathbf{z_2}(t_{k+1}) = \mathbf{z_3}(t_k)$$
$$\mathbf{z_3}(t_{k+1}) = \frac{5}{12}\mathbf{A}h \cdot \mathbf{z_1}(t_k) - \frac{4}{3}\mathbf{A}h \cdot \mathbf{z_2}(t_k) + \left[\mathbf{I}^{(\mathbf{n})} + \frac{23}{12}\mathbf{A}h\right] \cdot \mathbf{z_3}(t_k)$$

The Stability Domain II

Consequently, we can write:

$$\mathbf{z}(t_{k+1}) = \begin{pmatrix} \mathbf{O}^{(n)} & \mathbf{I}^{(n)} & \mathbf{O}^{(n)} \\ \mathbf{O}^{(n)} & \mathbf{O}^{(n)} & \mathbf{I}^{(n)} \\ \frac{5}{12}\mathbf{A}h & -\frac{4}{3}\mathbf{A}h & (\mathbf{I}^{(n)} + \frac{23}{12}\mathbf{A}h) \end{pmatrix} \cdot \mathbf{z}(t_k)$$

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i.e.:

$$\mathbf{z}(t_{k+1}) = \mathbf{F} \cdot \mathbf{z}(t_k)$$

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The F-matrix is three times larger than the A-matrix. Consequently, it contains three times as many eigenvalues.

Stability Domains of AB Algorithms

We are now ready to draw the *stability domains of the AB algorithms*.

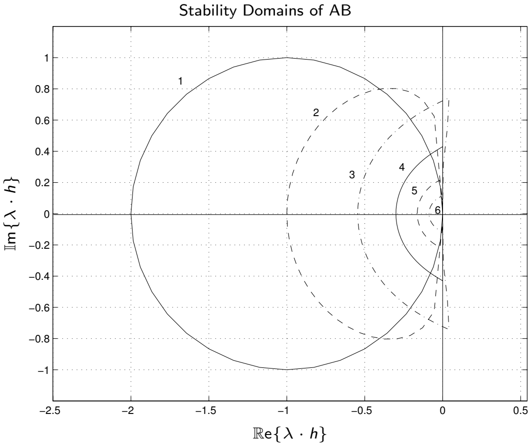

Figure: Stability domains of explicit AB algorithms

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- Although the stability domains of the higher-order AB algorithms approximate the imaginary axis better in the proximity of the origin, the size of the numerical stability domains shrinks with growing orders of approximation accuracy instead of growing.

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- Although the computational load associated with a single integration step is much lower for AB algorithms than for RK algorithms, we are forced to employ much smaller step sizes due to the reduced domains of numerical stability of these algorithms. For this reason, it is not at all clear that the AB algorithms in the end are more economical in their use than the RK algorithms.

Stability Domains of AB Algorithms III

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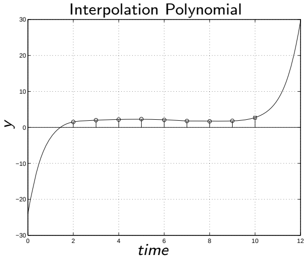

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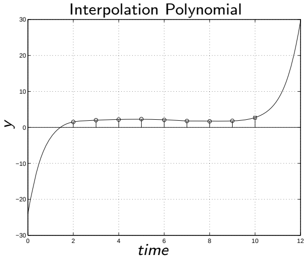

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This doesn't work very well.

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There results the family of formulae:

$$\mathbf{x}(t_{k+1}) = \mathbf{x}(t_k) + h\left(\mathbf{f}_{k+1} - \frac{1}{2}\nabla\mathbf{f}_{k+1} - \frac{1}{12}\nabla^2\mathbf{f}_{k+1} - \frac{1}{24}\nabla^3\mathbf{f}_{k+1} + \ldots\right)$$

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If we truncate this infinite time series after the quadratic term, we obtain:

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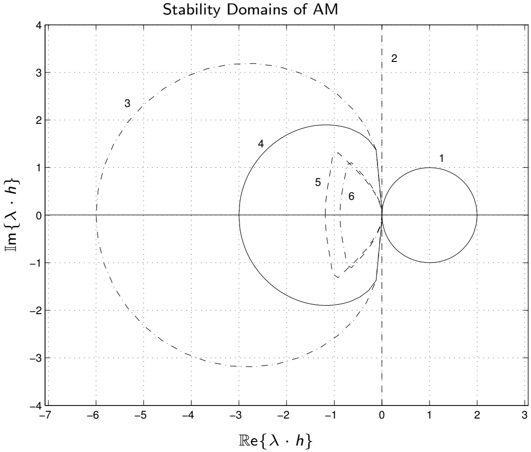
Stability Domains of AM Algorithms

We can draw the *stability domains of the AM algorithms*.



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- On average, we need three Newton iterations per integration step. Consequently, we perform on average three function evaluations during each step.
- Because of the larger stability domains of the AM algorithms, we can use step sizes that are on average three times larger than those used with the corresponding AB algorithms. The efficiencies of the AB and AM algorithms is therefore quite similar.

Adams-Bashforth-Moulton Predictor-Corrector Formulae

Sometimes a method is used that combines a predictor stage of AB with a subsequent corrector stage of AM, e.g.:

$$\text{predictor:} \quad \begin{aligned} \dot{\mathbf{x}}_{\mathbf{k}} &= \mathbf{f}(\mathbf{x}_{\mathbf{k}}, t_k) \\ \mathbf{x}^{\mathbf{P}}_{\mathbf{k+1}} &= \mathbf{x}_{\mathbf{k}} + \frac{h}{12}(23\dot{\mathbf{x}}_{\mathbf{k}} - 16\dot{\mathbf{x}}_{\mathbf{k-1}} + 5\dot{\mathbf{x}}_{\mathbf{k-2}}) \end{aligned}$$

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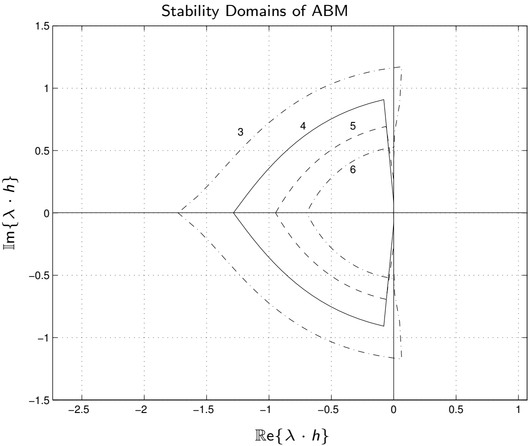

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We differentiate this polynomial with respect to time, t:

$$\dot{\mathbf{x}}(t) = \frac{1}{h} \left[\nabla \mathbf{x}_{k+1} + \left(s + \frac{1}{2} \right) \nabla^2 \mathbf{x}_{k+1} + \left(\frac{s^2}{2} + s + \frac{1}{3} \right) \nabla^3 \mathbf{x}_{k+1} + \ldots \right]$$

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We evaluate at $s = 0.0$:

$$\dot{\mathbf{x}}(t_{k+1}) = \frac{1}{h}\left[\nabla\mathbf{x}_{k+1} + \frac{1}{2}\nabla^2\mathbf{x}_{k+1} + \frac{1}{3}\nabla^3\mathbf{x}_{k+1} + \ldots\right]$$

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If we truncate this infinite series after the cubic term, we obtain:

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We may solve this differential equation for the state variable at the time instant t_{k+1}:

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The Backward Difference Formulae II

If we truncate this infinite series after the cubic term, we obtain:

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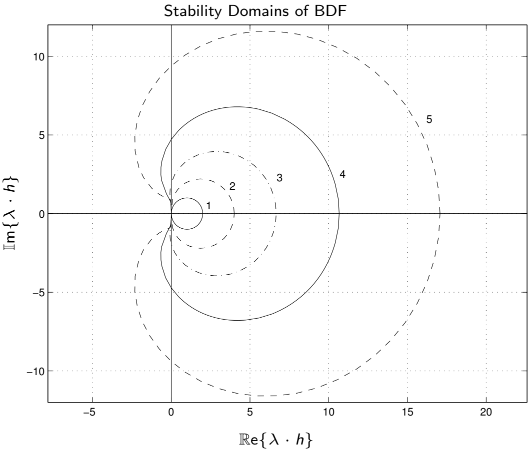
There results the well-known *third-order accurate backward difference formula (BDF3)*.

All BDF algorithms can be characterized by a vector α specifying the factor associated with the time derivative and by a matrix β that lists the weights of the past values of the state vector:

$$\alpha = \begin{pmatrix} 1 \\ 2/3 \\ 6/11 \\ 12/25 \\ 60/137 \end{pmatrix} \quad , \quad \beta = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 4/3 & -1/3 & 0 & 0 & 0 \\ 18/11 & -9/11 & 2/11 & 0 & 0 \\ 48/25 & -36/25 & 16/25 & -3/25 & 0 \\ 300/137 & -300/137 & 200/137 & -75/137 & 12/137 \end{pmatrix}$$

Stability Domains of BDF Algorithms

We can draw the *stability domains of the backward difference formulae (BDF)*.



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- The BDF algorithms are implicit methods. It is also possible to derive explicit BDF algorithms, but unfortunately, they are unstable everywhere.
- **Thanks to their suitability for the simulation of stiff systems and due to their simplicity, the BDF algorithms are among the most widely used numerical ODE solvers for the simulation of dynamic systems.**

The Explicit Nyström Formulae

We start with the same backward Newton-Gregory polynomial that we already used for the derivation of the AB algorithms:

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

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This time, we integrate the polynomial over the time interval $t \in [t_{k-1}, t_{k+1}]$, i.e., over the interval $s \in [-1.0, +1.0]$. We encounter the family of formulae:

$$\mathbf{x}(t_{k+1}) = \mathbf{x}(t_{k-1}) + h\left(2\mathbf{f}_k + \frac{1}{3}\nabla^2 \mathbf{f}_k + \frac{1}{3}\nabla^3 \mathbf{f}_k + \dots\right)$$

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If we truncate this infinite series after the cubic term, we obtain:

$$\mathbf{x}(t_{k+1}) = \mathbf{x}(t_{k-1}) + \frac{h}{3} (8\mathbf{f}_k - 5\mathbf{f}_{k-1} + 4\mathbf{f}_{k-2} - \mathbf{f}_{k-3})$$

This algorithm is called *fourth-order accurate Nyström algorithm (Ny4)*.

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The Nyström algorithms can be characterized by a vector α specifying the factor associated with the time step h and by a matrix β that lists the weights of the derivatives:

$$\alpha = \begin{pmatrix} 1 \\ 1 \\ 3 \\ 3 \\ 90 \end{pmatrix} \quad , \quad \beta = \begin{pmatrix} 2 & 0 & 0 & 0 & 0 \\ 2 & 0 & 0 & 0 & 0 \\ 7 & -2 & 1 & 0 & 0 \\ 8 & -5 & 4 & -1 & 0 \\ 269 & -266 & 294 & -146 & 29 \end{pmatrix}$$

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These algorithms can therefore not be used alone, but they may still be usable for *individual stages within blended or cyclic methods*.

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- **Dymola** uses **DASSL**, an implementation of a variable-step, variable-order BDF algorithm as its default ODE solver.