Order and stability for single and multivalue methods for differential equations

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For example time dependent partial differential equations, approximated by the Method of Lines, and problems in chemical kinetics with widely varying reaction rates.

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

$$y_n = y_{n-1} + hf(x_n, y_n)$$

Padé approximations to the exponential function

A rational function R given by

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

is an order p approximation to the exponential function if

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

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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

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

is A-stable if $|R(z)| \le 1$ whenever z is in the (closed) left half-plane.

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In this case

$$\begin{aligned} P(z) &= \det(I + z(\mathbf{1}b^T - A)), \\ Q(z) &= \det(I - zA). \end{aligned}$$

Generalized Padé approximations

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Φ is a generalized Padé approximation to $\exp$ if

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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

$$\Phi(w, z) = P(z)w^2 + Q(z)w + R(z)$$

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A general linear method

$$\begin{bmatrix} A & U \\ B & V \end{bmatrix}$$

has stability matrix

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Runge-Kutta methods possessing Padé stability functions

The 2 stage Gauss Runge-Kutta method has tableau

$$
\begin{array}{c|cc}
\frac{1}{2}-\frac{\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4}-\frac{\sqrt{3}}{6} \\
\frac{1}{2}+\frac{\sqrt{3}}{6} & \frac{1}{4}+\frac{\sqrt{3}}{6} & \frac{1}{4} \\
\hline
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$$R(z) = \frac{1+\frac{z}{2}+\frac{z^2}{12}}{1-\frac{z}{2}+\frac{z^2}{12}}$$

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

$|R(z)|$ is bounded by 1 for z 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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Each of these methods is A-stable.

The Runge-Kutta method

$$\begin{array}{c|cc} \frac{1}{3} & \frac{5}{12} & -\frac{1}{12} \\ 1 & \frac{3}{4} & \frac{1}{4} \\ \hline & \frac{3}{4} & \frac{1}{4} \end{array}$$

has stability function

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

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

$$|Q(iy)|^2 - |P(iy)|^2 = \frac{1}{36}y^4 \geq 0.$$

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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.

General linear methods with generalized Padé stability

Consider the following general linear method

$$\left[\begin{array}{cc|cc} \frac{2}{7} & -\frac{2}{7} & 1 & 0 \\ \frac{3}{7} & \frac{4}{7} & 1 & \frac{\sqrt{7}}{7} \\ \hline \frac{6-\sqrt{7}}{7} & \frac{1+\sqrt{7}}{7} & 1 & 0 \\ \frac{343-131\sqrt{7}}{98} & -\frac{\sqrt{7}}{49} & 0 & \frac{1}{7} \end{array}\right]$$

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

We have

$$\begin{aligned}
&(7-6z+2z^2)\exp(2z)-8\exp(z)+1\\
&\quad= (7-6z+2z^2)(1+2z+2z^2+\tfrac{4}{3}z^3+\tfrac{2}{3}z^4+\cdots)\\
&\qquad\quad -8(1+z+\tfrac{1}{2}z^2+\tfrac{1}{6}z^3+\tfrac{1}{24}z^4+\cdots)+1\\
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$$\begin{aligned}
w &= \tfrac{4+\sqrt{9+6z-2z^2}}{7-6z+2z^2} \\
&= 1+z+\tfrac{1}{2}z^2+\tfrac{1}{6}z^3-\tfrac{1}{72}z^4+\cdots \\
&= \exp(z)-\tfrac{1}{18}z^4-\cdots
\end{aligned}$$

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 $c_0w^2 + c_1w + c_2$ has both its roots in the open unit disc iff

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

(b) $(|c_0|^2 - |c_2|^2)^2 - |\overline{c}_0 c_1 - c_2\overline{c}_1|^2 > 0$.

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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

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For example,

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

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

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

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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 $d = 0, 1, 2$,

$$|Q(iy)|^2 - |P(iy)|^2 = Cy^{2s}, \quad \text{where} \quad C \geq 0.$$

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Write $Q_0, Q_1, \ldots, Q_{s-1}, Q_s = Q$ for the denominators of the sequence of $(0, 0)$, $(1, 1)$, …, $(s-1, s-1)$, $(s, s-d)$ Padé approximations.

From known relations between adjacent members of the Padé table, it can be shown that for $k = 2, \ldots, s-1$,

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

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In all cases, $\beta > 0$.

Consider the sequence of complex numbers, ζ_k, for $k = 1, 2, \dots, s$, defined by

$$\begin{aligned} \zeta_1 &= 2 - z, \\ \zeta_k &= 1 + \frac{1}{4(2k-1)(2k-3)} z^2 \zeta_{k-1}^{-1}, \quad k = 2, \dots, s-1, \\ \zeta_s &= (1 - \alpha z) + \beta z^2 \zeta_{s-1}^{-1}. \end{aligned}$$

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\end{aligned}$$

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

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

We see this by noting that

$$\begin{aligned}\frac{\zeta_k}{z} &= \frac{1}{z} + \frac{1}{4(2k-1)(2k-3)}\left(\frac{\zeta_{k-1}}{z}\right)^{-1}, \qquad 2 \le k < s,\\ \frac{\zeta_s}{z} &= \frac{1}{z} - \alpha + \beta\left(\frac{\zeta_{s-1}}{z}\right)^{-1}.\end{aligned}$$

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The fact that $Q_s(z)$ cannot vanish now follows by observing that

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$$Q_s(z) = \zeta_1\zeta_2\zeta_3\cdots\zeta_s.$$

Hence, $Q = Q_s$ does not have a zero in the left half plane.

Order stars

The set of points in the complex plane such that

$$|\exp(-z)R(z)| > 1,$$

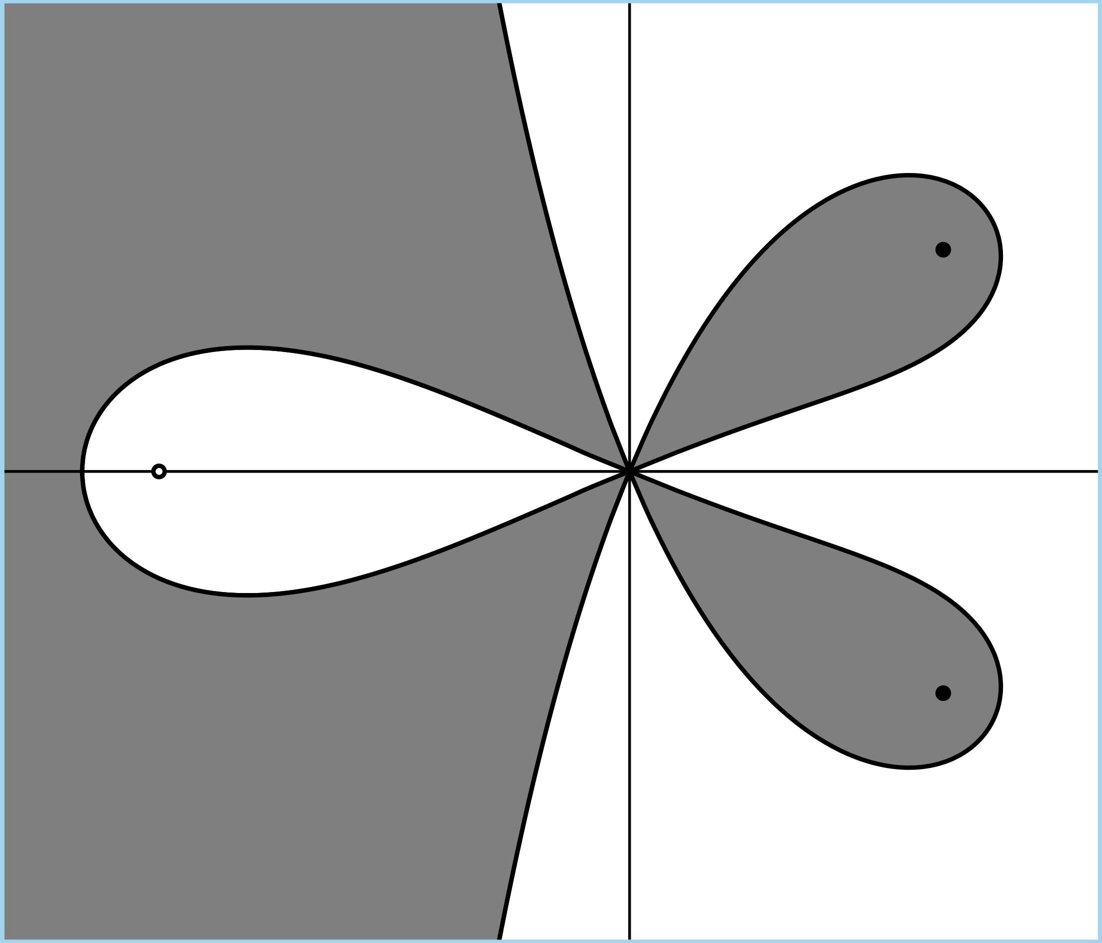
is known as the ‘order star’ of the method and the set

$$|\exp(-z)R(z)| < 1$$

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 disconects into 'fingers'

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The statements on the next two slides summarize the key properties of order stars.

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 $\lim_{\rho\to\infty} \theta_1(\rho) = \pi/2$ and $\lim_{\rho\to\infty} \theta_2(\rho) = 3\pi/2$.

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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.

Order arrows

As an alternative to the famous theory of Hairer, Nørsett and Wanner, I will introduce a slightly different tool for studying stability questions.

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.

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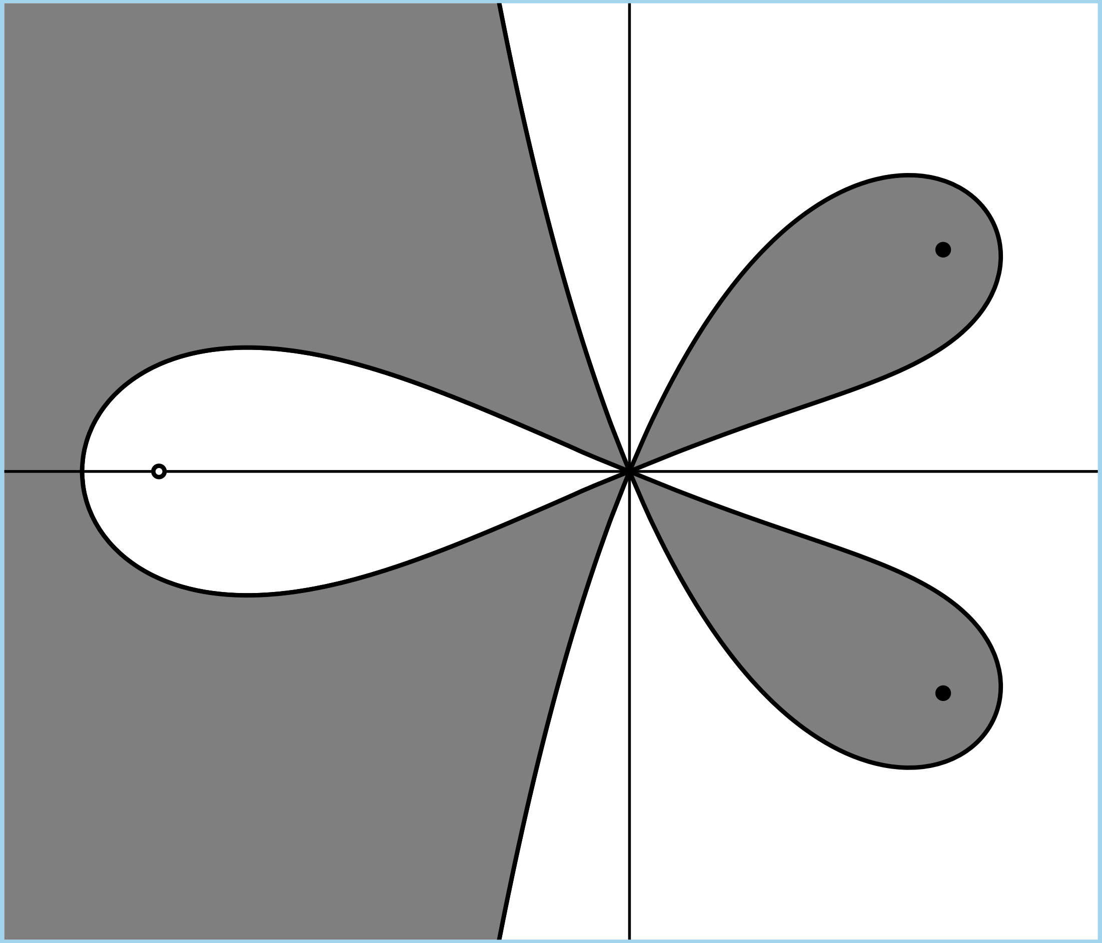

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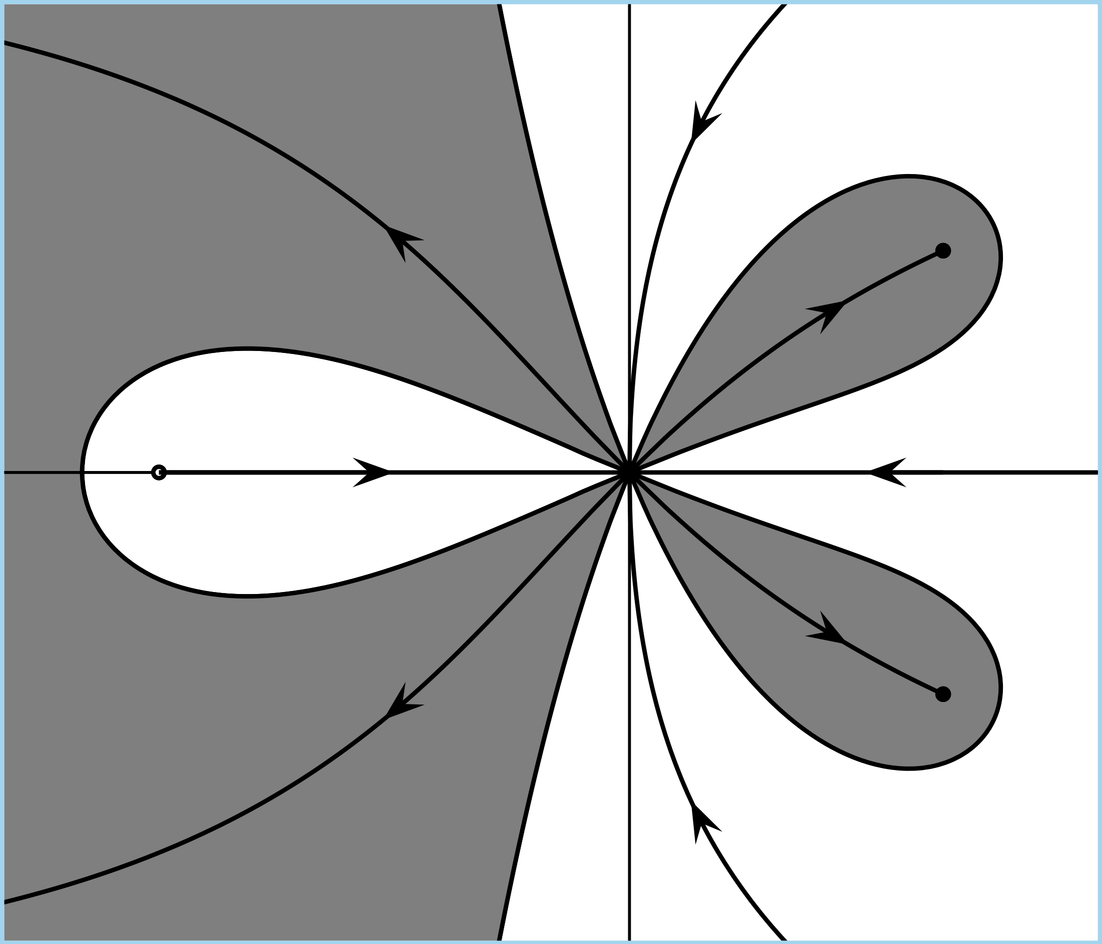

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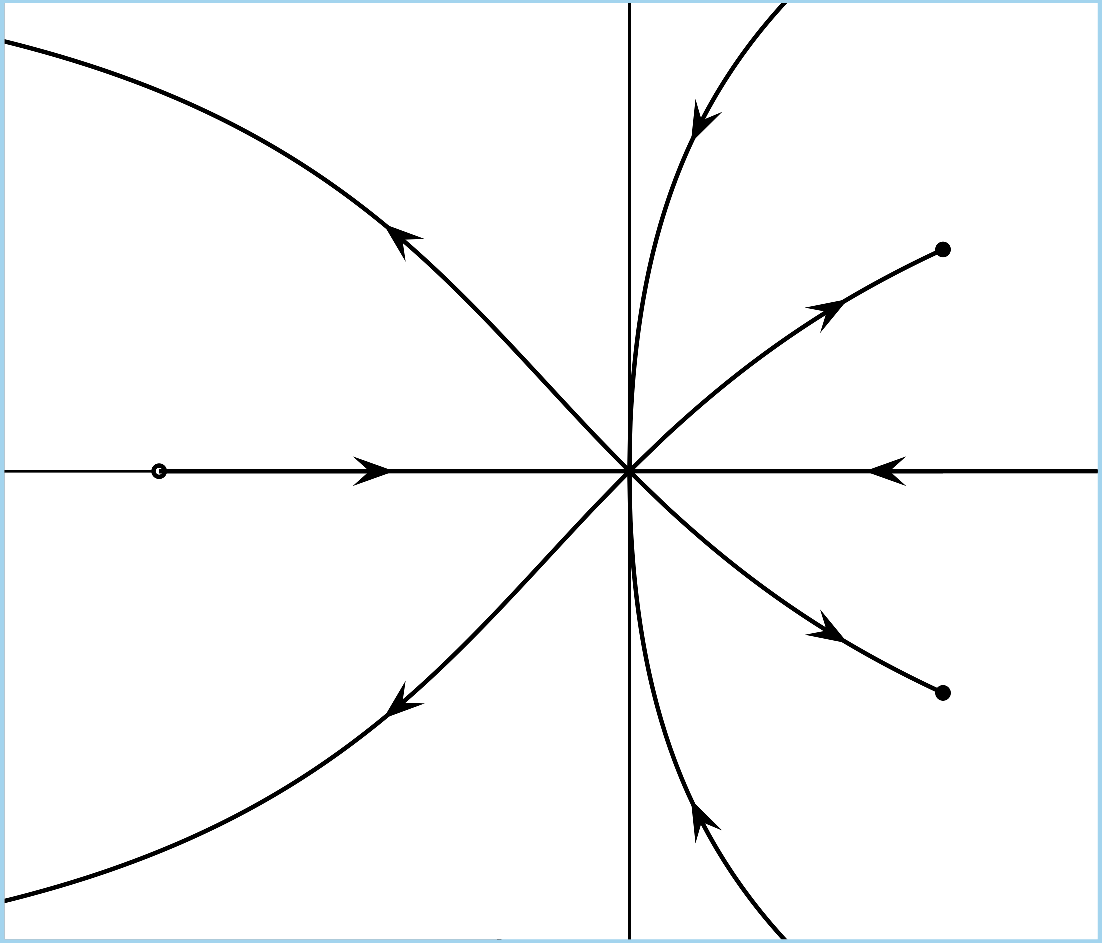

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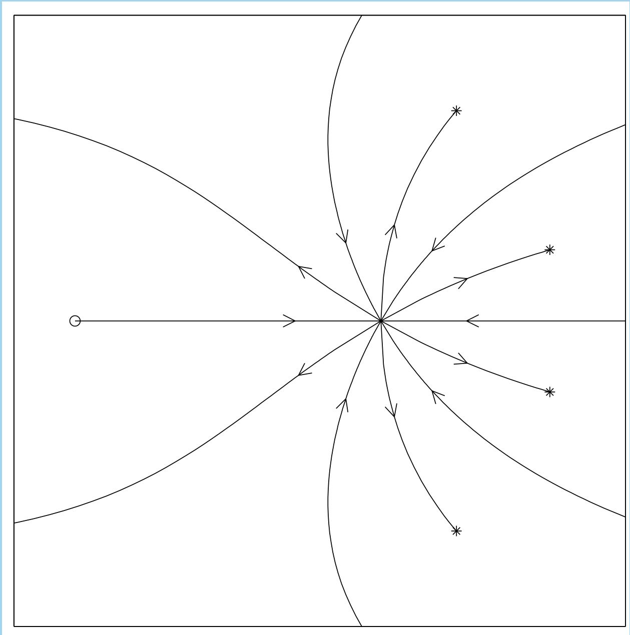

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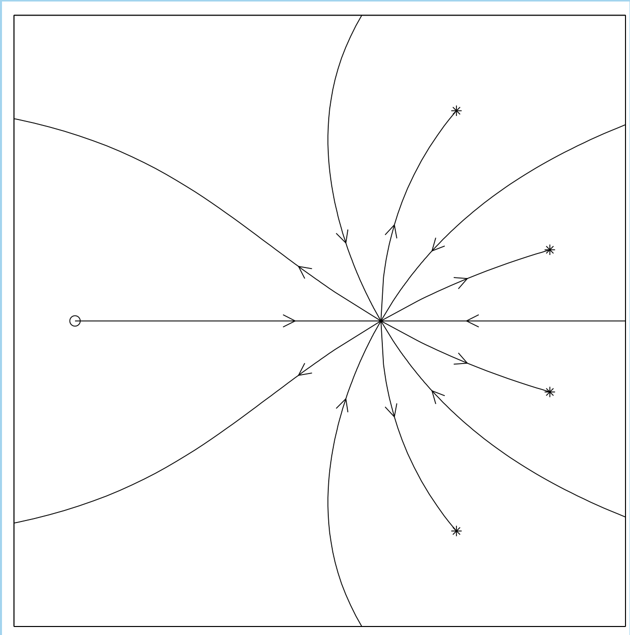

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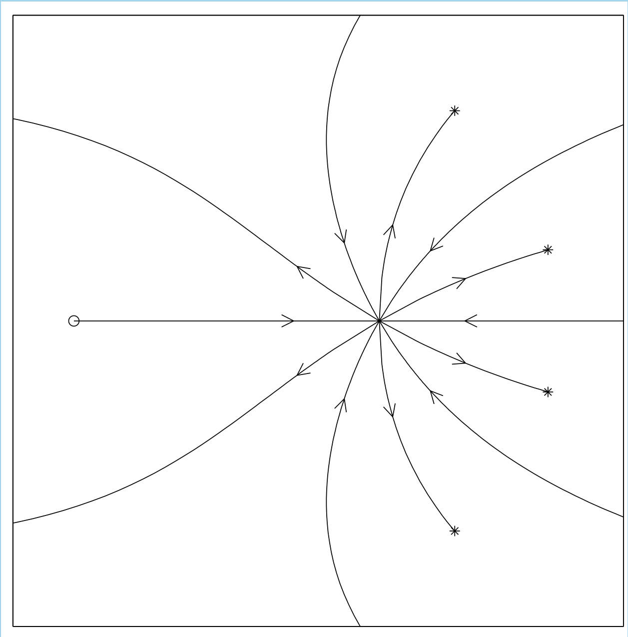

Note that the poles are marked $*$ and the single zero is marked $\circ$.
A method with this stability function cannot be A-stable because two of the up-arrows which terminate at poles subtend an angle π.

A dynamical system associated with Padé approximations

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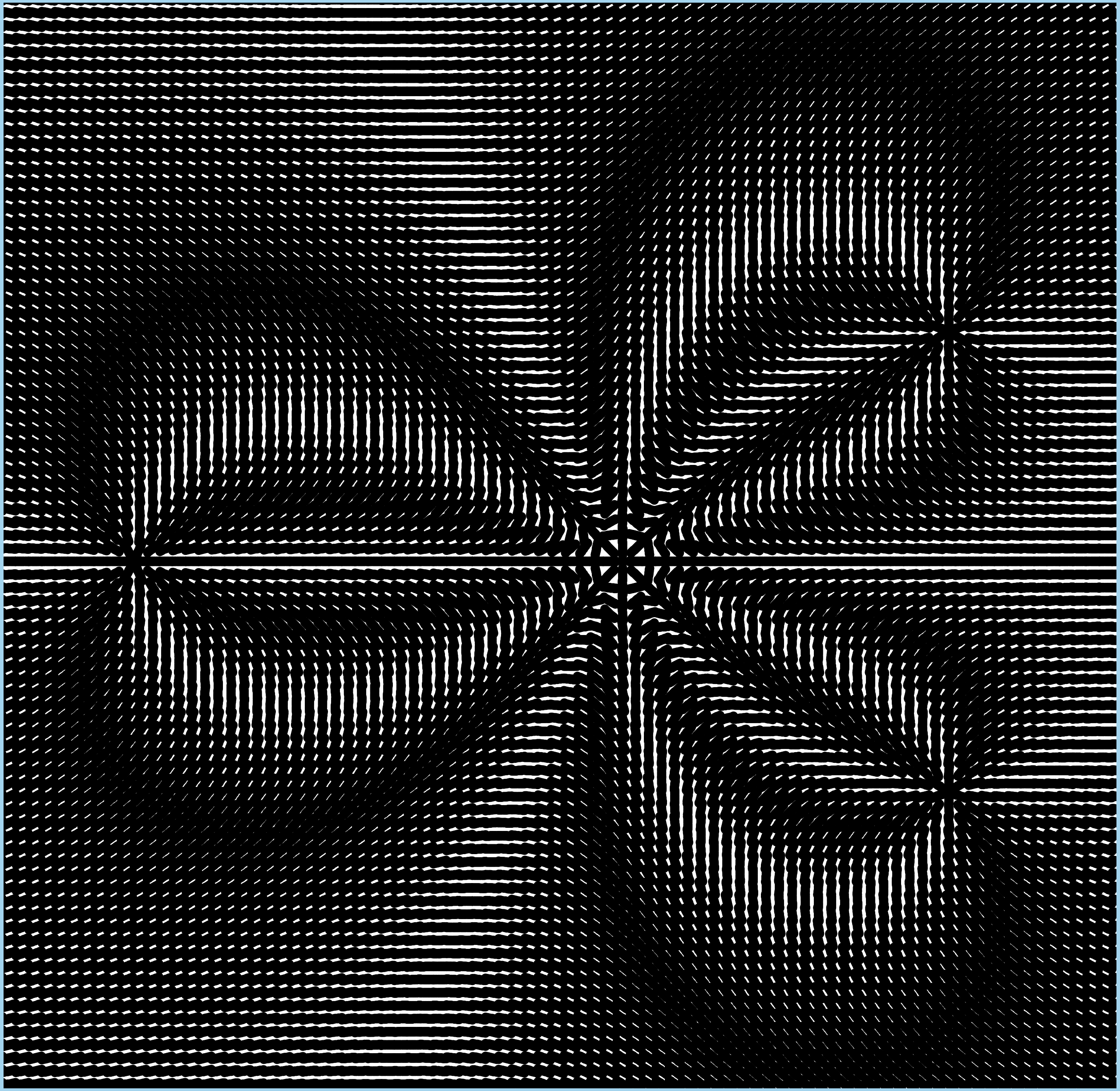
Similarly, the boundaries of the order star fingers are trajectories for the system

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

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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However, some of the fingers that contain poles may have worked their way up from a lower sheet of the Riemann surface.

Commentary on the conjecture by Gerhard Wanner

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Gerhard Wanner, in a review of the history of order stars (to celebrate the 25^{th} anniversary of order stars), reported some interesting and extensive calculations he had performed on the Butcher-Chipman conjecture.

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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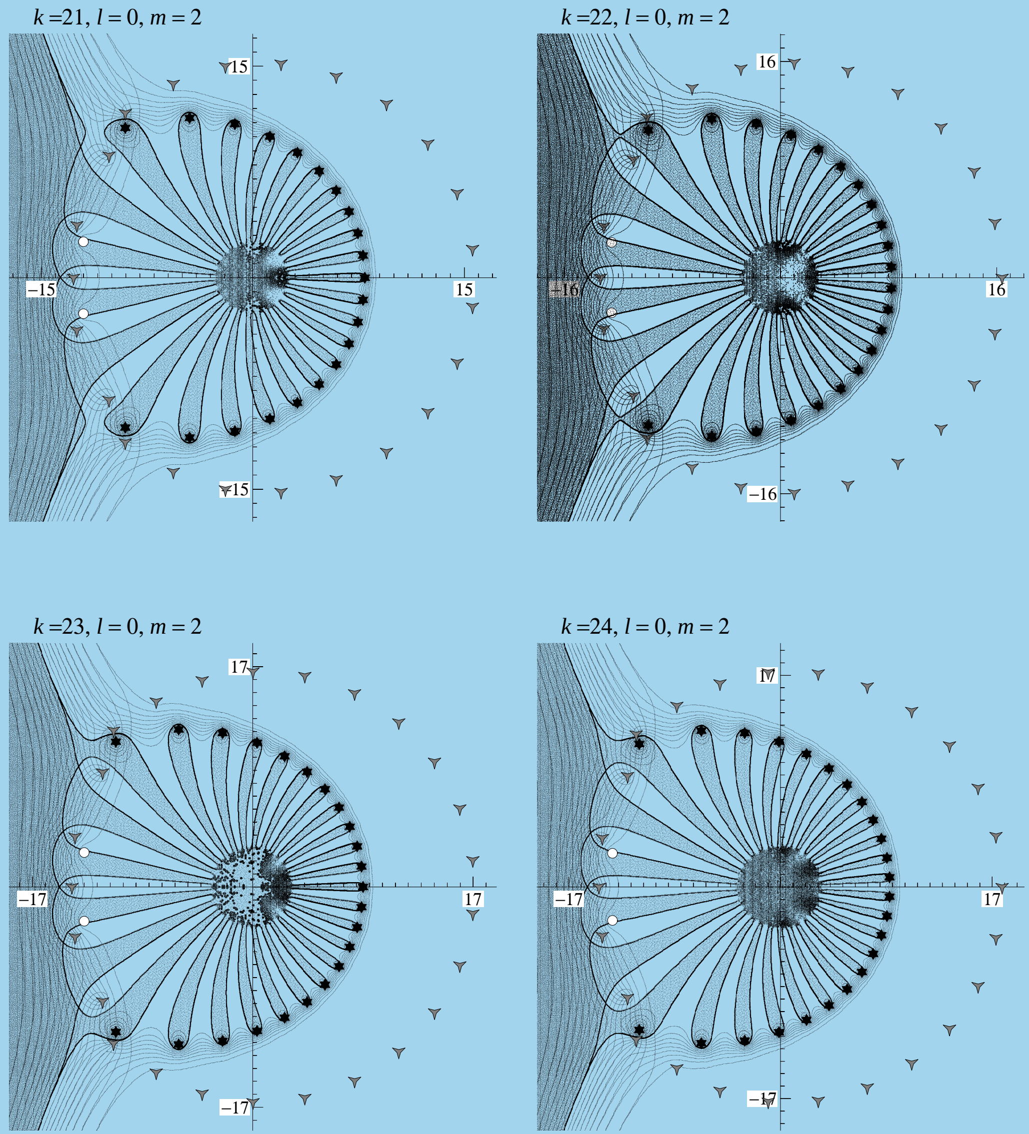
These order stars, which we present on the next slide, show that some of the bounded fingers merge in with some unbounded fingers and therefore are not evidence that we can always get sufficient poles linked to the origin by fingers on the principal sheet.


$k = 21, l = 0, m = 2$
15
−15
15
−15
$k = 22, l = 0, m = 2$
16
−16
16
−16
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17
−17
17
−17
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17
−17
17
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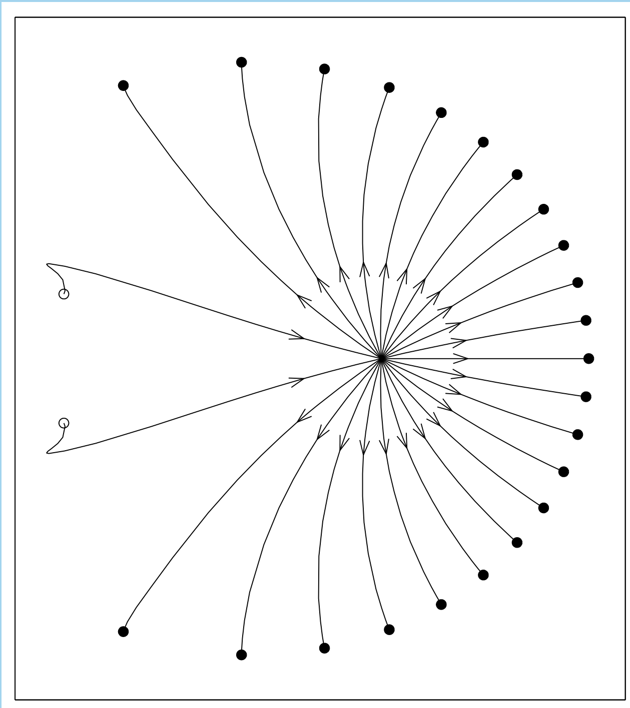

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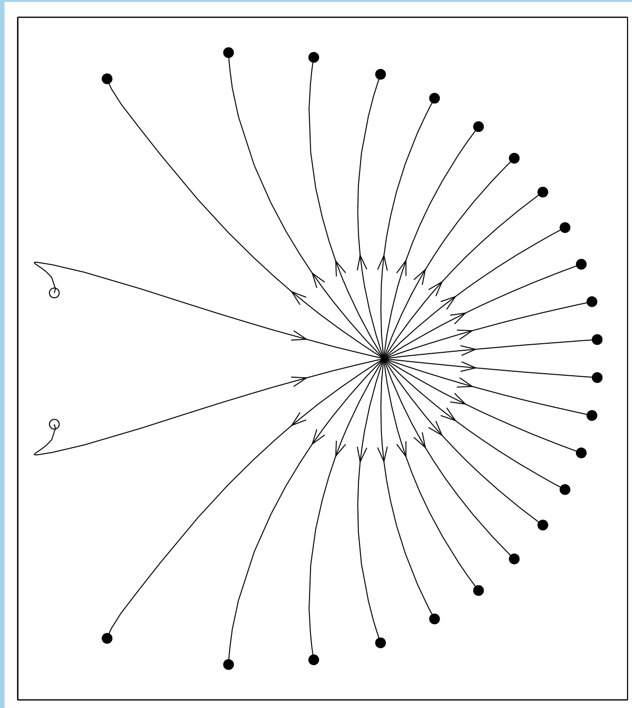

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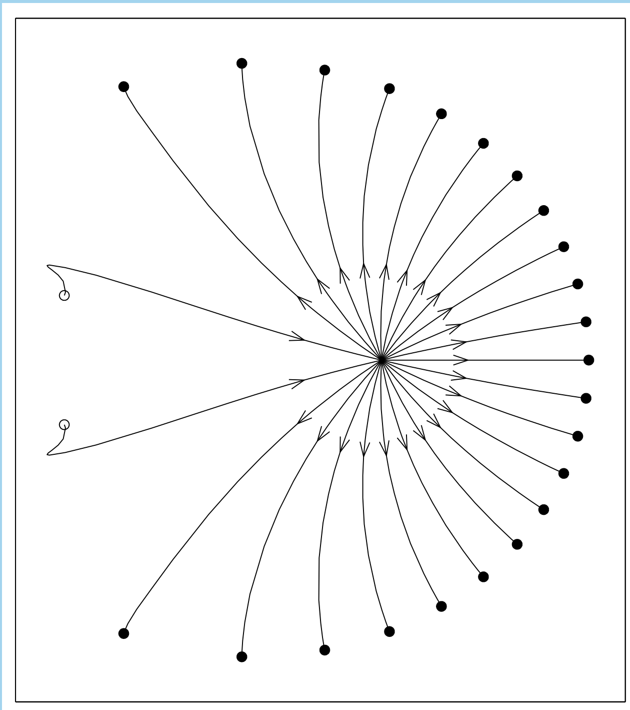

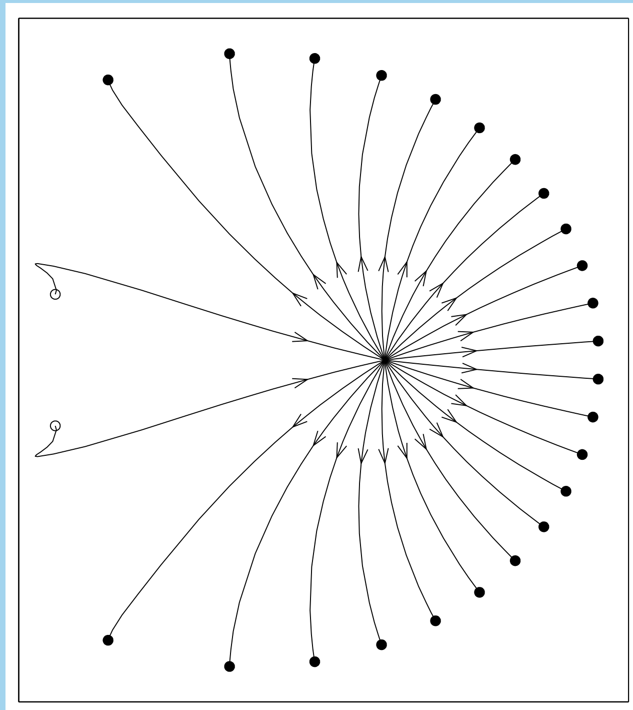

$(23, 0, 2)$ $(24, 0, 2)$

Undoubtedly the B-C conjecture applies to these cases.

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In particular the connection between the origin and poles by up-arrows.