Experiments with Order Arrows

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1 Introduction
- Order and stability
- Three Runge–Kutta methods
- Relative stability regions

2 Order stars and order arrows
- Example 1: the implicit Euler method
- Example 2: a third order implicit method
- Properties of order arrows

3 Applications
- The Ehle “conjecture”
- The Daniel-Moore “conjecture”
- The Butcher-Chipman conjecture

4 Drawing pictures
- Why arrow pictures are hard to draw
- Why arrow pictures are easy to draw
- A differential equation for order arrows

5 Gallery

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Order and stability

In the solution of stiff problems there are many aims such as

- High order
- Good stability
- Economical implementation

These attributes are not independent and there may be a conflict between them.

Order arrows are a tool for exploring restrictions on order for methods that are required to be A-stable.

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Three Runge–Kutta methods

I would like to talk about three special methods which I will call **Eu**, **Im** and **Th**.

$$\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array} \qquad \textbf{(Eu)}$$

$$\begin{array}{c|c} 1 & 1 \\ \hline & 1 \end{array} \qquad \textbf{(Im)}$$

$$\begin{array}{c|ccc} 0 & \frac{1}{6} & -\frac{4}{3} & \frac{7}{6} \\ \frac{1}{2} & \frac{1}{6} & \frac{2}{3} & -\frac{1}{3} \\ 1 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array} \qquad \textbf{(Th)}$$

Eu is the Euler method,

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The stability functions for the three methods are

$$R(z) = 1 + z \qquad = \exp(z) - \tfrac{1}{2}z^2 + O(z^3) \qquad \textbf{(Eu)}$$

$$R(z) = \frac{1}{1-z} \qquad = \exp(z) + \tfrac{1}{2}z^2 + O(z^3) \qquad \textbf{(Im)}$$

$$R(z) = \frac{1}{1 - z + \frac{1}{2}z^2 - \frac{1}{6}z^3} \qquad = \exp(z) + \tfrac{1}{24}z^4 + O(z^5) \qquad \textbf{(Th)}$$

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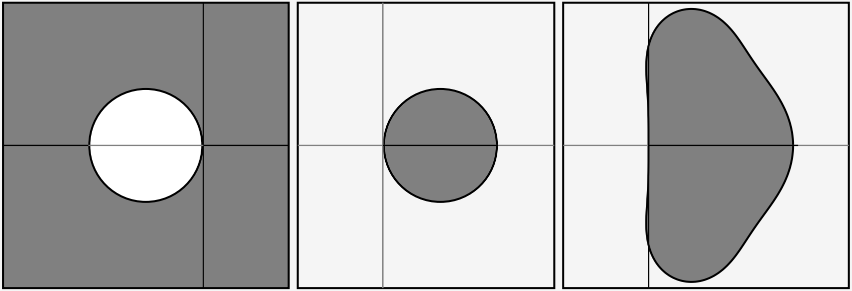

Eu **Im** **Th**

The Euler method has very poor stability and it should not be used with stiff problems.

The Implicit Euler method is A-stable and it can safely be used with most stiff problems.

The special third order method is not A-stable but it is A(α)-stable with $\alpha \approx 88^\circ$.

For many problems, such as pure diffusion problems, the special third order method will be completely satisfactory.

However, in this talk, we are interested in A-stability alone and the competition this property has with the order of methods.

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Relative stability regions

The "instability region" associated with a stability function $R(z)$ is the set of points in the complex plane such that

$$|R(z)| > 1.$$

The *relative* instability region is the set such that

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

The stability region and the relative stability regions are defined in a similar way but with $>$ replaced by $<$.

The relative instability region is known as the "order star" and the relative stability region is known as the dual order star.

These, and the closely related "order arrows", are introduced in the next section for the **Im** and **Th** methods.

Just as order stars are defined in terms of $|\exp(-z)R(z)|$, order arrows are defined as the paths traced out by the points for which $\exp(-z)R(z)$ is real and positive.

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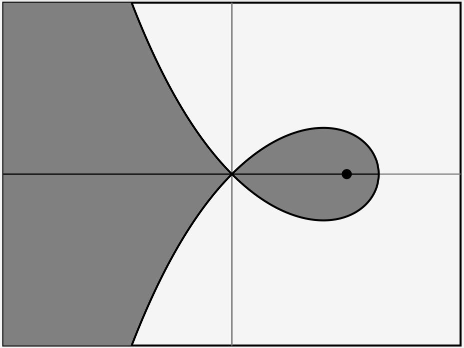
Example: 1 the **Im** method (order star)



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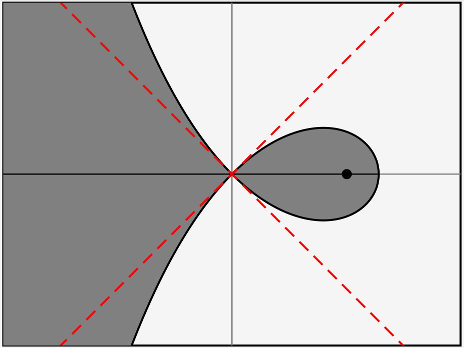

Note the behaviour near zero:
because $R(z)\exp(-z) = 1 + \frac{1}{2}z^2 + O(z^3)$,
the dashed red lines are tangent to the order star boundary at zero and the angle between these tangents is exactly $\pi/2$.

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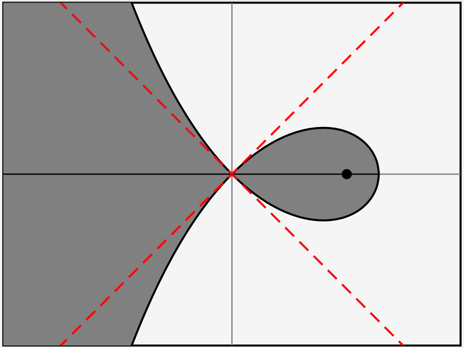

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Note also the existence of a pole in the "bounded finger"

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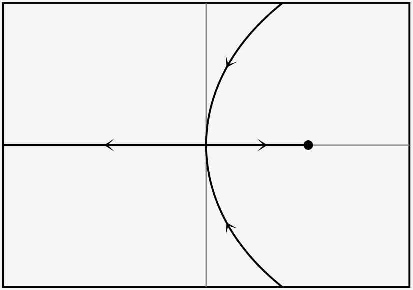

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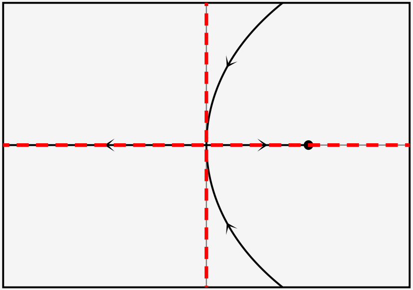

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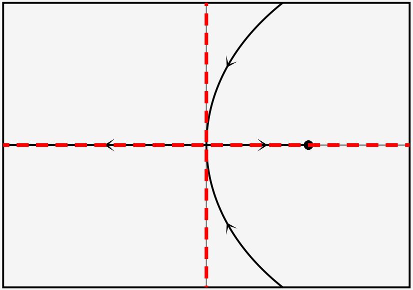

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Up-arrows (increasing values of $R(z)e^{-z}$) alternate with down-arrows.

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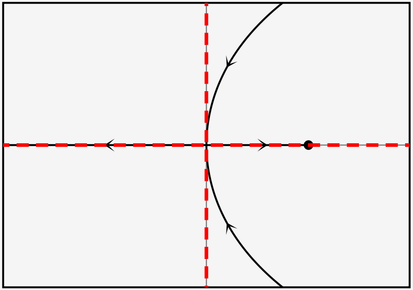

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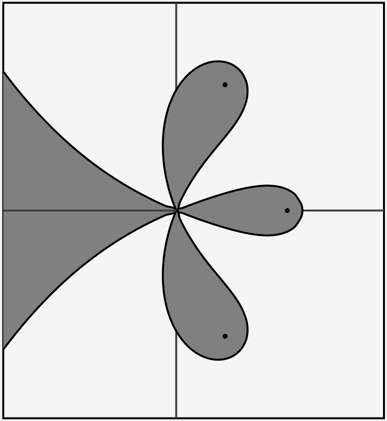
Up-arrows (increasing values of $R(z)e^{-z}$) alternate with down-arrows.

Note the existence of a pole as the termination point of an up-arrow.

Example 2: the **Th** method (order star)



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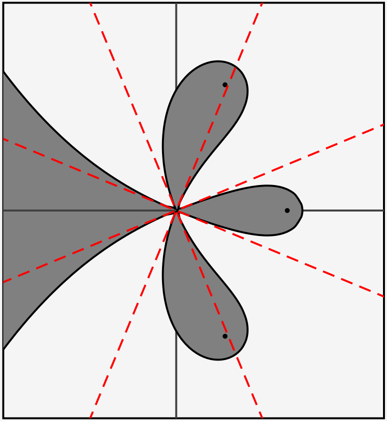

Fingers subtend angles $\pi/4$ at 0 because $\exp(-z)R(z) \approx 1 + \frac{1}{24}z^4$.

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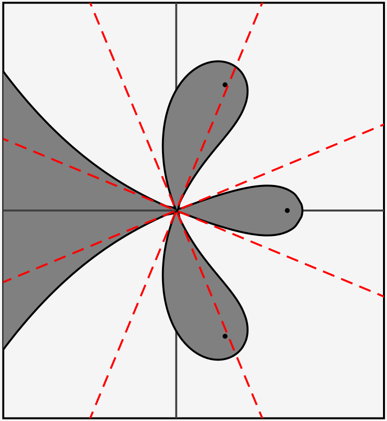

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Bounded fingers contain poles.

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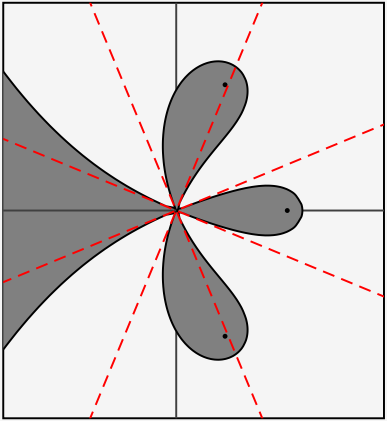

Fingers subtend angles $\pi/4$ at 0 because $\exp(-z)R(z) \approx 1 + \frac{1}{24}z^4$.

Bounded fingers contain poles.

Fingers overlap imaginary axis. Hence the method is not A-stable.

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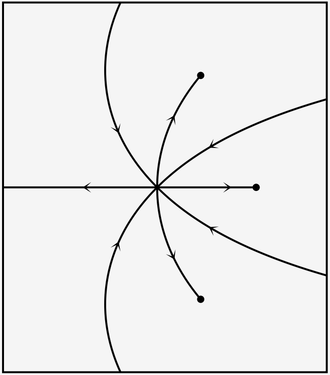

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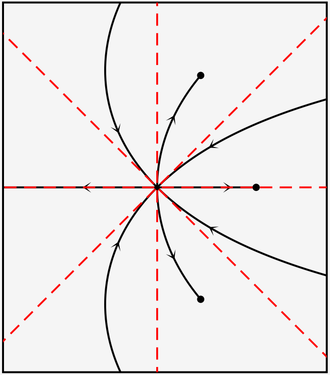

Angles $\pi/4$ between arrows at 0, because $\exp(-z)R(z) \approx 1 + \frac{1}{24}z^4$.

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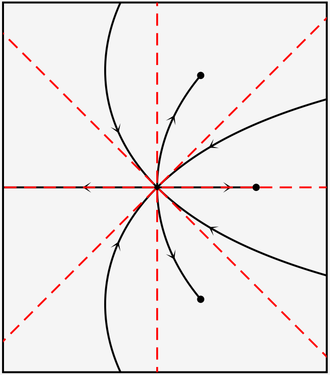

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Poles are at the ends of up-arrows from 0.

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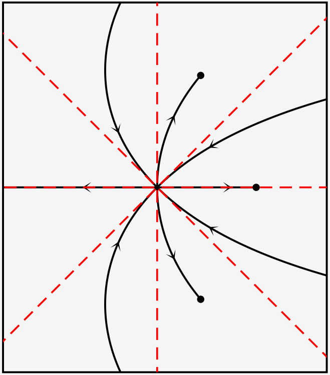

Angles $\pi/4$ between arrows at 0, because $\exp(-z)R(z) \approx 1 + \frac{1}{24}z^4$.

Poles are at the ends of up-arrows from 0.

There is an up-arrow tangential to the imaginary axis.
Hence the method is not A-stable.

Properties of order arrows

Order Stars were introduced in the classic 1978 paper[1] and are the subject of a 1991 monograph[2].

Order arrows have related properties such as

- Up-arrows from zero terminate at poles or at $-\infty$
- Down-arrows from zero terminate at zeros or at $+\infty$
- There is an arrow from zero in the direction of the positive real axis (up- or down- depending on the sign of the error constant)
- For an order p approximation, there are $p+1$ down-arrows from zero alternating with $p+1$ up-arrows from zero
- The angle between one arrow from zero and the next is $\pi/(p+1)$

[1] Wanner G., Hairer E. and Nørsett S. P., Order stars and stability theorems, BIT **18** (1978), 475–489

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If $R(z)$ is an A-function (the stability function of an A-stable method), then we can make further statements

Theorem

Let $R(z)$ be an A-function then

1. $\exp(-z)R(z)$ *has no poles in the left half-plane.*
2. *No up-arrow from zero can be tangential to the imaginary axis.*
3. *No up-arrow from zero can cross the imaginary axis.*

These properties follow from similar facts about $R(z)$ and the observation that multiplication by $\exp(-z)$ does not affect the poles or the behaviour of $|R(z)|$ on the imaginary axis.

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The Ehle "conjecture"

A Padé approximation is a rational function $R(z) = N(z)/D(z)$ such that

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$d \backslash n$	0	1	2	3	4	5
0	1	$1+z$	$1+z+\frac{1}{2}z^2$	$\cdots$	$\cdots$	$\cdots$
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Byron Ehle conjectured that A-stability implies $d \leq n + 2$.

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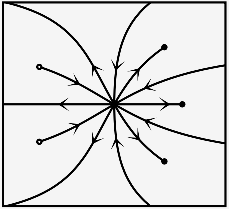

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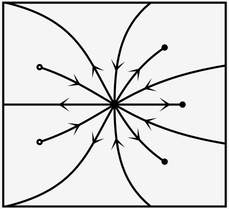

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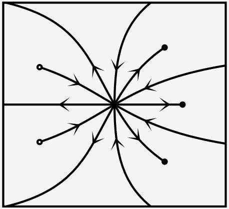

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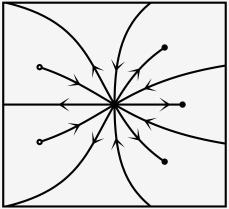

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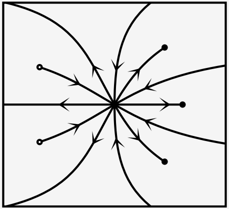

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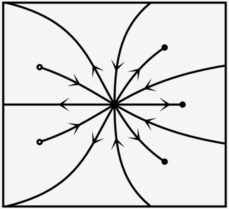

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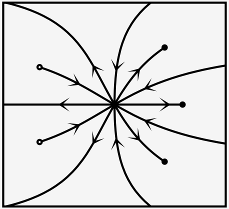

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Hence the sum of the two non-negative integers $n-\widetilde{n}$ and $d-\widetilde{d}$ is non-positive. Therefore $\widetilde{n} = n$ and $\widetilde{d} = d$.

Theorem (Hairer-Nørsett-Wanner Theorem)

A $[d,n]$ Padé approximation is an A-function only if

$$d - n \leq 2.$$

Let Θ be the set of angles in $(-\pi, \pi]$ at which an up-arrow leaves zero and terminates at a pole.

Because successive members of Θ differ by at least $2\pi/(n+d+1)$, it follows that

$$\max(\Theta) - \min(\Theta) \geq \frac{2\pi(d-1)}{n+d+1}.$$

This angle must be less than π, otherwise there will be up-arrows from zero which do one of the following

1. are tangential to the imaginary axis,
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The last two of these options are illustrated on the next slide.

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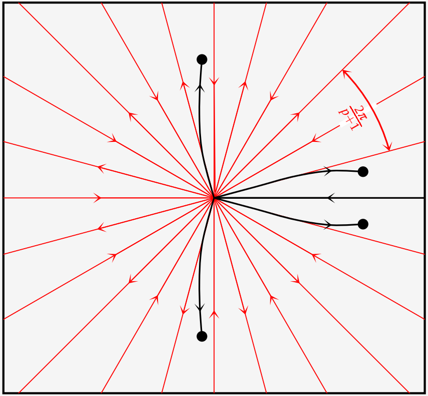
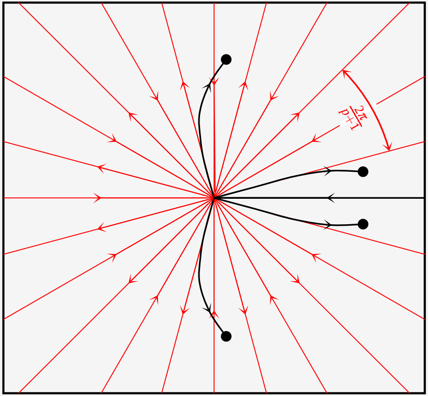

$\frac{2\pi}{p+1}$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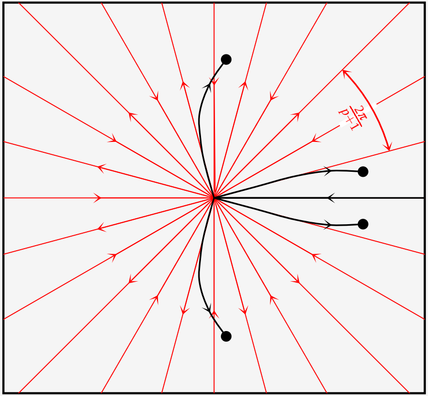
p+1



Since

$$\frac{2\pi(d-1)}{n+d+1} < \pi,$$

we deduce that

$$d-n<3.$$

The Daniel-Moore "conjecture"

This former conjecture was first proved using order stars in [1], but today I will outline an order arrow proof.

It concerns a more general type of approximation, in which $R(z)$ is replaced by a solution to a polynomial equation

$$\Phi(w,z) = w^m P_0(z) + w^{m-1} P_1(z) + \cdots + P_m(z) = 0,$$

and the degrees of $P_0, P_1, \ldots, P_m$ are $[d_0, d_1, \ldots, d_m]$.

Order arrows now live on a Riemann surface

Theorem

A multivalue approximation with degree vector $[d_0, d_1, \ldots, d_m]$ is an A-function only if

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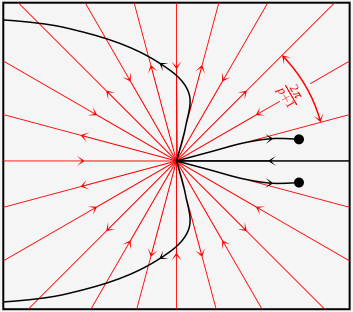

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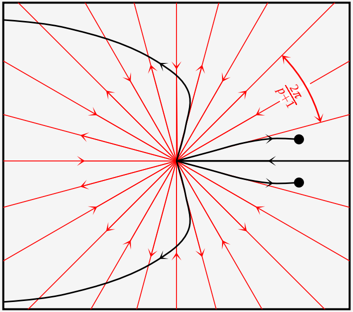

Hence,

$$\frac{2\pi(d_0+1)}{p+1} > \pi,$$

which implies $p \leq 2d_0$.

The Butcher-Chipman conjecture

This conjecture concerns a multivalue generalization of Padé approximations in which the order is

$$p = d_0 + d_1 + \cdots + d_m + m - 1.$$

The conjecture surmised that a necessary condition for an A-approximation is that

$$2d_0 - p \leq 2,$$

just as for the Ehle result.

It is not possible to include a proof of this result here but it can at least be noted that the crucial part of the proof is that every pole is at the end of an up-arrow from zero.

The simple argument which worked in the case $m = 1$ cannot be used in the more general situation because it might be possible for up-arrows from zero to cross down-arrows from zero if they lie on different sheets of the Riemann surface.

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Why arrow pictures are hard to draw

Because $w(z) = R(z)\exp(-z)$ is very close to 1 when z is close to zero, it is difficult to determine accurately when $w(z)$ is real.

To illustrate this, consider the $[5,5]$ Padé approximation

$$R(z) = \frac{1+\frac{1}{2}z+\frac{1}{9}z^2+\frac{1}{72}z^3+\frac{1}{1008}z^4+\frac{1}{30240}z^5}{1-\frac{1}{2}z+\frac{1}{9}z^2-\frac{1}{72}z^3+\frac{1}{1008}z^4-\frac{1}{30240}z^5}$$

In the next slide, we will present a figure constructed by evaluating the imaginary part of $R(z)\exp(-z)$ over a grid of points superimposed on the unit circle centred at 0.

The centre of each small square was regarded as a point on an order arrow if the sum of the signs of the imaginary parts of $w(z)$ at the corners was -1, 0 or $+1$ and the real part of $w(z)$ is positive.

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In the next slide, we will present a figure constructed by evaluating the imaginary part of $R(z)\exp(-z)$ over a grid of points superimposed on the unit circle centred at 0.

The centre of each small square was regarded as a point on an order arrow if the sum of the signs of the imaginary parts of $w(z)$ at the corners was -1, 0 or $+1$ and the real part of $w(z)$ is positive.

Why arrow pictures are hard to draw

Because $w(z) = R(z)\exp(-z)$ is very close to 1 when z is close to zero, it is difficult to determine accurately when $w(z)$ is real.

To illustrate this, consider the $[5,5]$ Padé approximation

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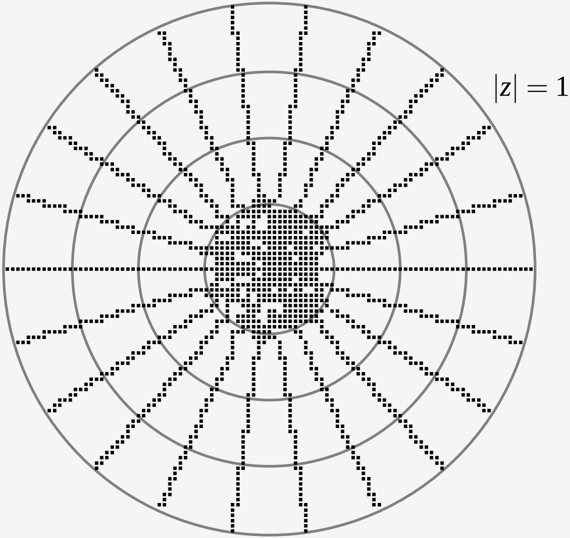
$|z| = 1$

Why arrow pictures are easy to draw

Even though we cannot obtain a clear picture of the arrows by this technique, we can take into account that, near zero, we know that the lines we want are approximately radial with arguments

$$\theta_k = 2\pi k/22, \qquad k = 0, 1, 2, \ldots, 21.$$

In the next figure, lines in these directions are shown but with each point replaced by the closest point arising in the previous figure.

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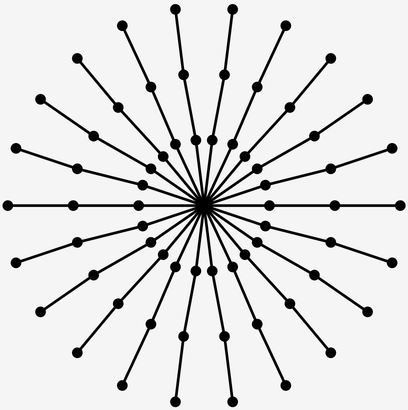
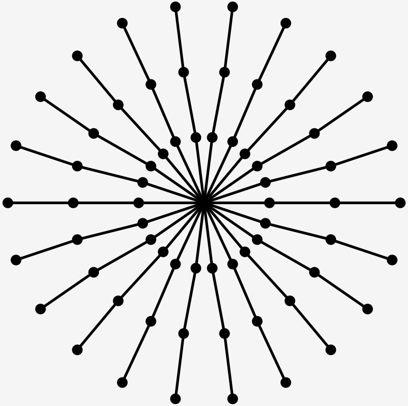


This gives a reasonable looking effect which can be improved by starting with a much finer grid and extending the region covered to a large rectangle centred at the origin.

Most of the pictures in this talk were drawn in this way.



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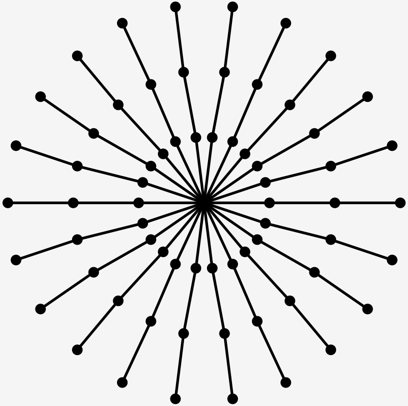

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A differential equation for order arrows

The difficulty caused by machine arithmetic can be eliminated in another way, in the case of a Padé approximation $N(z)/D(z)$.

Write $w = \exp(t)$ in the relationship $wD(z)\exp(z) - N(z) = 0$, so that

$$\exp(z+t)D(z) - N(z) = 0. \tag{1}$$

We can now construct a differential equation expressing the dependence of z on t. Differentiate (1) and it is found that

$$\exp(z+t)(z'(t)(D'(z)+D(z))+D(z)) - z'(t)N'(z) = 0. \tag{2}$$

Eliminate $\exp(z+t)$ from (1) and (2) to yield the differential equation

$$z'(t)F = N(z)D(z), \tag{3}$$

where

$$F = D(z)N'(z) - D'(z)N(z) - D(z)N(z). \tag{4}$$

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Interpret $\exp(z+t)D(z)-N(z)=0$ as defining t as a function of z for $|z|$ small, so that $t=-Cz^{p+1}+O(z^{p+2})$, where C is the error constant.

We can now say something about F. It is equal to

$$D(z)N'(z)-D'(z)N(z)-D(z)N(z)=-(p+1)Cz^{p}+O(z^{p+1}).$$

The $O(z^{p+1})$ term can be deleted because F is a polynomial of degree p.

Hence as t moves from zero in a positive direction (up-arrows) or a negative direction (down-arrows) the z value traces out a path satisfying the differential equation

$$C\frac{d(z^{p+1})}{dt}=-N(z)D(z),$$

This differential equation can be used to draw order arrows accurately.

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1 Introduction
- Order and stability
- Three Runge–Kutta methods
- Relative stability regions

2 Order stars and order arrows
- Example 1: the implicit Euler method
- Example 2: a third order implicit method
- Properties of order arrows

3 Applications
- The Ehle “conjecture”
- The Daniel-Moore “conjecture”
- The Butcher-Chipman conjecture

4 Drawing pictures
- Why arrow pictures are hard to draw
- Why arrow pictures are easy to draw
- A differential equation for order arrows

5 Gallery

Gallery

I would now like to show you a gallery of some order arrows pictures based on both rational and quadratic approximations.

Where an approximation is given in the form

$$\left[\ P_0(z), \quad P_1(z), \quad P_2(z)\ \right]$$

this denotes the quadratic function

$$\Phi(w,z) = P_0(z)w^2 + P_1(z)w + P_2(z).$$

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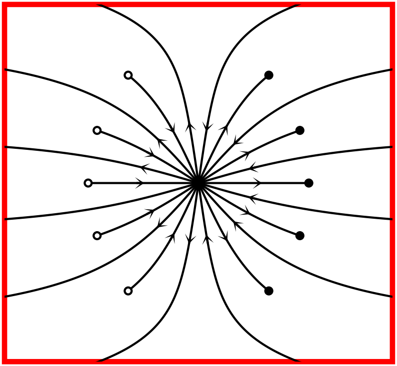
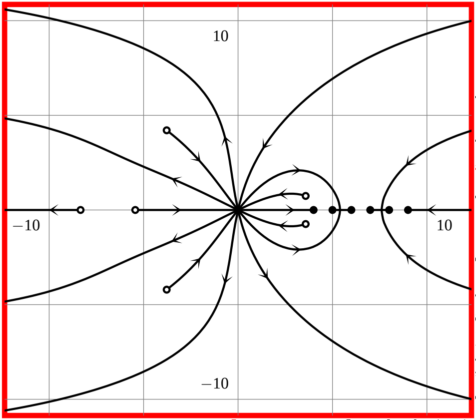
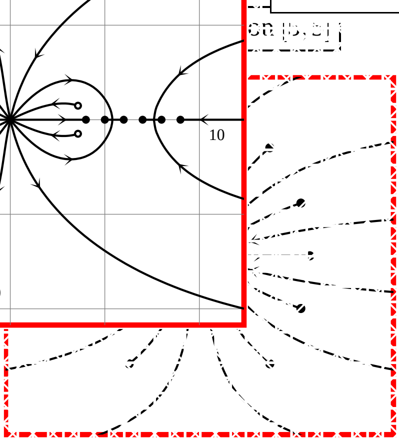
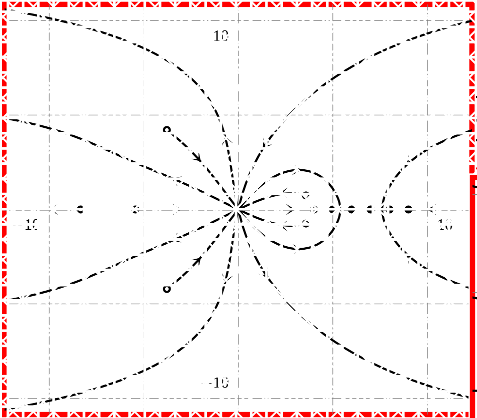
Padé approximation $[5,5]$





Sixth order with poles $\{4,5,6,7,8,9\}$





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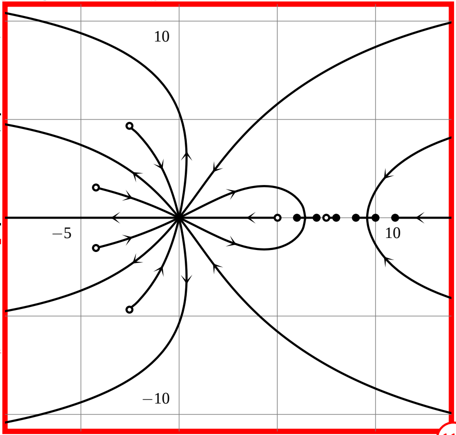
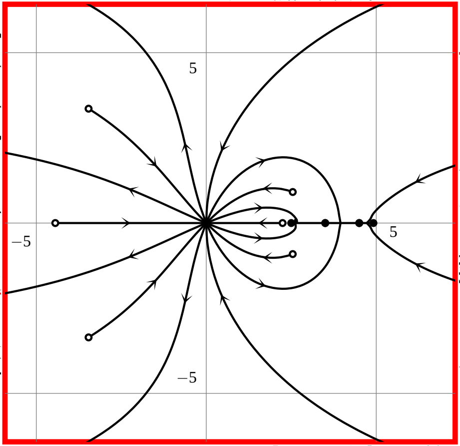
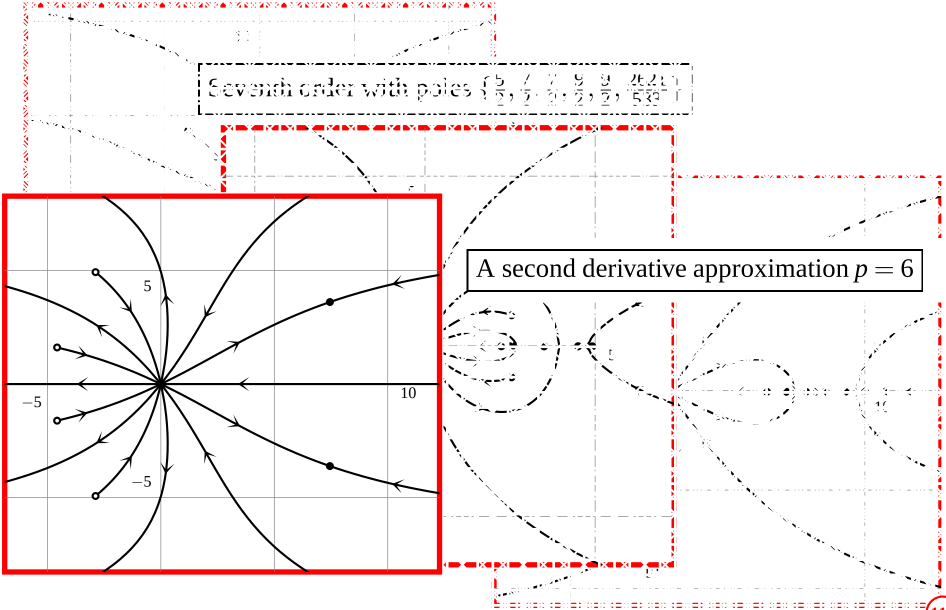


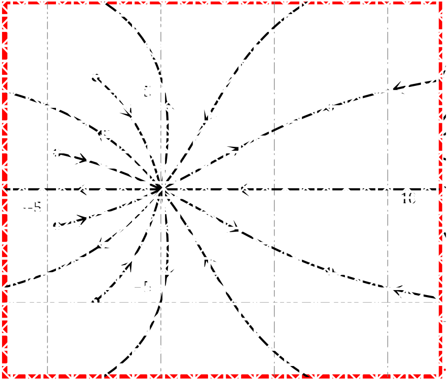
Sixth order with poles $\{6,7,8,9,10,11\}$

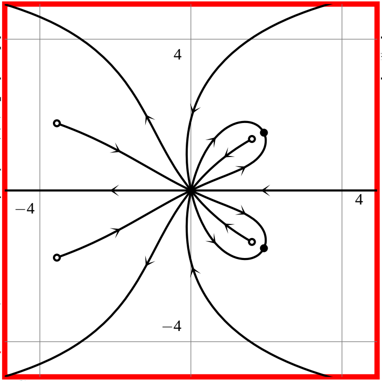
Seventh order with poles $\{\frac{5}{2}, \frac{7}{2}, \frac{7}{2}, \frac{9}{2}, \frac{9}{2}, \frac{2621}{533}\}$



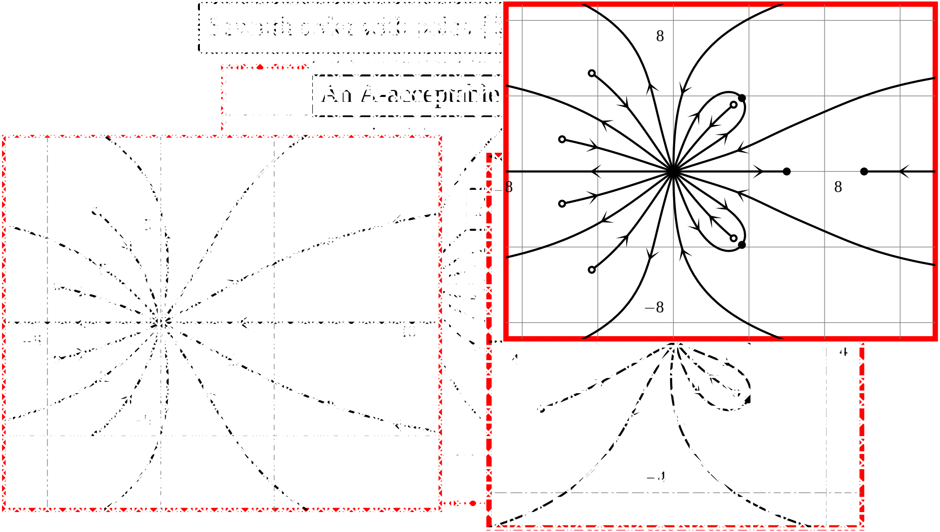

Seventh order with poles {5/2, 7/2, 7/2, 9/2, 9/2,
A second derivative approximation $p = 6$
5
−5
10
−5

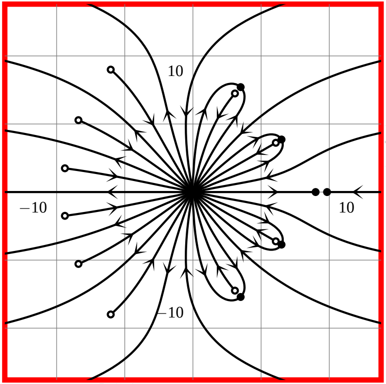
An A-acceptable second derivative approximation $p = 6$



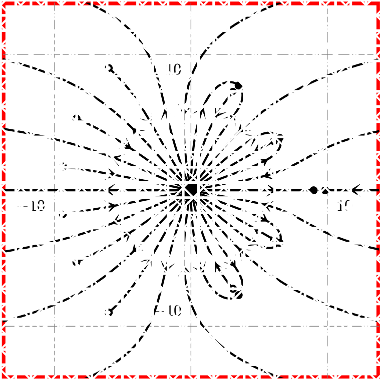


A ninth order approximation





A fifteenth order approximation



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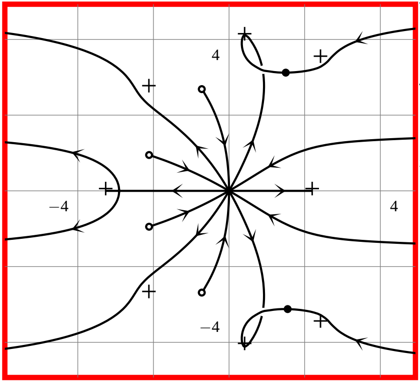
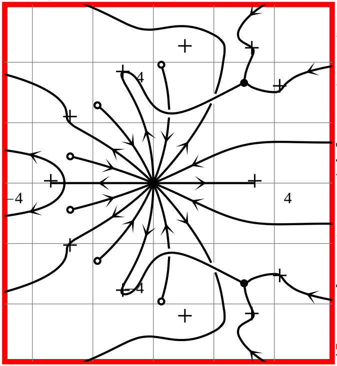
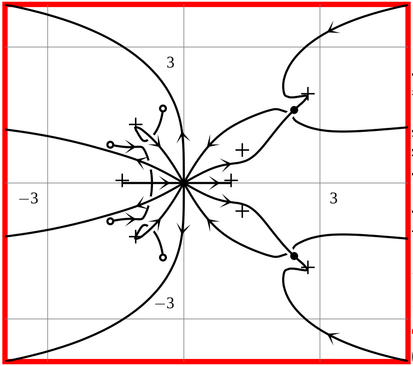


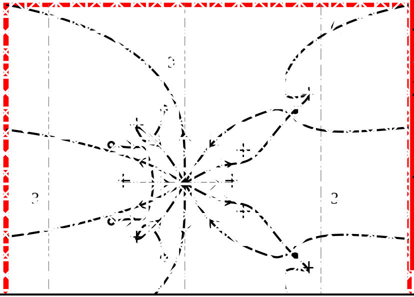
Fifth order method $\left[(1-\frac{1}{4}z+\frac{1}{12}z^2)^2, -\frac{61}{3}, \frac{58}{3}+\frac{113}{6}z+\frac{143}{16}z^2+\frac{95}{36}z^3+\frac{67}{144}z^4\right]$

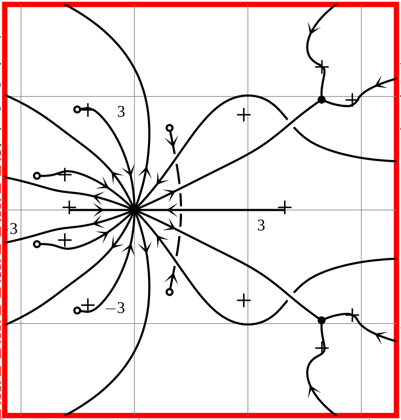
$$p=7:\ \left[(1-\tfrac{3}{10}z+\tfrac{1}{20}z^2)^3, -\tfrac{793}{50}, \tfrac{743}{50}+\tfrac{369}{25}z+\tfrac{731}{100}z^2+\tfrac{2387}{1000}z^3+\tfrac{3403}{6000}z^4+\tfrac{399}{4000}z^5+\tfrac{829}{72000}z^6\right]$$



$$\left[\left(1-\frac{4}{7}z+\left(\frac{2}{21}-\frac{\sqrt{31930}}{840}\right)z^2\right)^2, -\frac{3}{2}, \frac{1}{2}+\frac{9}{14}z+\left(\frac{529}{588}-\frac{\sqrt{31930}}{420}\right)z^2+\left(\frac{23}{88}-\frac{\sqrt{31930}}{294}\right)z^3+\left(\frac{26497}{70560}-\frac{4\sqrt{31930}}{2205}\right)z^4\right]$$

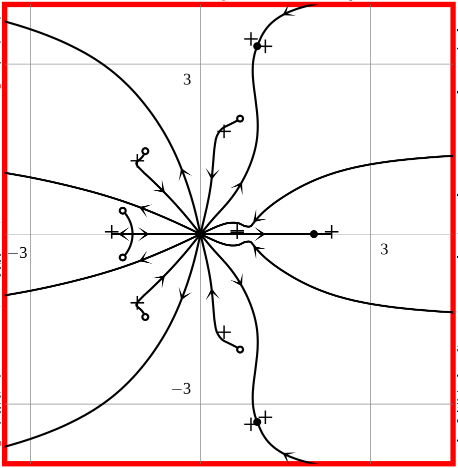




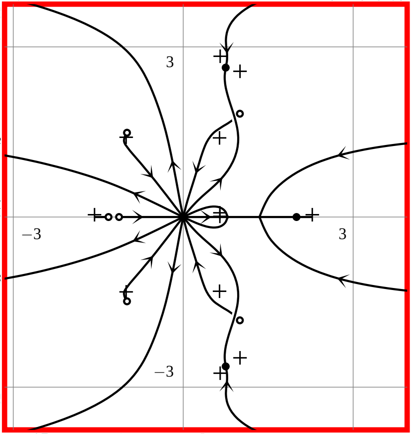


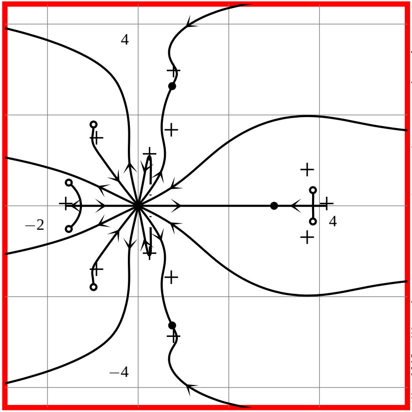
$$\left[\left(1-\frac{3}{10}z+\frac{1}{33}z^2\right)^3, -\frac{131092}{99825}, \frac{31267}{99825}+\frac{42569}{199650}z+\frac{38213}{399300}z^2+\frac{542213}{11979000}z^3+\frac{27532}{1497375}z^4+\frac{30599}{5989500}z^5+\frac{14519}{17968500}z^6\right]$$

$$\left[(1-\tfrac{1}{6}z+\tfrac{1}{12}z^2)^2(1-\tfrac{1}{2}z)^2, -\tfrac{3}{2}, \tfrac{1}{2}+\tfrac{5}{6}z+\tfrac{23}{36}z^2+\tfrac{1}{3}z^3+\tfrac{7}{48}z^4+\tfrac{121}{2160}z^5+\tfrac{49}{2880}z^6\right]$$

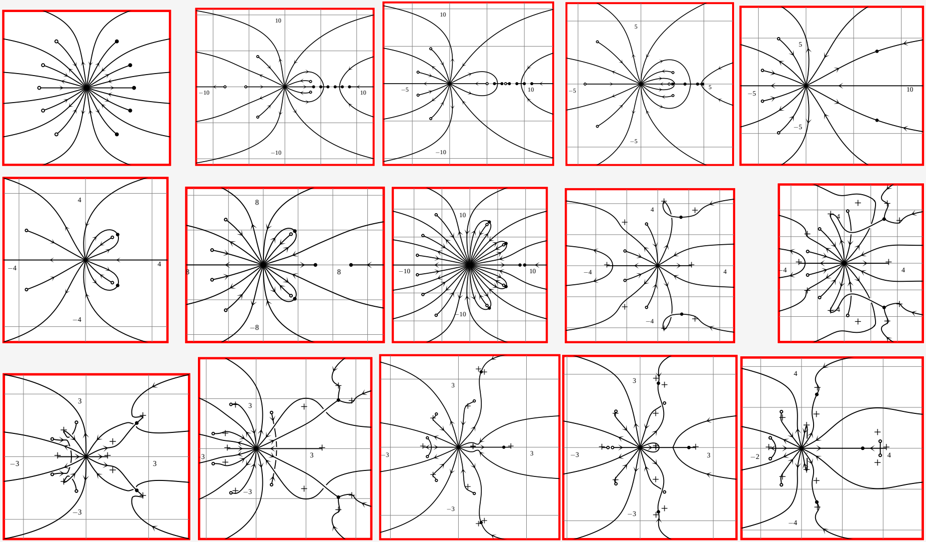


$$\left[(1-\tfrac{1}{5}z+\tfrac{2}{15}z^2)^2(1-\tfrac{1}{2}z)^2, -\tfrac{3}{2}, \tfrac{1}{2}+\tfrac{9}{10}z+\tfrac{89}{150}z^2+\tfrac{79}{300}z^3+\tfrac{437}{3600}z^4+\tfrac{71}{1200}z^5+\tfrac{7}{288}z^6\right]$$





$$\left[(1-\tfrac{1}{5}z+\tfrac{2}{15}z^2)^2(1-\tfrac{1}{3}z)^2, -\tfrac{3}{2}, \tfrac{1}{2}+\tfrac{17}{30}z+\tfrac{179}{900}z^2-\tfrac{1}{60}z^3-\tfrac{73}{2160}z^4-\tfrac{89}{10800}z^5+\tfrac{199}{64800}z^6\right]$$



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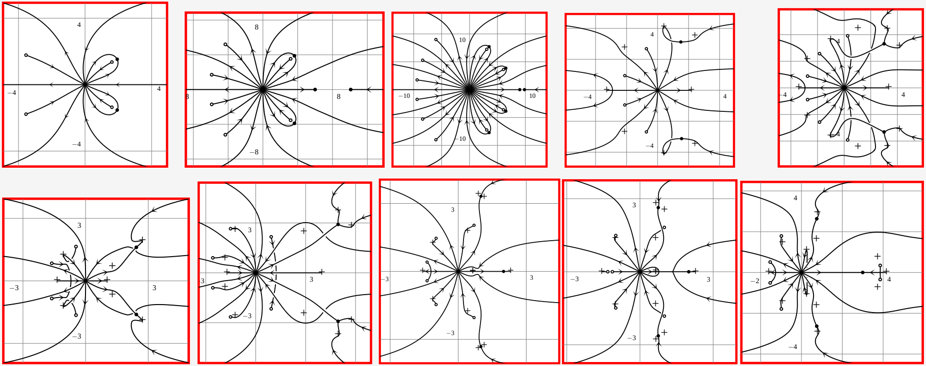

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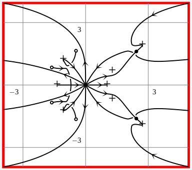

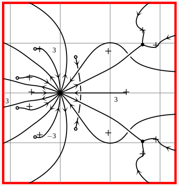

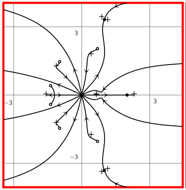

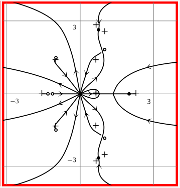

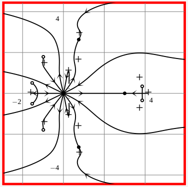

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