Order and stability for general linear methods

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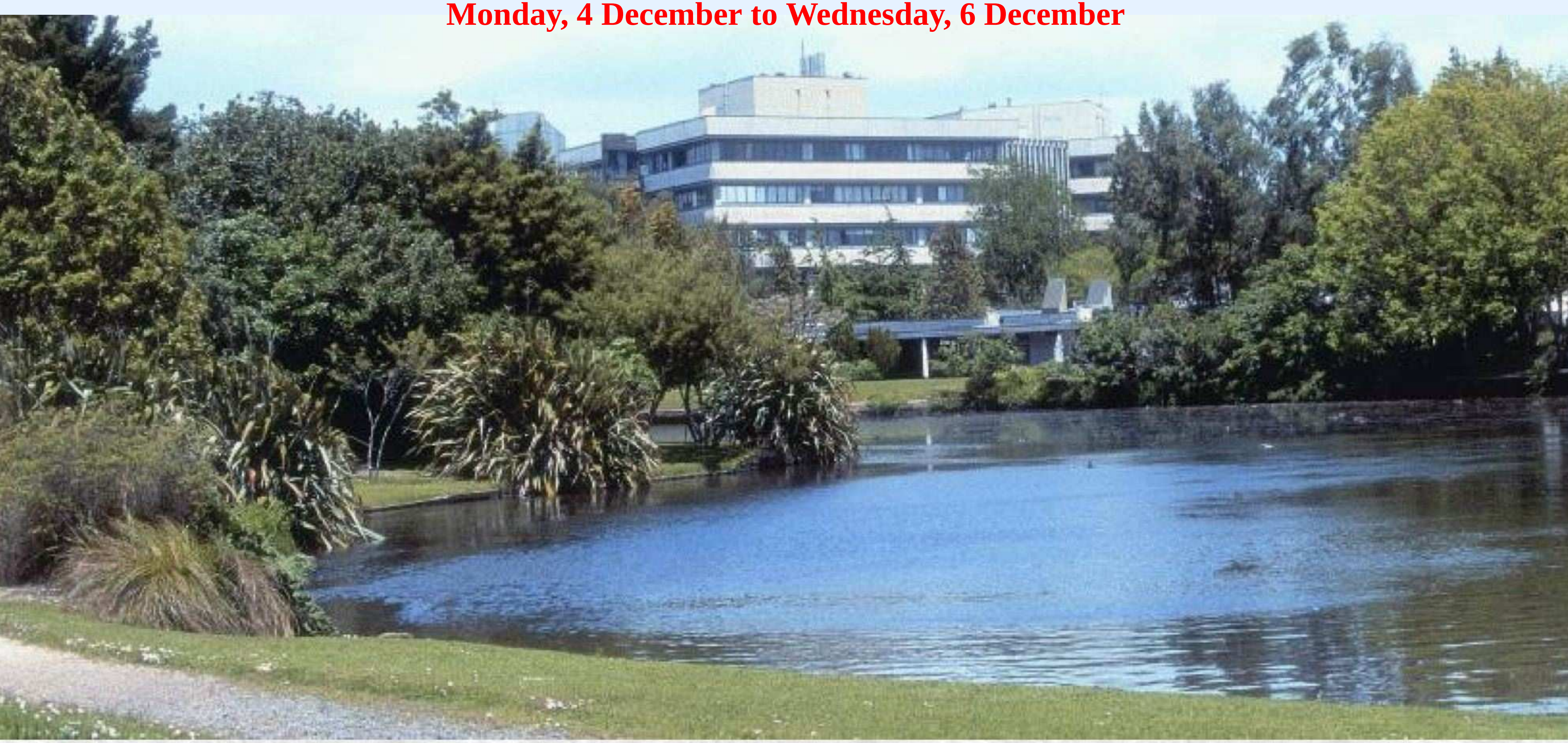

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Padé approximations to the exponential function

Given non-negative integers n_0, n_1 a rational function $N(z)/D(z)$ is the $[n_0, n_1]$ Padé approximation to the exponential function if

$$\frac{N(z)}{D(z)} = \exp(z) + O(z^{p+1}),$$

where $\deg(D) = n_0, \quad \deg(N) = n_1, \quad p = n_0 + n_1$.

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Some examples are

p	n_0	n_1	$D(z)$	$N(z)$
1	0	1	1	$1+z$
1	1	0	$1-z$	1
2	0	2	1	$1+z+\frac{1}{2}z^2$
2	1	1	$1-\frac{1}{2}z$	$1+\frac{1}{2}z$
2	2	0	$1-z+\frac{1}{2}z^2$	1

Generalized Padé approximations to exponential

Given a sequence of integers $[n_0, n_1, \ldots, n_r]$, consider a sequence of polynomials

$$(P_0, P_1, \ldots, P_r),$$

with degrees n_0, n_1, $\ldots$, n_r, and the corresponding polynomial in two variables

$$\Phi(w, z) = P_0(z)w^r + P_1(z)w^{r-1} + \cdots + P_r(z).$$

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$$p = \sum_{i=0}^{r}(n_i + 1) - 1.$$

To within a scale factor, $(P_0, P_1, \dots, P_r)$ is unique.

This is an approximation to the exponential function in the sense that the polynomial equation

$$P_0(z)w^r + P_1(z)w^{r-1} + \cdots + P_r(z) = 0,$$

regarded as a function of w, has solutions some of which are approximations to $\exp(z)$.

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Under certain conditions, there is a single "principal solution" $w(z)$, which exists in a neighbourhood of 0, such that

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In the case $r = 1$, $w = -P_1(z)/P_0(z)$ is the $[n_0, n_1]$ Padé approximation to $\exp(z)$.

Generalized Padé approximations arise naturally when a numerical method is applied to the linear problem

$$y' = qy, \qquad (\star)$$

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If for any z in the left half-plane, all zeros of $\Phi(w, z)$ are in the unit disc then Φ is said to be "A-stable".

This is an important property of numerical methods for solving "stiff" problems.

Examples of generalized Padé approximations

The first example is the $[2,0,0,0]$ approximation

$$(1 - \tfrac{66}{85}z + \tfrac{18}{85}z^2)w^3 - \tfrac{108}{85}w^2 + \tfrac{27}{85}w - \tfrac{4}{85}.$$

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This approximation is related to the Obreshkov method

$$y_n = \tfrac{66}{85}hy'_n - \tfrac{18}{85}h^2y''_n + \tfrac{108}{85}y_{n-1} - \tfrac{27}{85}y_{n-2} + \tfrac{4}{85}y_{n-3},$$

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The order can also be verified using Taylor’s theorem.

The second example has order 5 and corresponds to the Obreshkov method

$$y_n = \frac{60}{83} h y_n' - \frac{72}{415} h^2 y_n'' + \frac{576}{415} y_{n-1} - \frac{216}{415} y_{n-2} + \frac{64}{415} y_{n-3} - \frac{9}{415} y_{n-4},$$

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leading to the stability function

$$(1 - \tfrac{60}{83} z + \tfrac{72}{415} z^2) w^4 - \tfrac{576}{415} w^3 + \tfrac{216}{415} w^2 - \tfrac{64}{415} w + \tfrac{9}{415}.$$

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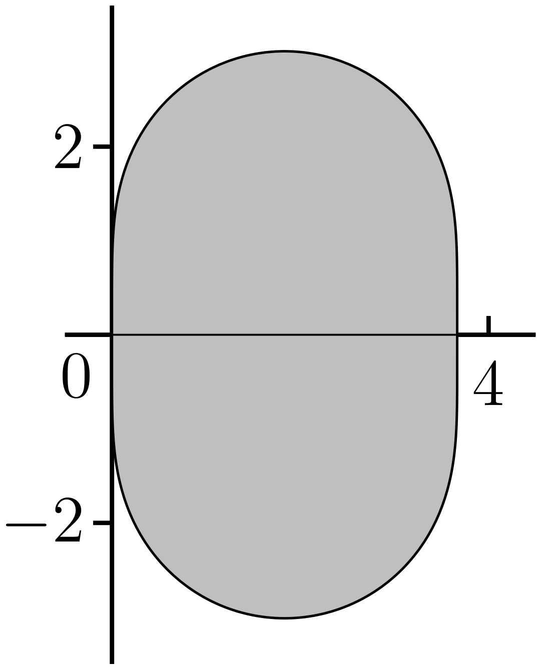
This is the $[2, 0, 0, 0, 0]$ approximation.

The stability regions of these two methods are the unshaded regions in the diagrams:



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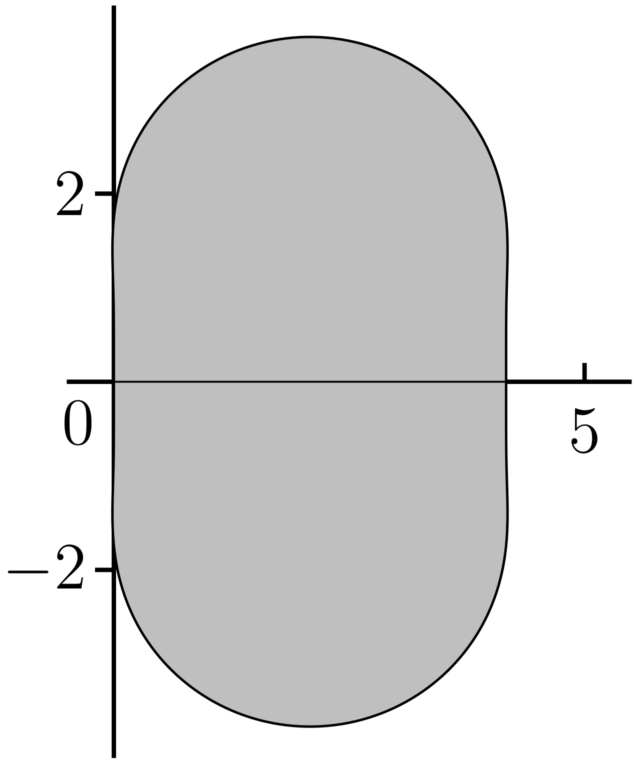

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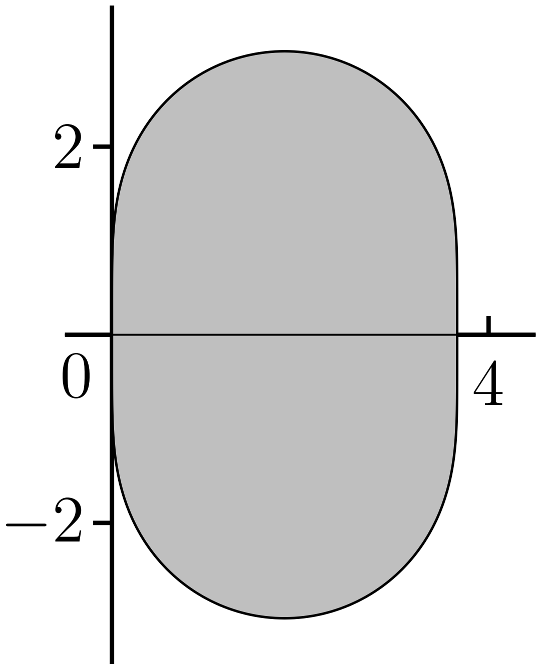

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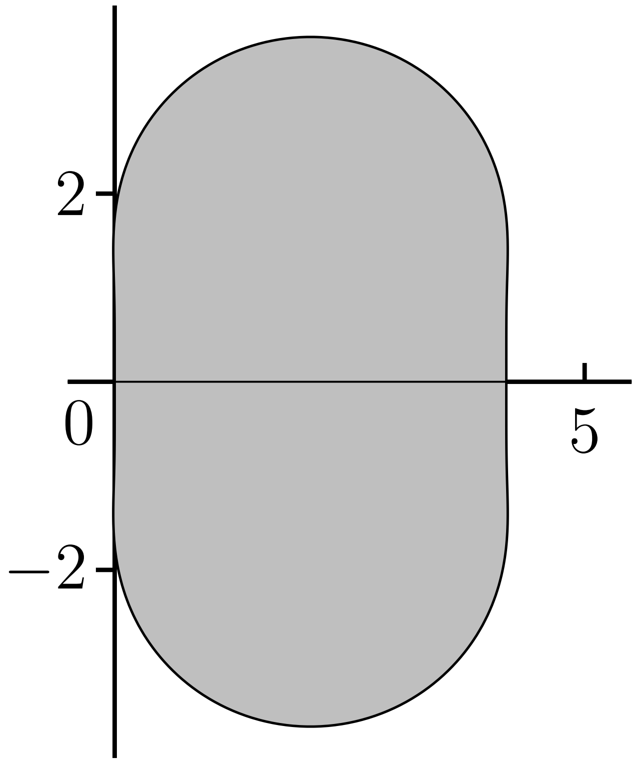

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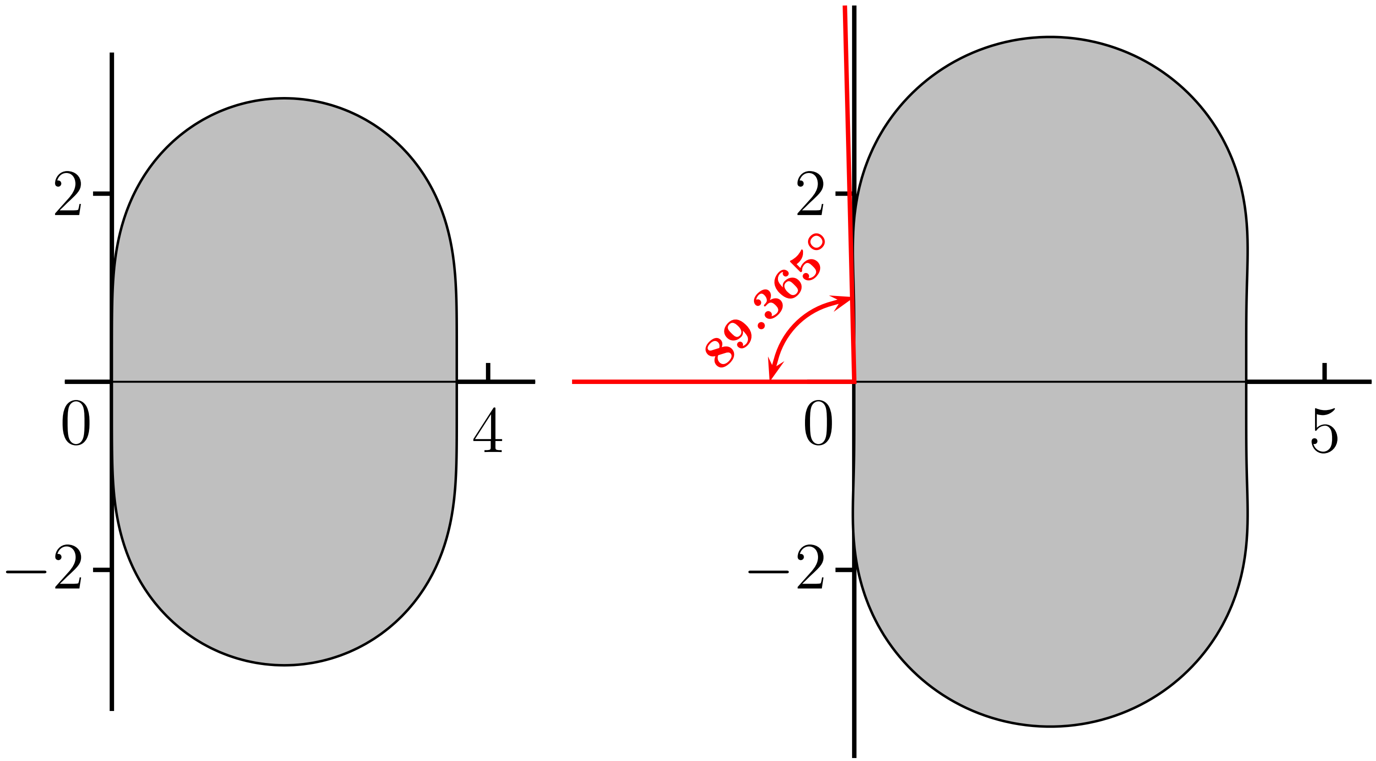

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The methods are A-stable and A$(89.365°)$-stable respectively.

Order stars and order arrows

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For order arrows we consider the set of (w, z) pairs satisfying $(\star)$, such that w is real and positive.

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We consider the example of the $[2, 1]$ Padé approximation for which

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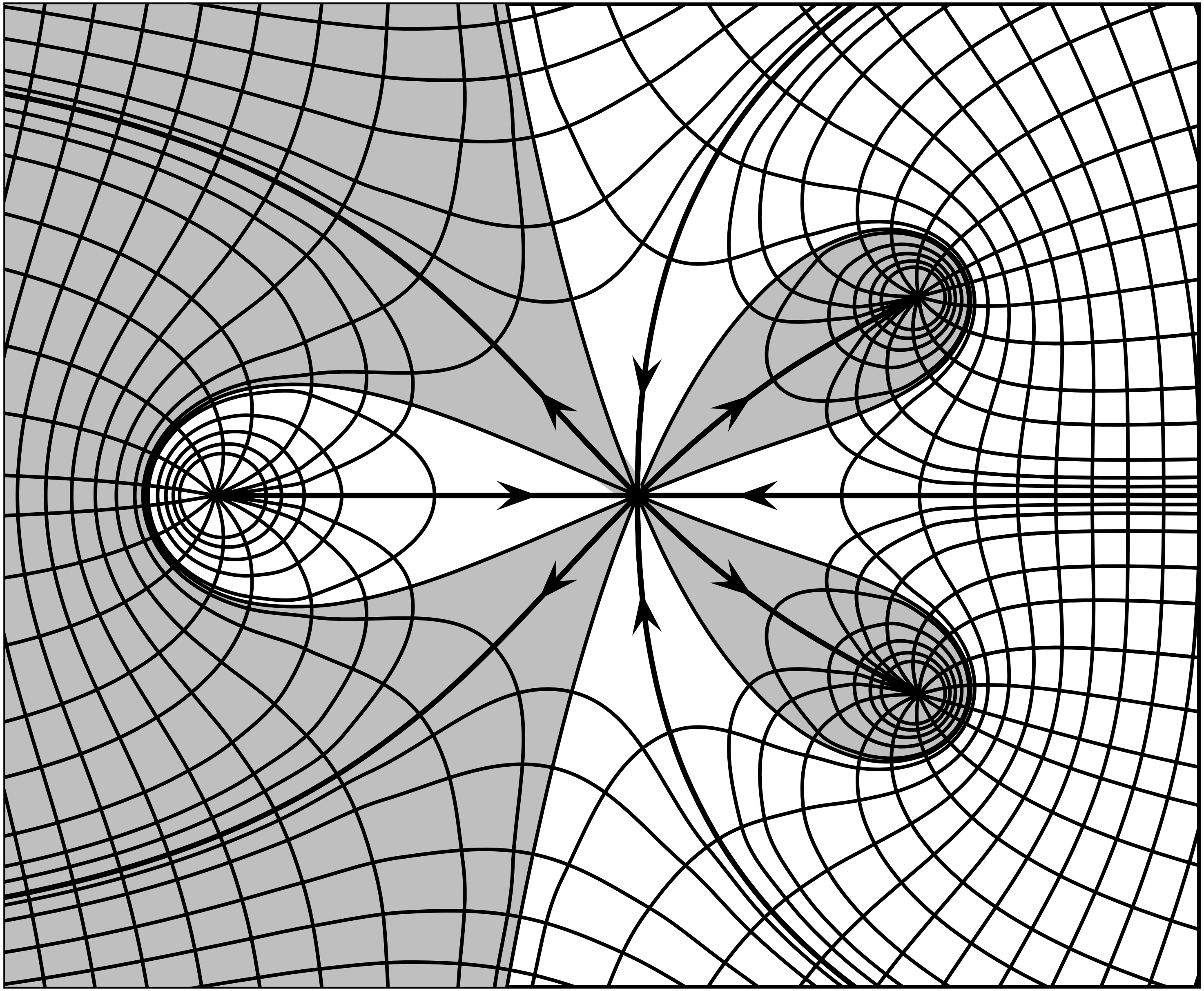
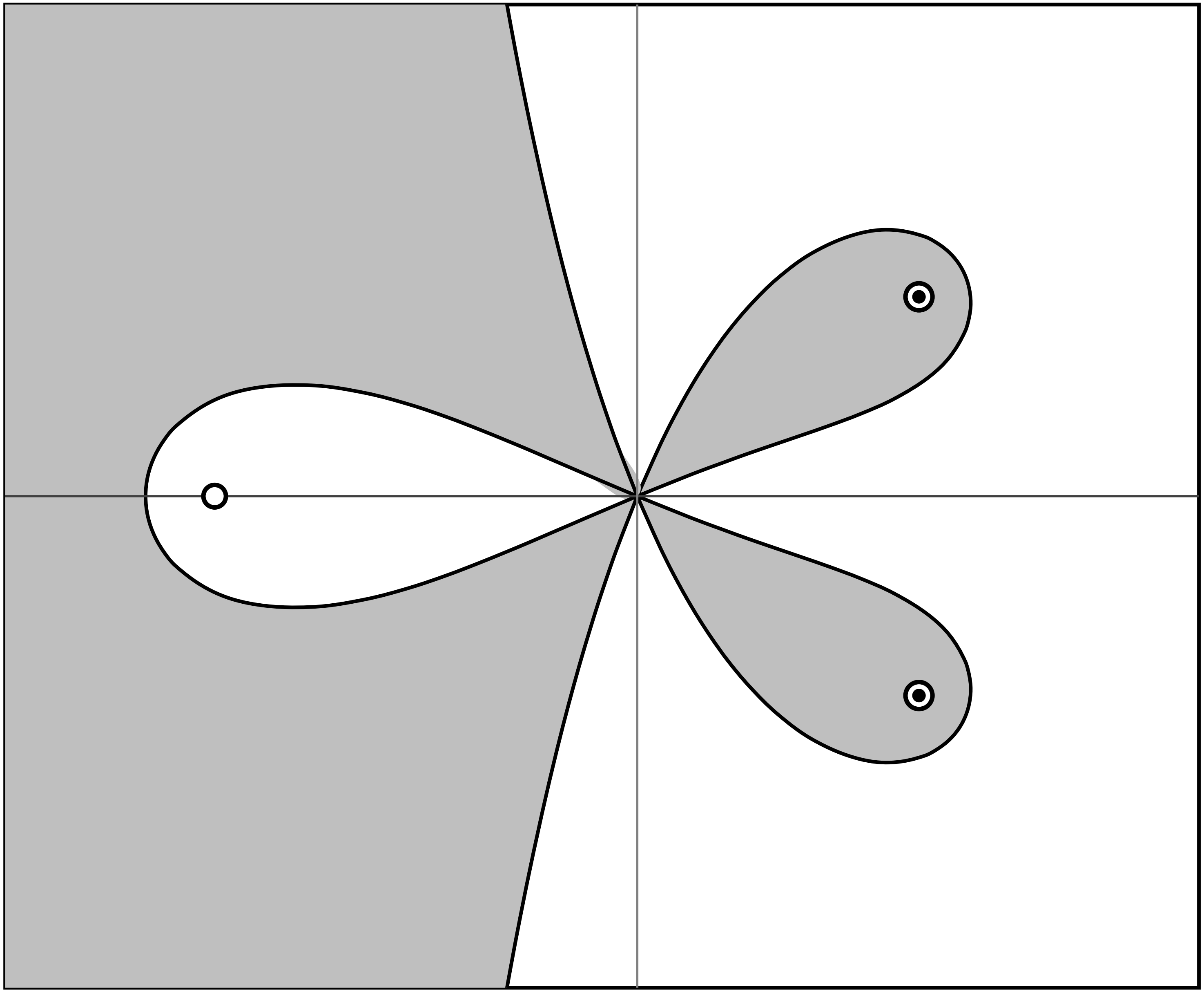
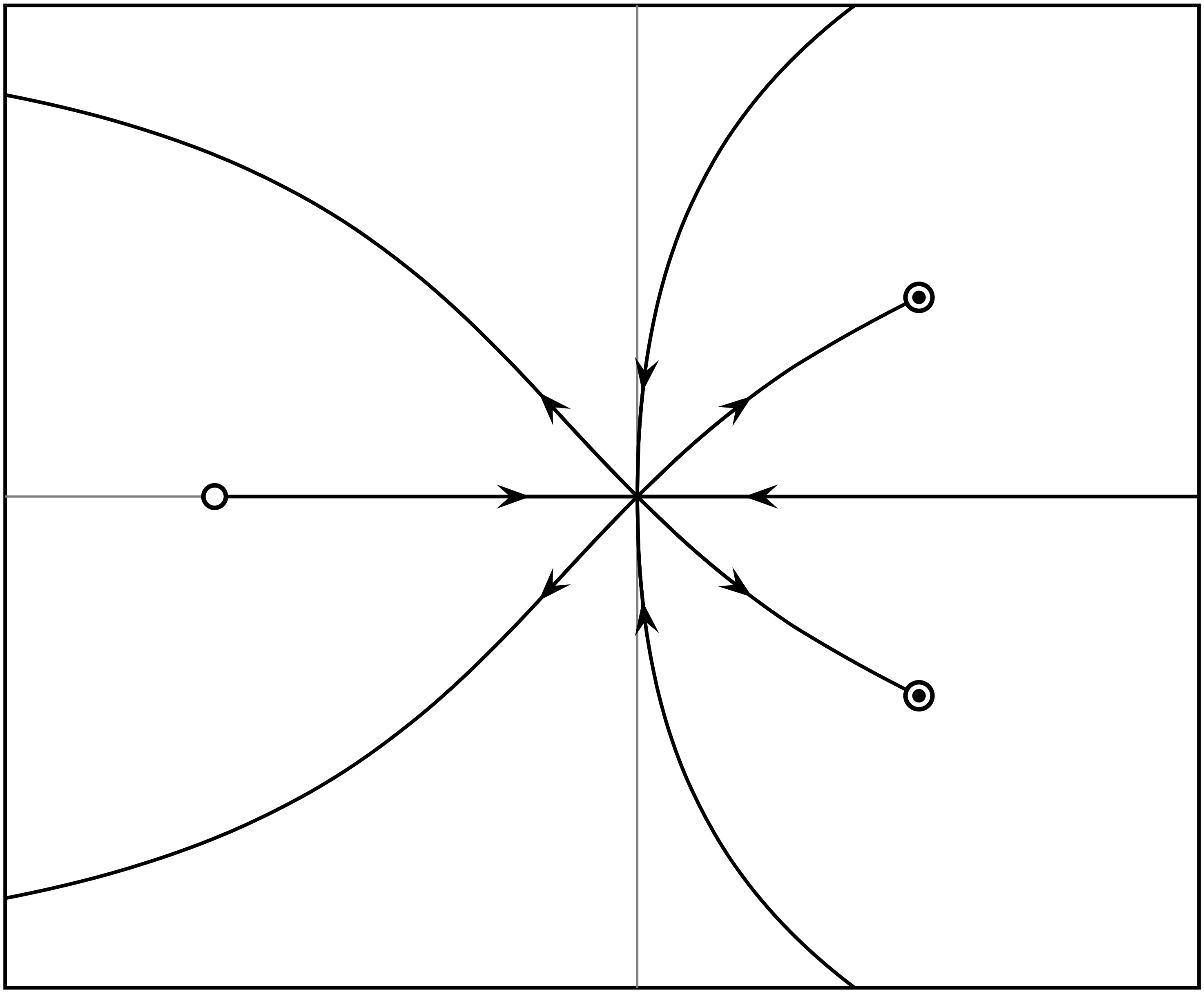
The figure on the next slide gives information on both the order star and the order arrows:



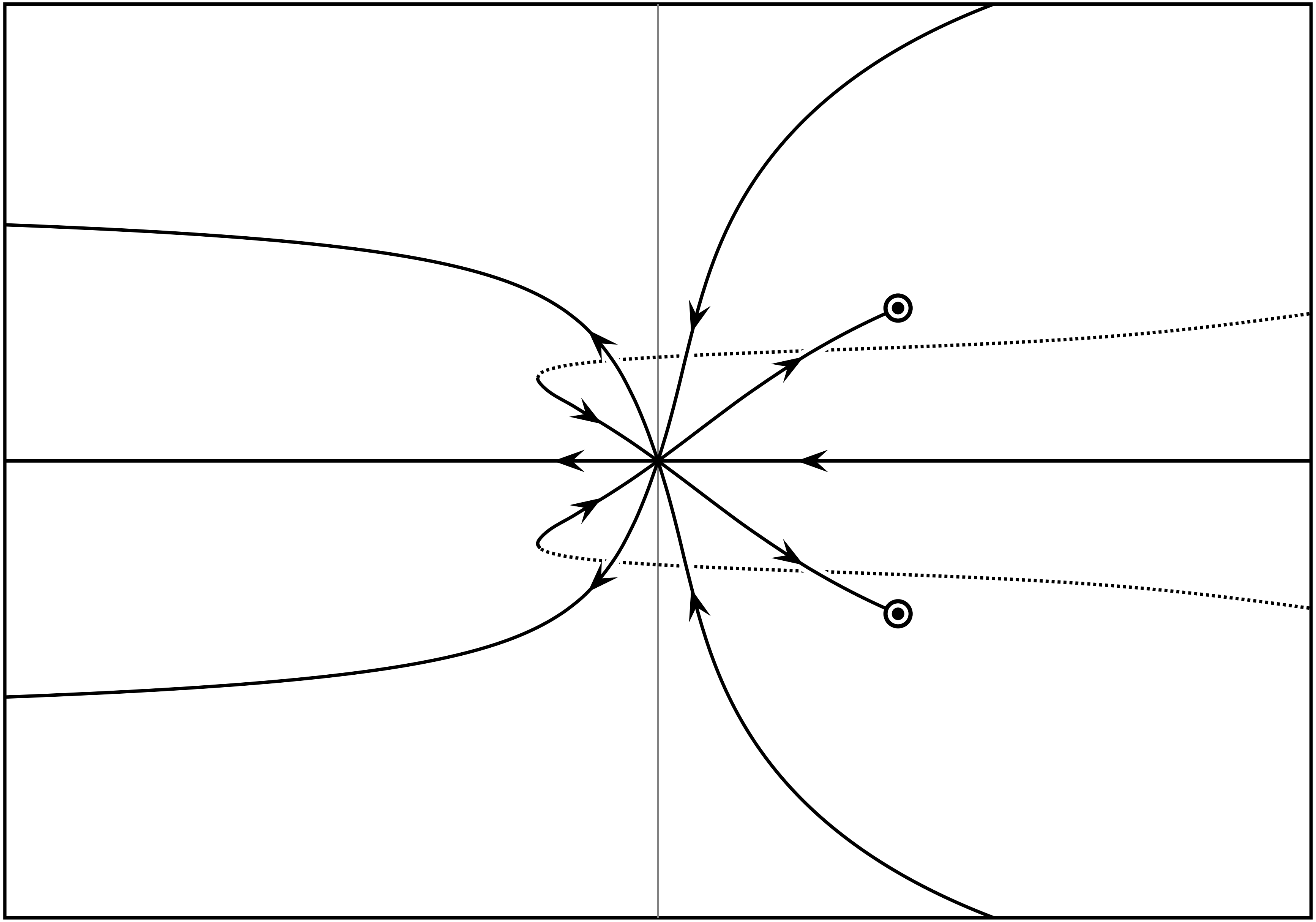
We can separate out the order star picture



And the order arrow picture



Now consider the $[2, 0, 0, 0]$ ***approximation***



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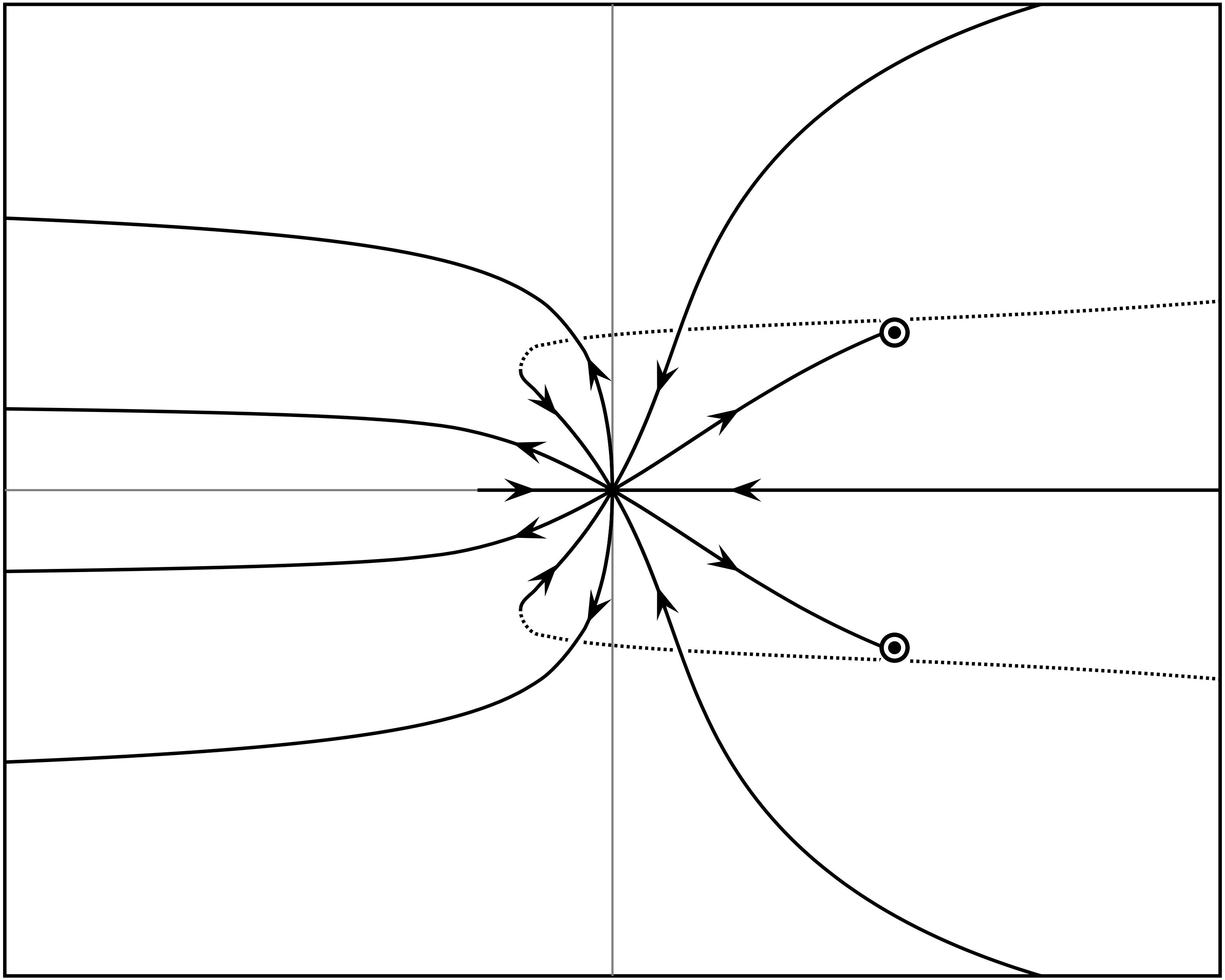

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This is similar to the observation that, in the order star analysis, a finger cannot overlap the imaginary axis if the method is to be A-stable.

In each case we also use the behaviour near zero of the locally defined function $w(z) = 1 + Cz^{p+1}$.

The Daniel-Moore theorem

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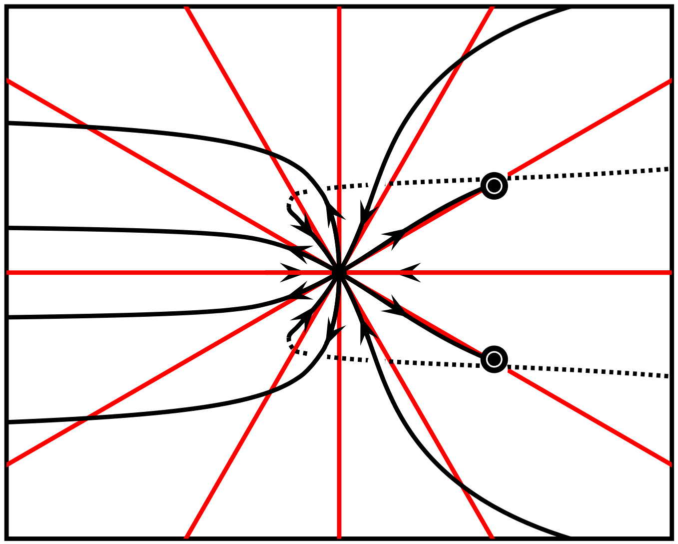

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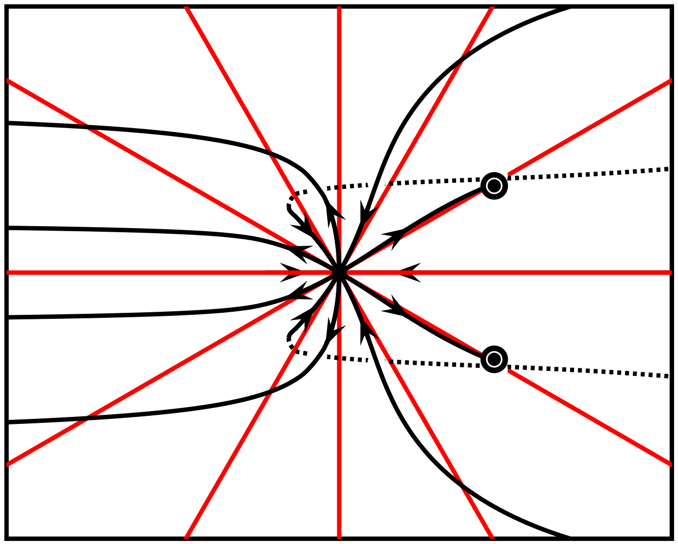

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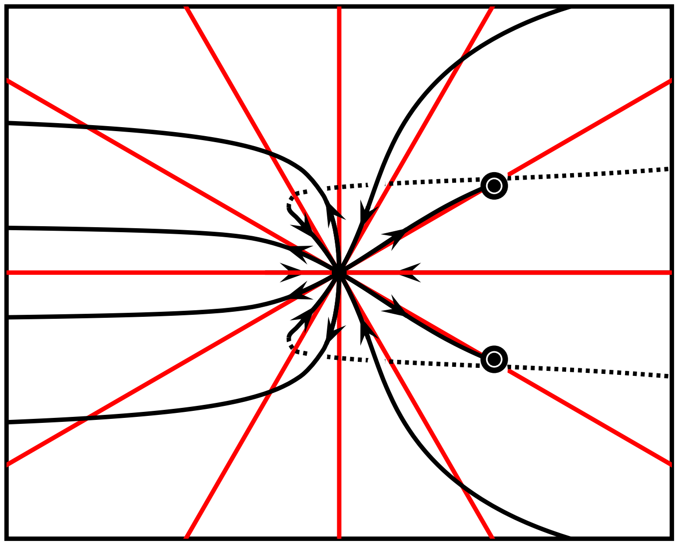

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Hence there exist up-arrows tangent to the imaginary axis.

The Ehle theorem

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This question will be discussed later.

Because adjacent up-arrows subtend an angle

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

and n_0 of them terminate at poles, the total angle subtended is at least

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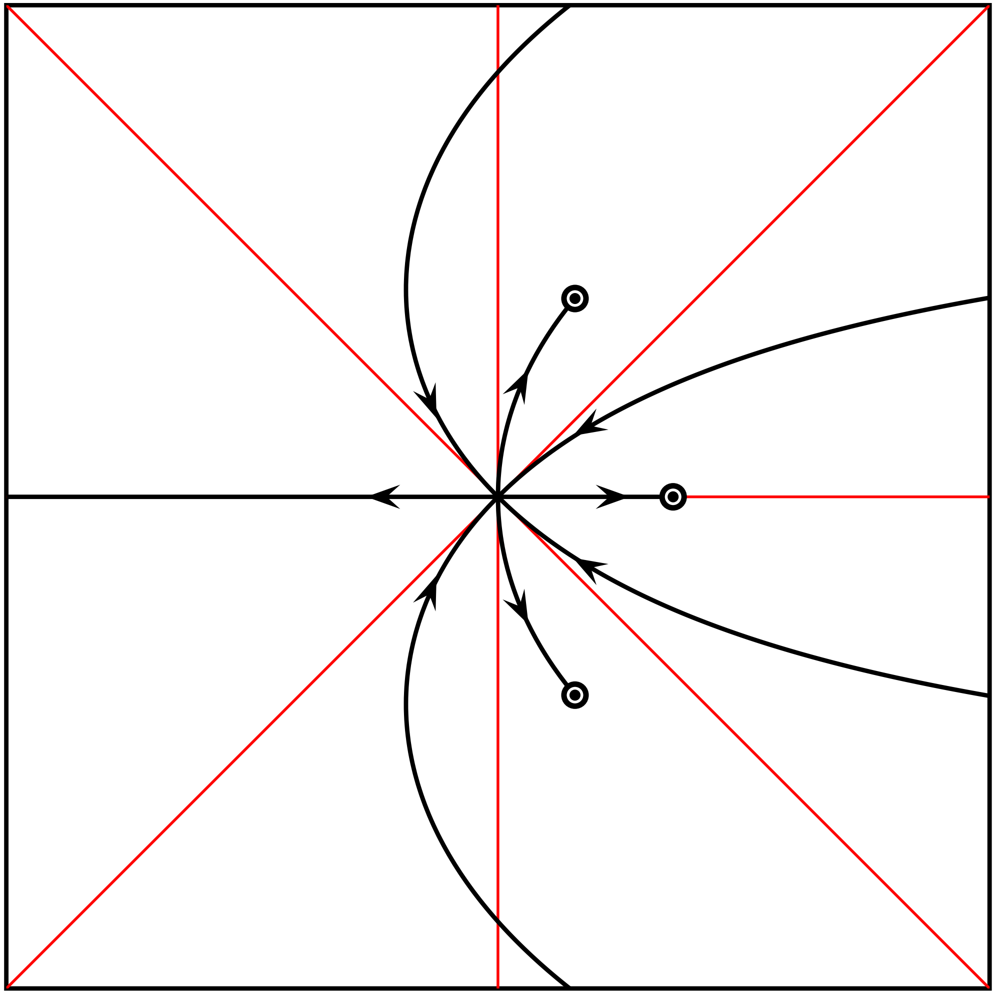
Hence, either up-arrows terminating at poles are tangential to the imaginary axis or protrude into the left half-plane.

In the latter case, there are poles in the left half-plane or an up-arrow crosses back across the imaginary axis.

We will illustrate this result in the $[3, 0]$ case.



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But in the general case, where everything happens on a Riemann surface, we cannot use this argument in a simple way.

Our approach will be based on modified arrows and homotopy.

Modifications to the arrow system

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We will remove all poles by replacing a polynomial sequence

$$(P_0, P_1, \dots, P_r) \quad \text{by} \quad (-t, P_0, P_1, \dots, P_r)$$

and take the limit as $t \to 0$. Although the limit does not exist on the Riemann surface, its projection onto the Z plane does.

Modifications to the arrow system

We want to simplify what happens when an arrow interacts with a stagnation point, a branch point, a pole or a zero.

We will adopt a "pass on the right" convention by moving each arrow, drawn in the increasing w sense, by an infinitesimal amount to the right.

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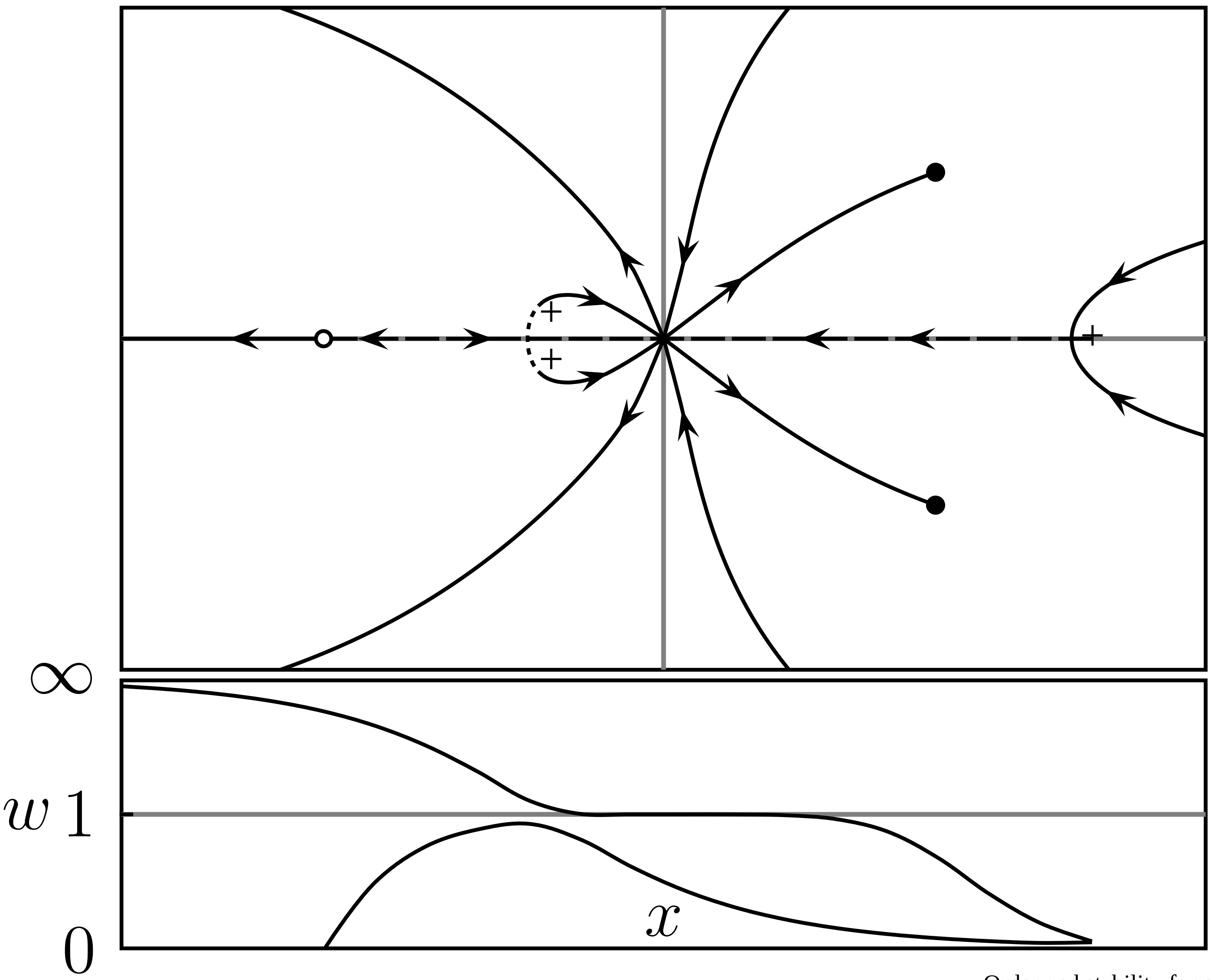
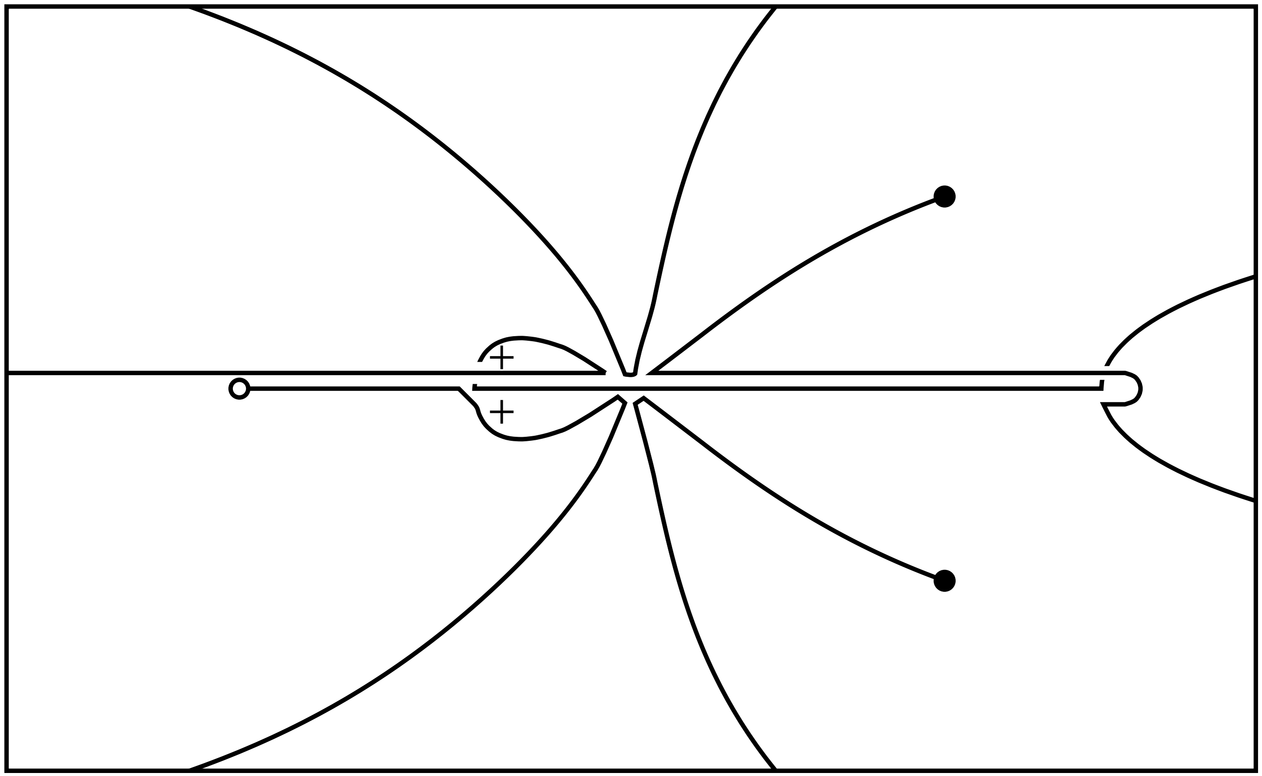
Do the same with zeros.

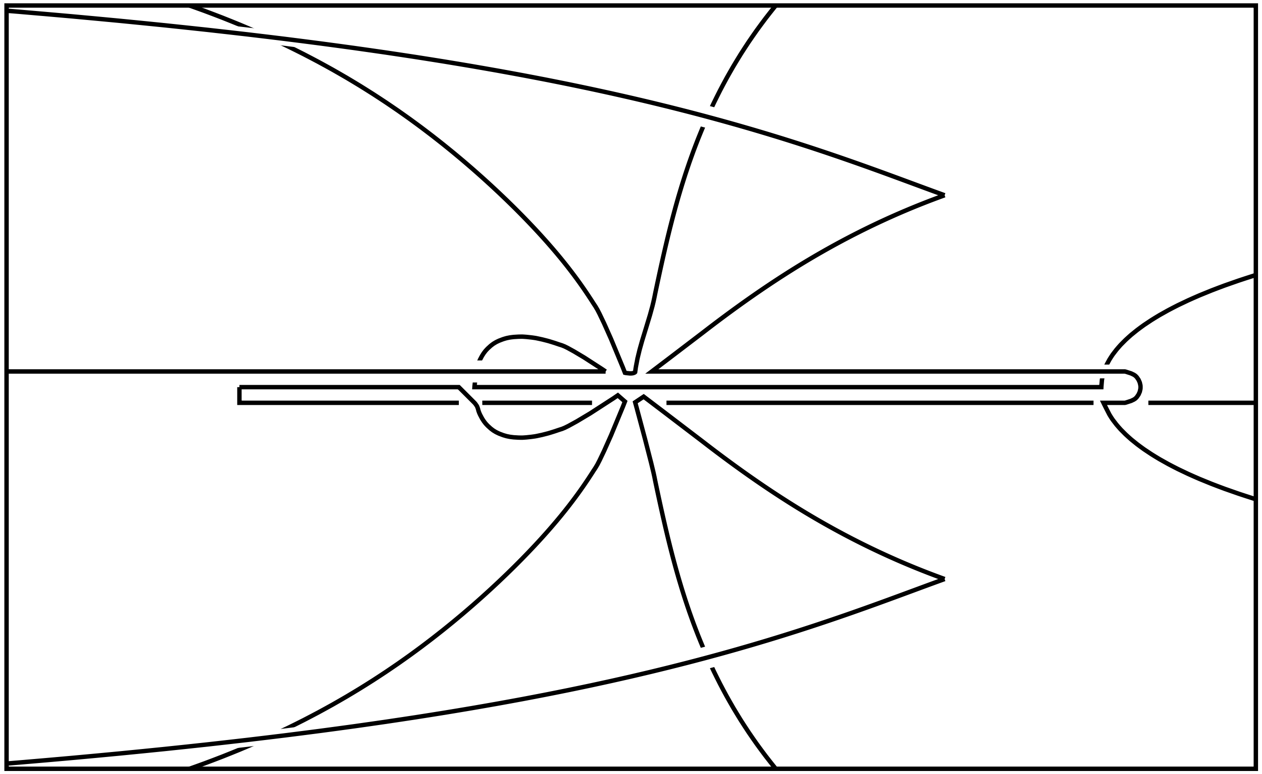
We will illustrate these ideas with the $[2, 0, 1]$ approximation



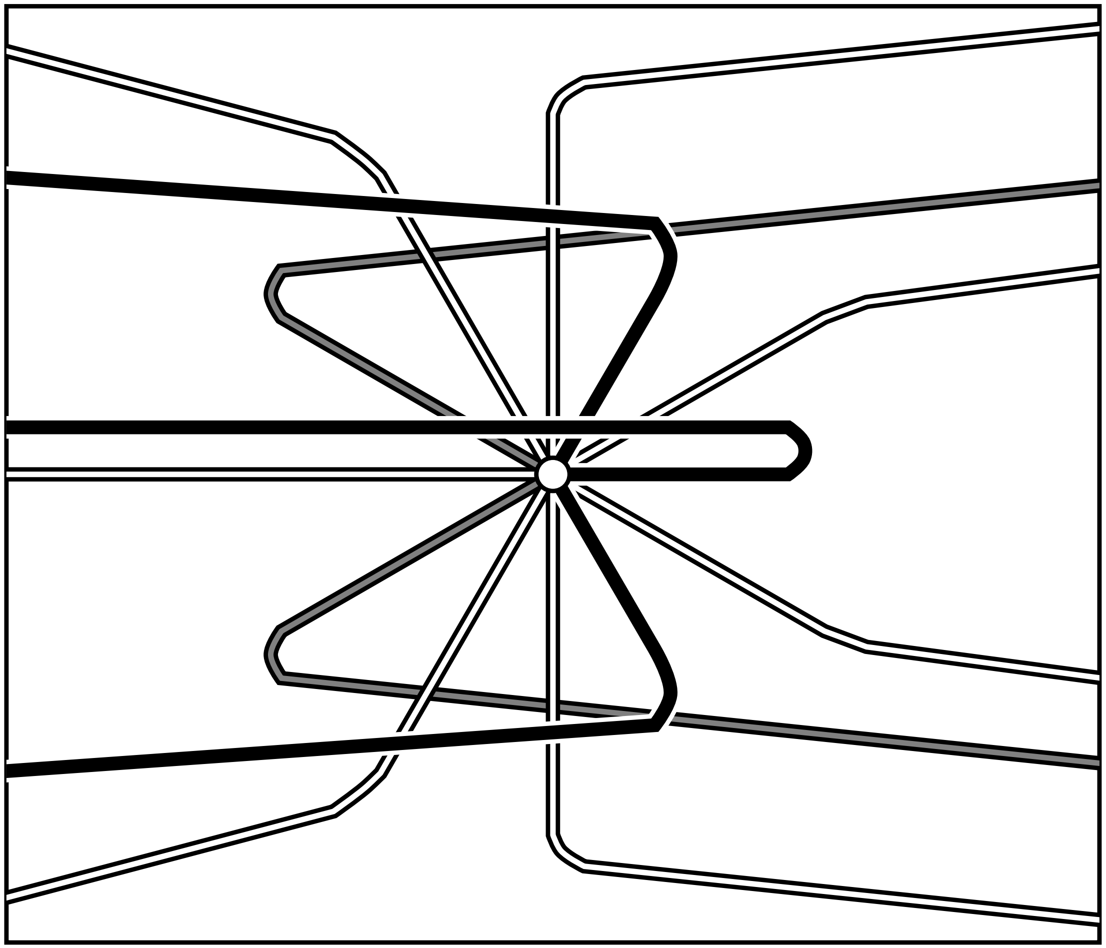
Use right-oriented arrows



Replace poles and zeros using extra sheets



Now a generic diagram for $n_0 = 3$, $p = 5$:



It could be $[3, 2]$, $[3, 1, 0]$, $[3, 0, 1]$ etc

The Butcher–Chipman conjecture

After extensive searching, Fred Chipman and I formulated the following audacious statement:

For generalized Padé approximations to the exponential function, the necessary condition for A-stability of linear Padé approximations also holds in the general case:

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- The proof outline I will give makes use of homotopy from lower order approximations

Proof outline

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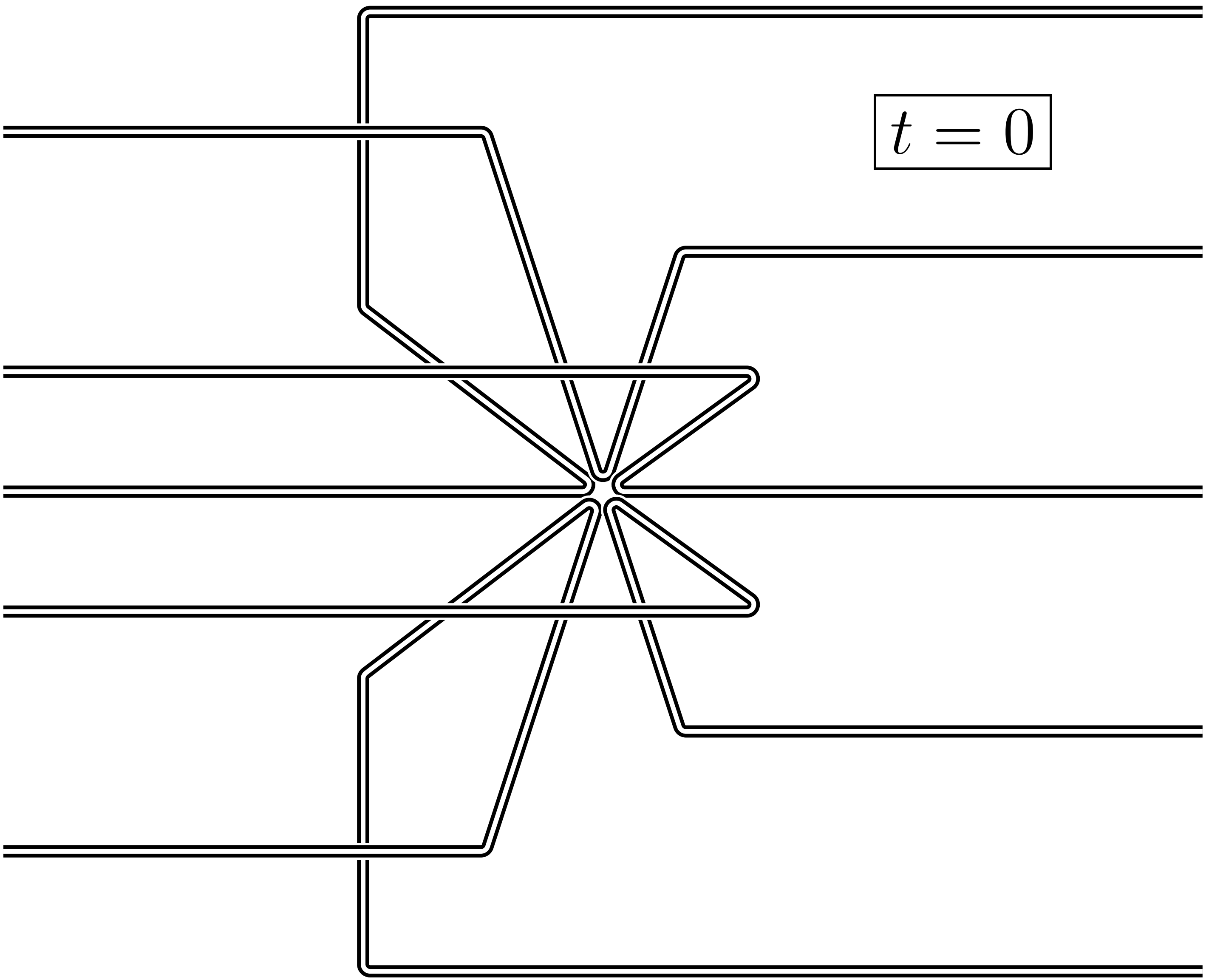
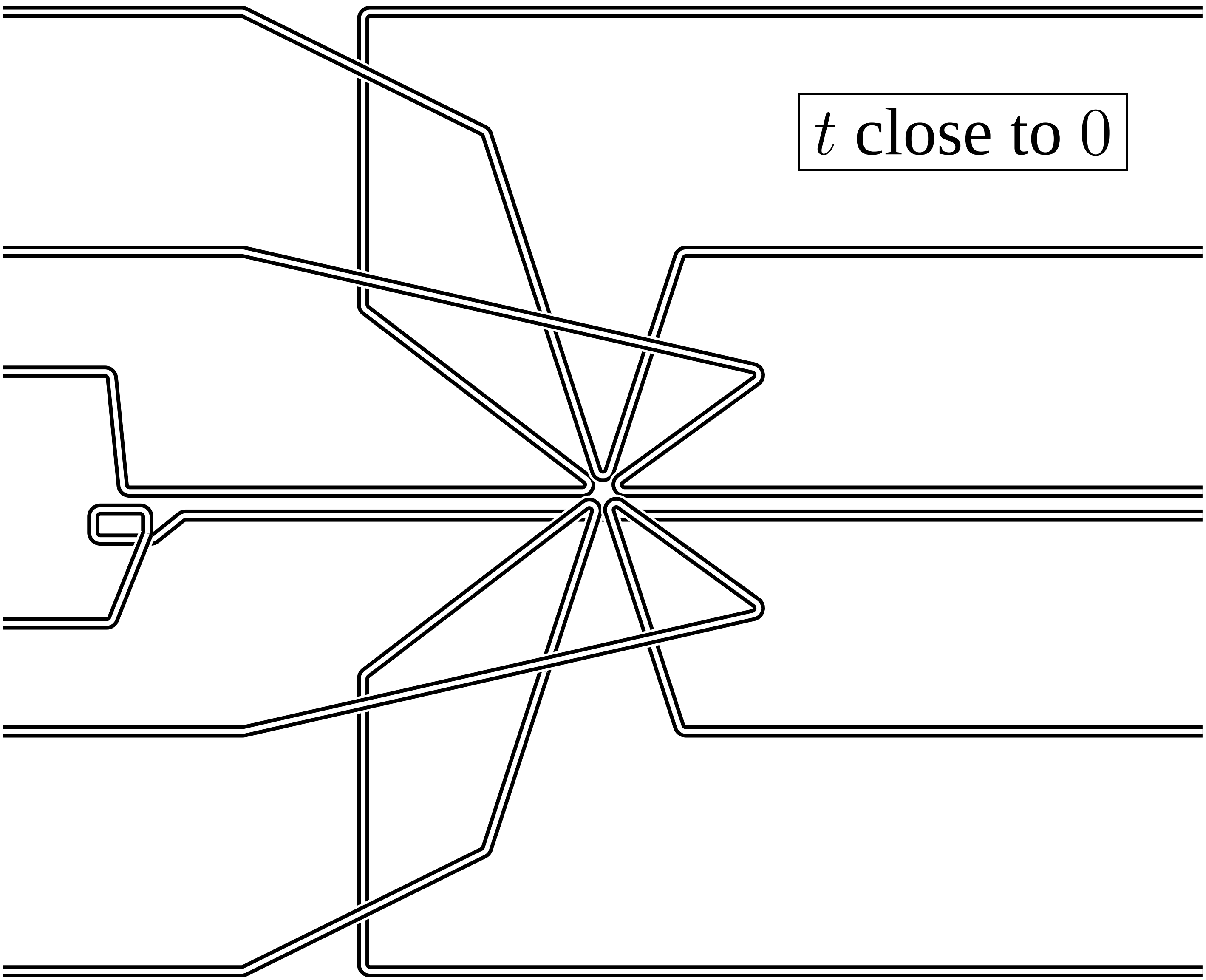
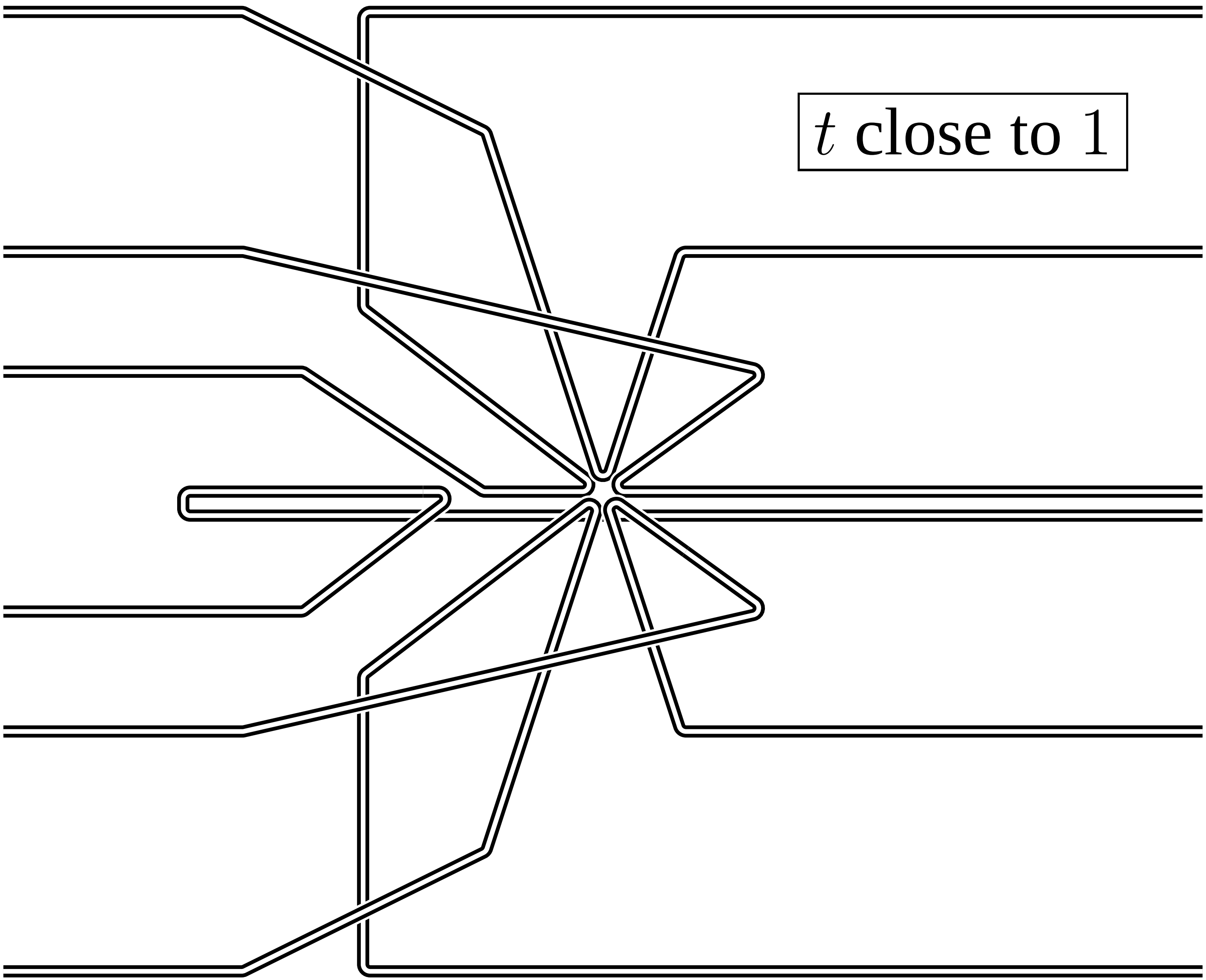
First see how the order increases as t approaches 1


$t = 0$


t close to 0


t close to 1

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This is impossible, because of the uniqueness of generalized Padé approximations.

Thank you