Order and stability for single and multivalue methods for differential equations

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“Stiff” differential equations arise in many modelling situations’
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Stiff problems are characterised by the existence of rapidly decaying transients.

We can isolate such transients by considering the one-dimensional linear problem

$$y'(x) = qy(x),$$

where $q$ is a complex number with negative real part.
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A famous example of a method which is not A-stable is the (forward) Euler method

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A famous example of a method which is not A-stable is the (forward) Euler method

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An equally famous example of a method which is A-stable is the backward Euler method

\[ y_n = y_{n-1} + hf(x_n, y_n) \]
A rational function $R$ given by

$$R(z) = \frac{P(z)}{Q(z)}$$

is an order $p$ approximation to the exponential function if

$$R(z) - \exp(z) = C z^{p+1} + O(z^{p+2})$$
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If $P$ has degree $n$ and $Q$ has degree $d$ and $p = n + d$ then $R$ is a Padé approximation.
A Runge-Kutta method with stability function given by

\[ R(z) = 1 + zb^T(I - zA)^{-1}1 \]

is A-stable if \(|R(z)| \leq 1\) whenever \(z\) is in the (closed) left half-plane.
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In this case

\[ P(z) = \det(I + z(1b^T - A)), \quad Q(z) = \det(I - zA). \]
Let $\Phi(w, z)$ be a polynomial in two variables.
Generalized Padé approximations

Let $\Phi(w, z)$ be a polynomial in two variables.

Let $d_0, d_1, \ldots, d_n$ be the $z$ degrees of the coefficients of $w^n, w^{n-1}, \ldots, w^1$ and $w^0$ terms.
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$\Phi$ is a generalized Padé approximation to $\exp$ if

$$\Phi(\exp(z), z) = Cz^{p+1} + O(z^{p+2})$$

where the ‘order’ is $p = \sum_{i=0}^{n} (d_i + 1) - 2$. 
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We will emphasise the ‘quadratic’ case $n = 2$ as an important example and write

$$\Phi(w, z) = P(z)w^2 + Q(z)w + R(z)$$
We will write the degrees as $d_0 = k$, $d_1 = l$, $d_2 = m$. 
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A general linear method

\[
\begin{bmatrix}
A & U \\
B & V
\end{bmatrix}
\]

has stability matrix

\[
M = V + zB(I - zA)^{-1}U.
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This method is A-stable if $M$ is power bounded for $z$ in the left half-plane.
Runge-Kutta methods possessing Padé stability functions

The 2 stage Gauss Runge-Kutta method has tableau

\[
\begin{array}{ccc}
\frac{1}{2} - \frac{\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4} - \frac{\sqrt{3}}{6} \\
\frac{1}{2} + \frac{\sqrt{3}}{6} & \frac{1}{4} + \frac{\sqrt{3}}{6} & \frac{1}{4} \\
\frac{1}{2} & \frac{1}{2} & \frac{1}{2}
\end{array}
\]
The 2 stage Gauss Runge-Kutta method has tableau

\[
\begin{array}{c|ccc}
\frac{1}{2} & - & \frac{\sqrt{3}}{6} \\
\frac{1}{2} & + & \frac{\sqrt{3}}{6} \\
\hline
\frac{1}{4} & + & \frac{\sqrt{3}}{6} & \frac{1}{4} & - & \frac{\sqrt{3}}{6} \\
\frac{1}{2} & + & \frac{\sqrt{3}}{6} & \frac{1}{4} & - & \frac{\sqrt{3}}{6} \\
\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\
\end{array}
\]

It has stability function

\[
R(z) = \frac{1 + \frac{z}{2} + \frac{z^2}{12}}{1 - \frac{z}{2} + \frac{z^2}{12}}
\]
Runge-Kutta methods possessing Padé stability functions

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\hline
\frac{1}{2} & \frac{1}{2} & \frac{1}{2}
\end{array}
\]

It has stability function

\[R(z) = \frac{1 + \frac{z}{2} + \frac{z^2}{12}}{1 - \frac{z}{2} + \frac{z^2}{12}}\]

\[|R(z)|\text{ is bounded by 1 for } z \text{ in the left half plane because there are no poles there and } |R(iy)| = 1.\]
For this method, $R(z)$ is the $(2, 2)$ member of the Padé table.
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In general, the stability function for the \(s\) stage Gauss-Legendre method is the \((s, s)\) diagonal Padé approximation.
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In general, the stability function for the \(s\) stage Gauss-Legendre method is the \((s, s)\) diagonal Padé approximation.

Each of these methods is A-stable.
The Runge-Kutta method

\[
\begin{array}{c|ccc}
1 & 5 & -1 \\
3 & 12 & 12 \\
1 & 3 & 4 \\
3 & 4 & 4 \\
\end{array}
\]

has stability function

\[
R(z) = \frac{P(z)}{Q(z)} = \frac{1 + \frac{z}{3}}{1 - \frac{2z}{3} + \frac{z^2}{6}}
\]
The Runge-Kutta method

\[
\begin{array}{c|ccc}
\frac{1}{3} & \frac{5}{12} & -\frac{1}{12} \\
1 & \frac{3}{4} & \frac{1}{4} \\
\frac{3}{4} & 1 & 0
\end{array}
\]

has stability function

\[
R(z) = \frac{P(z)}{Q(z)} = \frac{1 + \frac{z}{3}}{1 - \frac{2z}{3} + \frac{z^2}{6}}
\]

Again \( |R(z)| \) is bounded by 1 for \( z \) in the left half plane because there are no poles there and because

\[
|Q(iy)|^2 - |P(iy)|^2 = \frac{1}{36}y^4 \geq 0.
\]
This stability function is the \((2, 1)\) member of the Padé table.
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In general, the $s$ stage Radau IIA method is A-stable (and because $R(\infty) = 0$, is also L-stable) and its stability function is the $(s, s - 1)$ member of the Padé table.
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In general, the \(s\) stage Radau IIA method is A-stable (and because \(R(\infty) = 0\), is also L-stable) and its stability function is the \((s, s - 1)\) member of the Padé table.

Methods are also known corresponding to the \((s, s - 2)\) members of the Padé table. These are also L-stable.
Consider the following general linear method

\[
\begin{bmatrix}
\frac{2}{7} & -\frac{2}{7} & 1 \\
\frac{3}{7} & \frac{4}{7} & 0 \\
\frac{6-\sqrt{7}}{7} & \frac{1+\sqrt{7}}{7} & \frac{\sqrt{7}}{7} \\
\frac{343-131\sqrt{7}}{98} & -\frac{\sqrt{7}}{49} & 0 \\
\end{bmatrix}
\]
Consider the following general linear method

\[
\begin{bmatrix}
\frac{2}{7} & -\frac{2}{7} & 1 & 0 \\
\frac{3}{7} & \frac{4}{7} & 1 & \frac{\sqrt{7}}{7} \\
\frac{6-\sqrt{7}}{7} & \frac{1+\sqrt{7}}{7} & 1 & 0 \\
\frac{343-131\sqrt{7}}{98} & -\frac{\sqrt{7}}{49} & 0 & \frac{1}{7}
\end{bmatrix}
\]

The characteristic polynomial of the stability matrix is

\[
(7 - 6z + 2z^2)w^2 - 8w + 1.
\]
General linear methods with generalized Padé stability

Consider the following general linear method

\[
\begin{bmatrix}
\frac{2}{7} & -\frac{2}{7} & 1 & 0 \\
\frac{3}{7} & \frac{4}{7} & 1 & \frac{\sqrt{7}}{7} \\
\frac{6-\sqrt{7}}{7} & \frac{1+\sqrt{7}}{7} & 1 & 0 \\
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\end{bmatrix}
\]

The characteristic polynomial of the stability matrix is

\[(7 - 6z + 2z^2)w^2 - 8w + 1.\]

To test the order of this method, substitute \( w = \exp(z) \) and calculate the Taylor expansion.
We have

\[(7 - 6z + 2z^2) \exp(2z) - 8 \exp(z) + 1\]

\[= (7 - 6z + 2z^2)(1 + 2z + 2z^2 + \frac{4}{3}z^3 + \frac{2}{3}z^4 + \cdots) - 8(1 + z + \frac{1}{2}z^2 + \frac{1}{6}z^3 + \frac{1}{24}z^4 + \cdots) + 1\]

\[= \frac{1}{3}z^4 + \cdots\]
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\[= \frac{1}{3}z^4 + \cdots \]

An alternative verification of order is to solve for \(w\) and check that one of the solutions is a good approximation to \(\exp(z)\).
We have

\[(7 - 6z + 2z^2) \exp(2z) - 8 \exp(z) + 1 = (7 - 6z + 2z^2)(1 + 2z + 2z^2 + \frac{4}{3}z^3 + \frac{2}{3}z^4 + \cdots) - 8(1 + z + \frac{1}{2}z^2 + \frac{1}{6}z^3 + \frac{1}{24}z^4 + \cdots) + 1 = \frac{1}{3}z^4 + \cdots\]

An alternative verification of order is to solve for \(w\) and check that one of the solutions is a good approximation to \(\exp(z)\). We have

\[w = \frac{4+\sqrt{9+6z-2z^2}}{7-6z+2z^2} = 1 + z + \frac{1}{2}z^2 + \frac{1}{6}z^3 - \frac{1}{72}z^4 + \cdots = \exp(z) - \frac{1}{18}z^4 - \cdots\]
To test the possible A-stability of this method use the Schur criterion.
To test the possible A-stability of this method use the Schur criterion: a polynomial $c_0 w^2 + c_1 w + c_2$ has both its roots in the open unit disc iff

(a) $|c_0|^2 - |c_2|^2 > 0$, 

(b) $(|c_0|^2 - |c_2|^2)^2 - |c_0 c_1 - c_2 c_1|^2 > 0$. 
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In the present case, for $z = iy$ with $y$ real, we have

(a) $48 + 8y^2 + 4y^4$,

(b) $192y^4 + 64y^6 + 16y^8$. 
Multiderivative–multistep (Obreshkov) methods

If, in addition to a formula for $y'$ given by a differential equation, a formula is also available for $y''$ and possibly higher derivatives, then Obreshkov methods become available.

For example,

$$y(x_n) \approx \frac{6}{7}hy'(x_n) - \frac{2}{7}h^2y''(x_n) + \frac{8}{7}y(x_{n-1}) - \frac{1}{7}y(x_{n-2})$$

The stability function for this method is just the auxiliary polynomial for the difference equation

$$\left(1 - \frac{6}{7}z + \frac{2}{7}z^2\right)u_n - \frac{8}{7}u_{n-1} + \frac{1}{7}u_{n-2} = 0$$

Hence we have a second method with the same A-stability as for the previous general linear method.
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Hence we have a second method with the same A-stability as for the previous general linear method.
A-stability of diagonal and first two sub-diagonals

It is easy to show that, for the \((s, s - d)\) Padé approximation, with \(d = 0, 1, 2,\)

\[
|Q(iy)|^2 - |P(iy)|^2 = C y^{2s}, \quad \text{where} \quad C \geq 0.
\]
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To complete the proof that these methods are all A-stable, we need to show that if \(z\) has negative real part, then \(Q(z) \neq 0.\)
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To complete the proof that these methods are all A-stable, we need to show that if \(z\) has negative real part, then \(Q(z) \neq 0\).

Write \(Q_0, Q_1, \ldots, Q_{s-1}, Q_s = Q\) for the denominators of the sequence of \((0, 0), (1, 1), \ldots, (s - 1, s - 1), (s, s - d)\) Padé approximations.
From known relations between adjacent members of the Padé table, it can be shown that for $k = 2, \ldots, s - 1$,

$$Q_k(z) = Q_{k-1}(z) + \frac{1}{4(2k-1)(2k-3)}z^2Q_{k-2},$$
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\[
Q_k(z) = Q_{k-1}(z) + \frac{1}{4(2k-1)(2k-3)} z^2 Q_{k-2},
\]

and that

\[
Q_s(z) = (1 - \alpha z) Q_{s-1} + \beta z^2 Q_{s-2},
\]

where the constants \( \alpha \) and \( \beta \) will depend on the value of \( d \) and \( s \).
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However, $\alpha = 0$ if $d = 0$ and $\alpha > 0$ for $d = 1$ and $d = 2$. 
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where the constants \( \alpha \) and \( \beta \) will depend on the value of \( d \) and \( s \).

However, \( \alpha = 0 \) if \( d = 0 \) and \( \alpha > 0 \) for \( d = 1 \) and \( d = 2 \).

In all cases, \( \beta > 0 \).
Consider the sequence of complex numbers, $\zeta_k$, for $k = 1, 2, \ldots, s$, defined by

\[
\begin{align*}
\zeta_1 &= 2 - z, \\
\zeta_k &= 1 + \frac{1}{4(2k-1)(2k-3)} z^2 \zeta_{k-1}^{-1}, \quad k = 2, \ldots, s-1, \\
\zeta_s &= (1 - \alpha z) + \beta z^2 \zeta_{s-1}^{-1}.
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This means that $\zeta_1/z = -1 + 2/z$ has negative real part.
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\end{align*}
\]

This means that $\zeta_1/z = -1 + 2/z$ has negative real part.

We prove by induction that $\zeta_k/z$ also has negative real part for $k = 2, 3, \ldots, s$. 
We see this by noting that

\[
\frac{\zeta_k}{z} = \frac{1}{z} + \frac{1}{4(2k-1)(2k-3)} \left( \frac{\zeta_{k-1}}{z} \right)^{-1}, \quad 2 \leq k < s,
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\frac{\zeta_s}{z} = \frac{1}{z} - \alpha + \beta \left( \frac{\zeta_{s-1}}{z} \right)^{-1}.
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The fact that \( Q_s(z) \) cannot vanish now follows by observing that

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Hence, \( Q = Q_s \) does not have a zero in the left half plane.
The set of points in the complex plane such that

\[ |\exp(-z) R(z)| > 1, \]

is known as the ‘order star’ of the method and the set

\[ |\exp(-z) R(z)| < 1 \]

is the ‘dual star’.

We will illustrate this for the \((2, 1)\) Padé approximation

\[ R(z) = \frac{1 + \frac{1}{3}z}{1 - \frac{2}{3}z + \frac{1}{6}z^2} \]
The interior of the shaded area is the ‘order star’ and the unshaded region is the ‘dual order star’.
The order star for a particular rational approximation to the exponential function disconnects into ‘fingers’
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Note that $S$ denotes the order star for a specific ‘method’ and $I$ denotes the imaginary axis.
1. A method is A-stable iff $S$ has no poles in the negative half-plane and $S \cup I = \emptyset$. 
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2. The exists $\rho_0 > 0$ such that, for all $\rho \geq \rho_0$, functions $\theta_1(\rho)$ and $\theta_2(\rho)$ exist such that the intersection of $S$ with the circle $|z| = \rho$ is the set 
\[ \{ \rho \exp(i\theta) : \theta_1 < \theta < \theta_2 \} \] 
and where 
\[ \lim_{\rho \to \infty} \theta_1(\rho) = \pi/2 \] \[ \text{and} \] \[ \lim_{\rho \to \infty} \theta_2(\rho) = 3\pi/2. \]
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$\lim_{\rho \to \infty} \theta_1(\rho) = \pi/2$ and $\lim_{\rho \to \infty} \theta_2(\rho) = 3\pi/2$.

3. For a method of order $p$, the arcs
$\{r \exp(i(j + \frac{1}{2})\pi/(p + 1)) : 0 \leq r\}$, where
$j = 0, 1, \ldots, 2p + 1$, are tangential to the boundary of $S$ at 0.
4. Each bounded finger of $S$, with multiplicity $m$, contains at least $m$ poles, counted with their multiplicities.
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5. Each bounded dual finger of $S$, with multiplicity $m$, contains at least $m$ zeros, counted with their multiplicities.
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The basic idea is to use, rather than the fingers and dual fingers as in order star theory, the lines of steepest ascent and descent from the origin.

Since these lines correspond to values for which $R(z) \exp(-z)$ is real and positive, we are in reality looking at the set of points in the complex plane where this is the case.
For the special method we have been considering, we recall its order star
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There are \( p + 1 \) down-arrows and \( p + 1 \) up-arrows emanating, alternately, from the origin.
A new proof of the Ehle ‘conjecture’

There are $p + 1$ down-arrows and $p + 1$ up-arrows emanating, alternately, from the origin.

The up-arrows terminate at poles or at $-\infty$ and the down-arrows terminate at zeros or at $+\infty$. 
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and it follows that \( n = \tilde{n} \) and \( d = \tilde{d} \).
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If a Padé method is A-stable, the angle subtending the up-arrows which end at poles is bounded by

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Hence \(d - n \leq 2\).
For example, consider the $(4, 1)$ Padé approximation
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![Diagram with arrows and markers](image.png)

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A method with this stability function cannot be A-stable because two of the up-arrows which terminate at poles subtend an angle $\pi$. 
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$$\frac{dz}{dt} = \bar{z}^{n+d} P(z)Q(z).$$

(*)
A dynamical system associated with Padé approximations

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\frac{dz}{dt} = \bar{z}^{n+d} P(z) Q(z).
\]

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The order arrows are trajectories for this system.

Similarly, the boundaries of the order star fingers are trajectories for the system
\[
\frac{dz}{dt} = i\bar{z}^{n+d} P(z) Q(z).
\]
For the approximation

\[ \exp(z) \approx \frac{1 + \frac{1}{3}z}{1 - \frac{2}{3}z + \frac{1}{6}z^2} \]

the vector field associated with (*) is shown on the next slide.
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The ‘Butcher-Chipman conjecture’

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The order star theory is complicated by the need to work on Riemann surfaces.
It seems natural to aim to prove that bounded fingers still contain poles.
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However, some of the fingers that contain poles may have worked their way up from a lower sheet of the Riemann surface.
Gerhard Wanner, in a review of the history of order stars (to celebrate the 25th anniversary of order stars), reported some interesting and extensive calculations he had performed on the Butcher-Chipman conjecture.
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Although his results strongly support the conjecture, they suggest that the method of proof motivated by the order star proof of the Ehle conjecture, will not work, even for the quadratic case.
In particular he presented order stars for the \((k, 0, 2)\) cases where \(k = 21, 22, 23, 24\).
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These order stars, which we present on the next slide, show that some of the bounded fingers merge in with some unbounded fingers and therefore are not evidence that we can always get sufficient poles linked to the origin by fingers on the principal sheet.
A-stable numerical methods
Padé approximations to $\exp$
Generalized Padé approximations
Runge-Kutta methods with Padé stability
General linear methods with generalized Padé stability
Multiderivative–multistep methods
A-stability of diagonal and first two sub-diagonals
Order stars
Order arrows
A new proof of the Ehle ‘conjecture’
A dynamical system
The ‘B-C conjecture’
Wanner commentary
Commentary on the commentary
Known and strongly-believed results

$k = 21, l = 0, m = 2$

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If we use order arrows, we can still be optimistic.
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(23, 0, 2)  (24, 0, 2)
If we use order arrows, we can still be optimistic. Here are two of the unpromising cases.

Undoubtedly the B-C conjecture applies to these cases.
Summary of known and strongly-believed results

I will conclude by saying what I know at present about the BC conjecture and how I believe I can obtain a comprehensive result.
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(i) $2d_0 - p \equiv 3 \mod 4$

and

(ii) $2d_0 - p \equiv 0 \mod 4$ with $2d_0 - p > 0$. 
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Extension to the non-quadratic case of (i).
Preservation of many properties under homotopy.
In particular the connection between the origin and poles by up-arrows.