Methods for Computing Complex Singularity Structure in DEs

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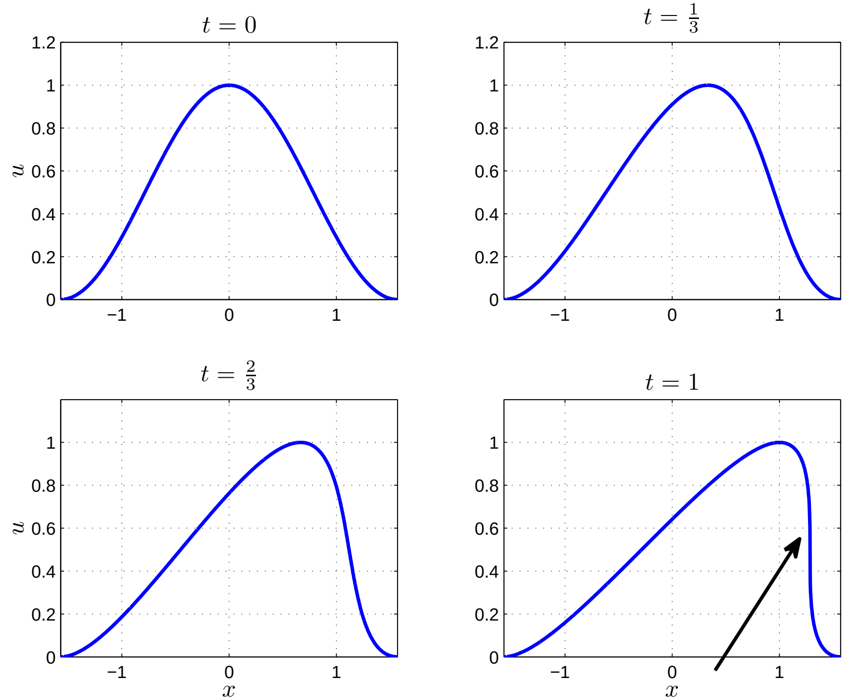
Motivational Example: Burgers' Equation $u_t + u\,u_x = 0$

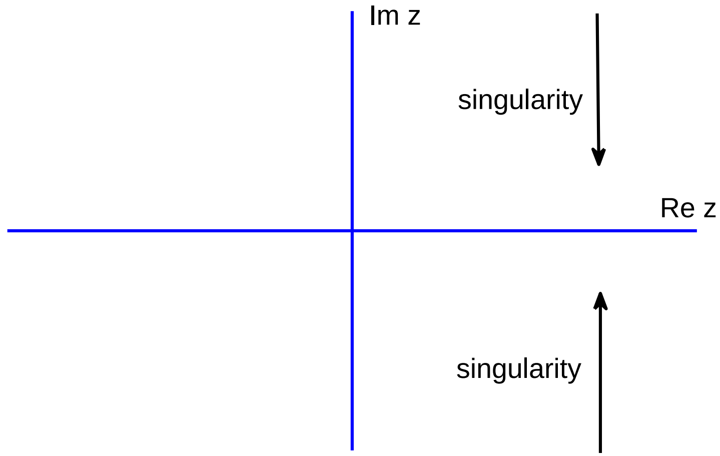
$$u(x,0) = \cos^2 x, \quad -\frac{1}{2}\pi \leq x \leq \frac{1}{2}\pi$$



Shock forms at $(x, t) = (1.285, 1)$

Bessis & Fournier [1984]

Explanation of shock in terms of complex singularities that reach the real axis



How to compute this?

Plan for the talk:

Part I: PDEs (published work (*))

(a) Burgers' Equation

(b) A Nonlinear Heat Equation

(*) JACW, "Computing the Dynamics of Complex Singularities of Nonlinear PDEs", SIAM J. Appl. Dyn. Syst., 2003

Part II: ODEs (unpublished)

(a) Painlevé

(b) Chazy

General Strategy:

(A) Solve ODE/PDE using Fourier or Chebyshev spectral method

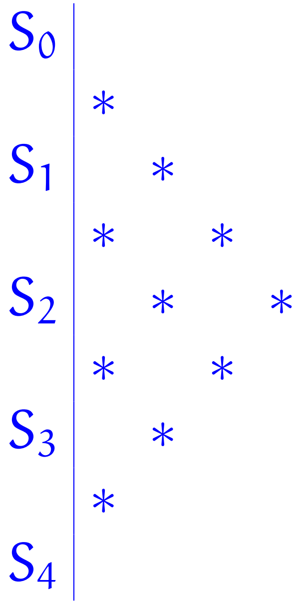
(B) Continue numerical solution into the complex plane using Padé approximation, implemented via the ϵ-algorithm

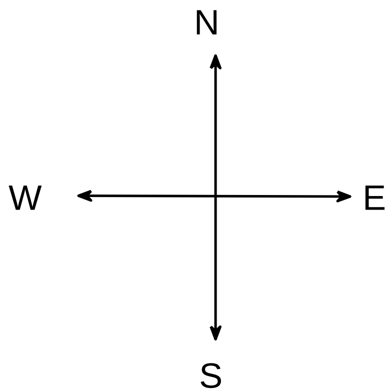
Review of Padé approximation and ϵ-algorithm:

$[L, M]$ Padé approximation of $f(z) = \sum_{k=0}^{\infty} c_k z^k$ is defined by

$$r_{L,M}(z) = \frac{a_0 + a_1 z + \cdots + a_L z^L}{1 + b_1 z + \cdots + b_M z^M} \iff f(z) - r_{L,M}(z) = O(z^{L+M+1})$$

ϵ-algorithm:
Wynn
[1961]





$$E \longleftarrow W + \frac{1}{S - N}$$

Part I: PDEs

(A) Solve PDE using Fourier spectral method (assume 2π-periodicity)

$$u(x,t) \approx \sum_{n=-N}^{N} c_n(t) e^{inx}$$

Burgers:

$$u_t + \tfrac{1}{2}(u^2)_x = 0$$

$$\frac{dc_n}{dt} + \tfrac{1}{2} in \sum_{\substack{j+k=n \\ |j|,|k|\leq N}} c_j c_k = 0$$

Nonlinear Heat:

$$u_t - u_{xx} - u^2 = 0$$

$$\frac{dc_n}{dt} + n^2 c_n - \sum_{\substack{j+k=n \\ |j|,|k|\leq N}} c_j c_k = 0$$

Integrate in time using ODE solver. In this case MATLAB ODE45.

How to continue $u(x,t) \approx \sum_{n=-N}^{N} c_n(t) e^{inx}$ into complex x-plane?

(B) Continue numerical solution into the complex plane

Fourier-Padé approximation: define $z_+ = e^{ix}, \quad z_- = e^{-ix}$:

$$\sum_{n=-N}^{N} c_n e^{inx} = \sum_{n=0}^{N} c_n z_+^n + \sum_{n=0}^{N} c_{-n} z_-^n - c_0$$

Convert two series on the right to Padé form using ϵ-algoritm.

(Similar to Driscoll & Fornberg [2001])

(a) Burgers

$$u_t + \tfrac{1}{2}(u^2)_x = 0$$

With the special initial condition

$$u(x,0) = e^{ix}$$

an explicit solution in terms of Lambert's W-function is obtained

$$u = f(x - ut) \quad \Longrightarrow \quad u = e^{ix}e^{-iut} \quad \Longrightarrow \quad \underbrace{(iut)}_{w}\, e^{iut} = \underbrace{ite^{ix}}_{z}$$

$$\Longrightarrow \quad w\, e^{w} = z \quad \Longrightarrow \quad w = W(z) \quad \Longrightarrow \quad u(x,t) = \frac{1}{it} W(ite^{ix})$$

Singularity structure of W-function is well understood.
(See, e.g., Corless, Gonnet, Hare, Jeffrey, Knuth [1996])

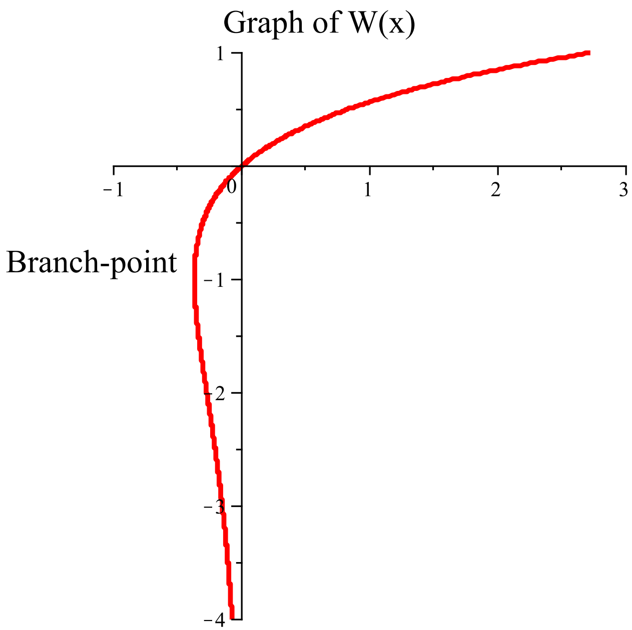
Branch-point at $x = -\frac{1}{e}$

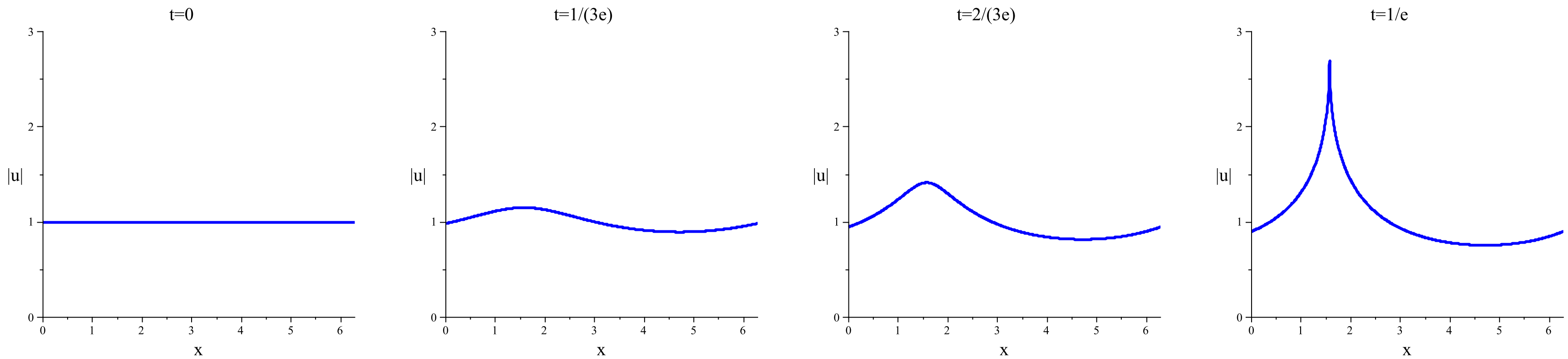
Transplant this to Burgers on $[0, 2\pi]$

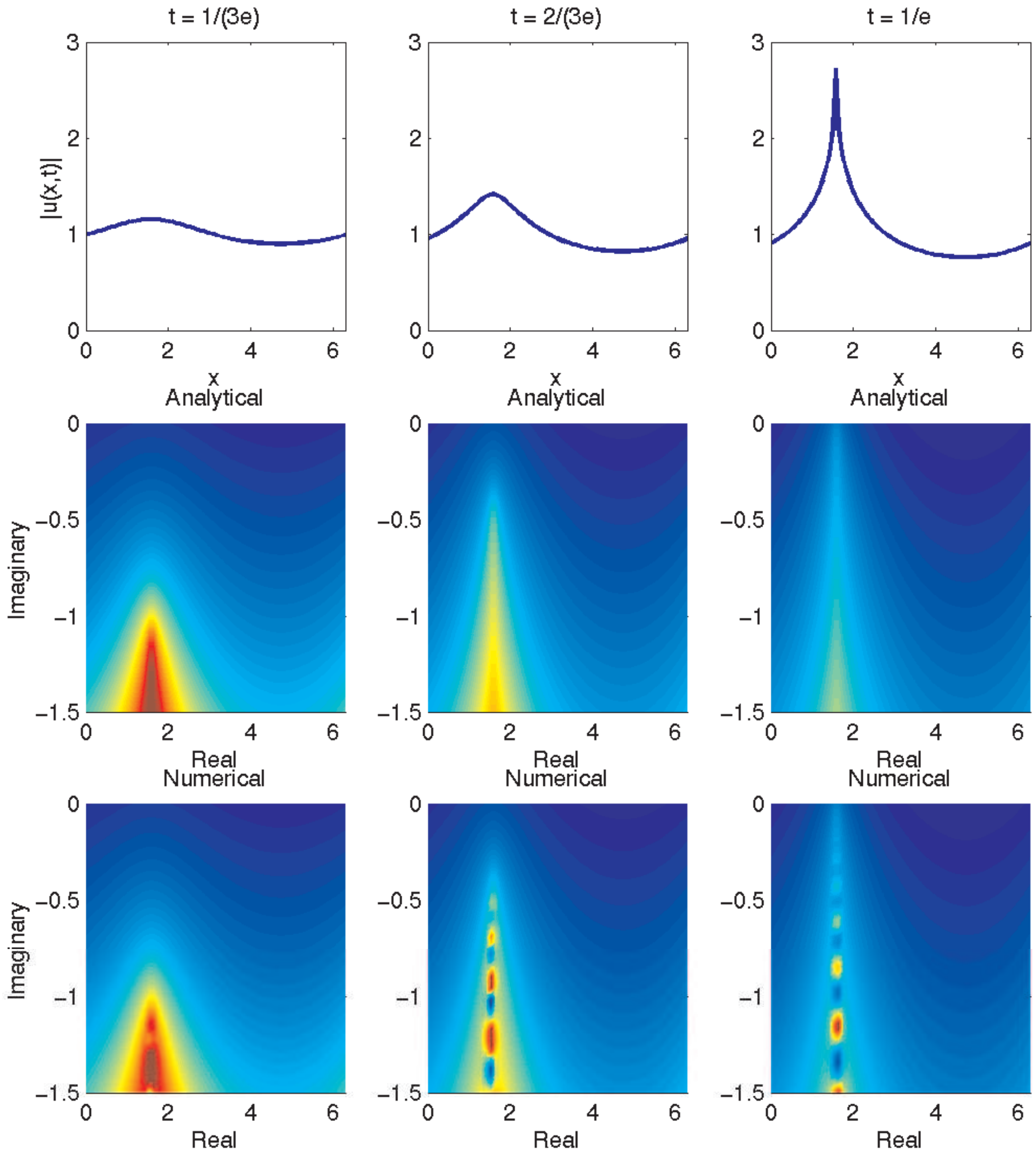
$$ite^{iz} = -\frac{1}{e} \quad \Longrightarrow \quad z = \frac{\pi}{2} + i(1 + \log t)$$

Shock forms at

$$(x, t) = \left(\frac{\pi}{2}, \frac{1}{e}\right)$$



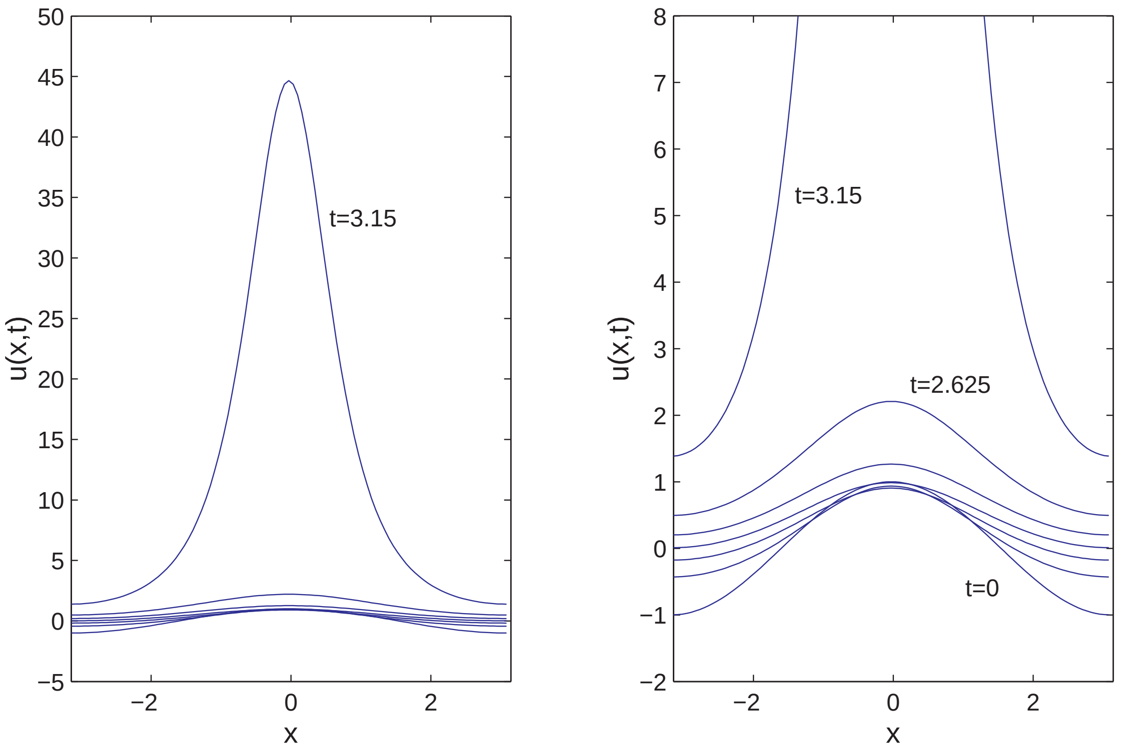


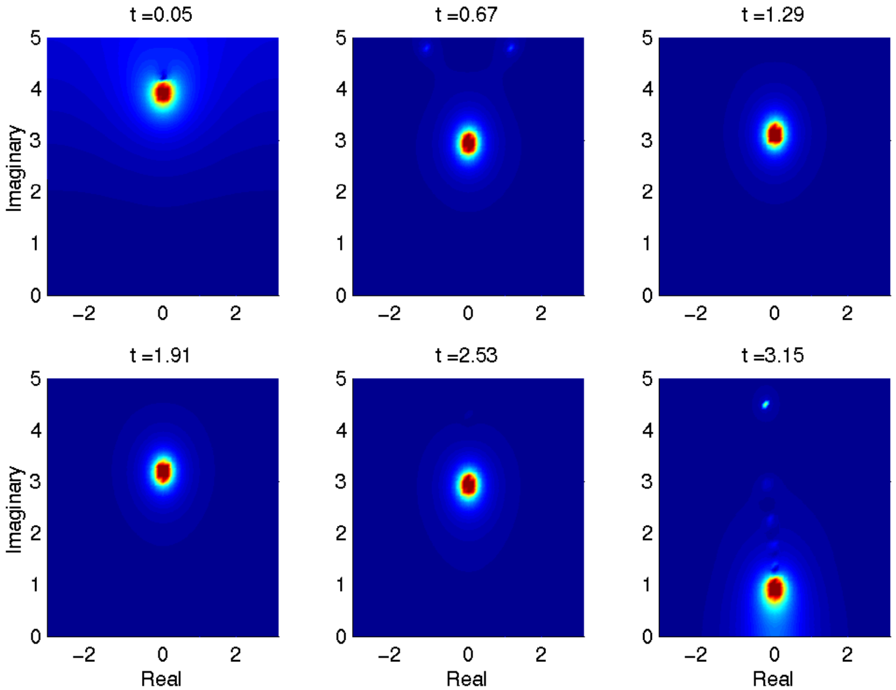

t = 1/(3e)
t = 2/(3e)
t = 1/e
|u(x,t)|
x
Analytical
Numerical
Imaginary
Real

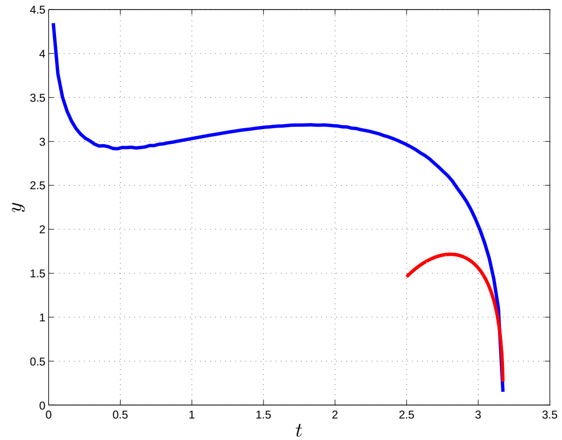
(a) Nonlinear Heat Equation on $[0, 2\pi]$

$$u_t - u_{xx} - u^2 = 0$$
$$u(x, 0) = \cos x$$

Nonlinear blow-up near $t = 3.17$







Red curve is theoretical asymptotic estimate

$$y \sim \sqrt{8(T-t)|\log(T-t)|}$$

as $t \to T$ (blow-up time)

Part II: ODEs

Strategy 1: BVP

(A) Chebyshev spectral on an interval

(B) Analytic continuation with Chebyshev-Padé

(Both steps implemented in chebfun system of Trefethen & Team)

Strategy 2: IVP

(A) Maclaurin coefficients via recursion

(B) Analytic continuation with Padé, implemented with the ϵ-algorithm

Painlevé 1

$$y'' = 6y^2 + z, \quad y(0) = y_0, \quad y'(0) = y_1$$

Step A: Compute power series by recurrences

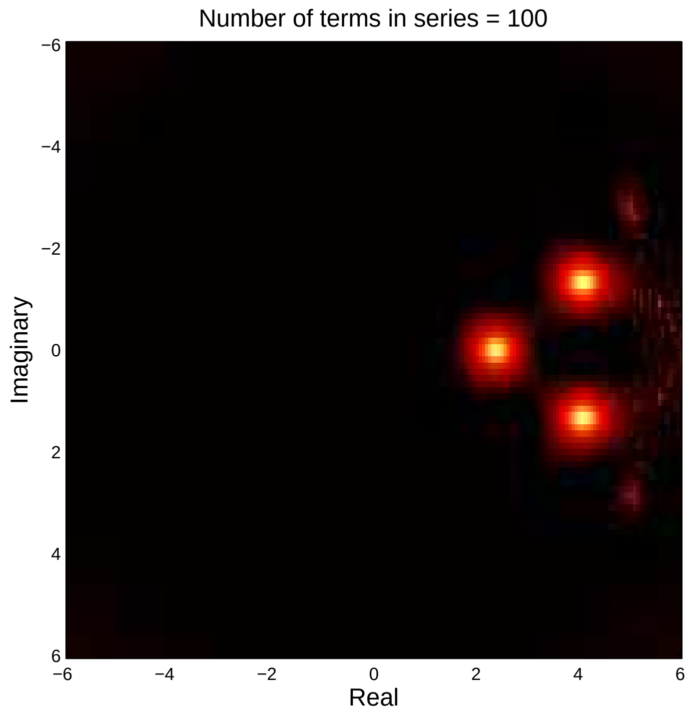
$$y = \sum_{n=0}^{\infty} c_n z^n \quad \Longrightarrow \quad c_0 = y_0, \quad c_1 = y_1$$

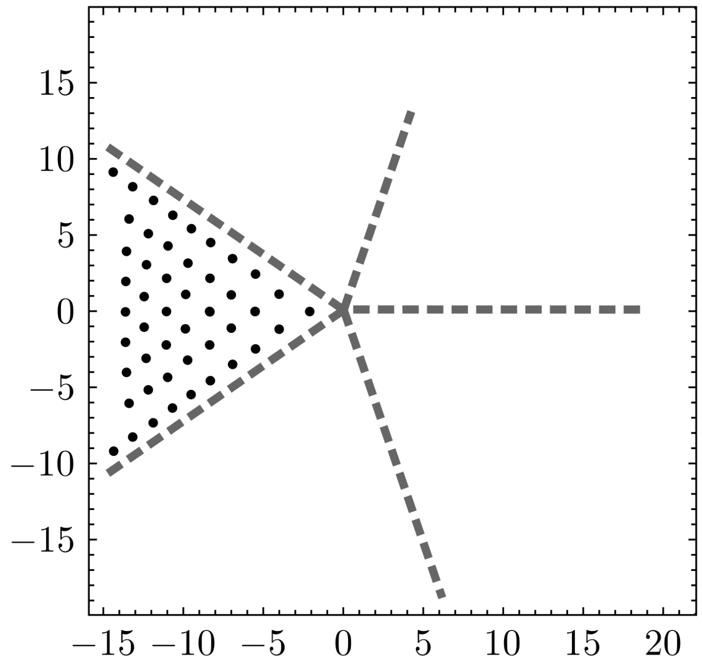
$$y^2 = \sum_{n=0}^{\infty} d_n z^n \quad \Longrightarrow \quad d_n = \sum_{j=0}^{n} c_j c_{n-j}$$

$$c_2 = \frac{6d_0}{1 \cdot 2}, \quad c_3 = \frac{6d_1 + 1}{2 \cdot 3}, \quad c_4 = \frac{6d_2}{3 \cdot 4}, \quad \cdots \quad , \quad c_n = \frac{6d_{n-2}}{(n-1)n}$$

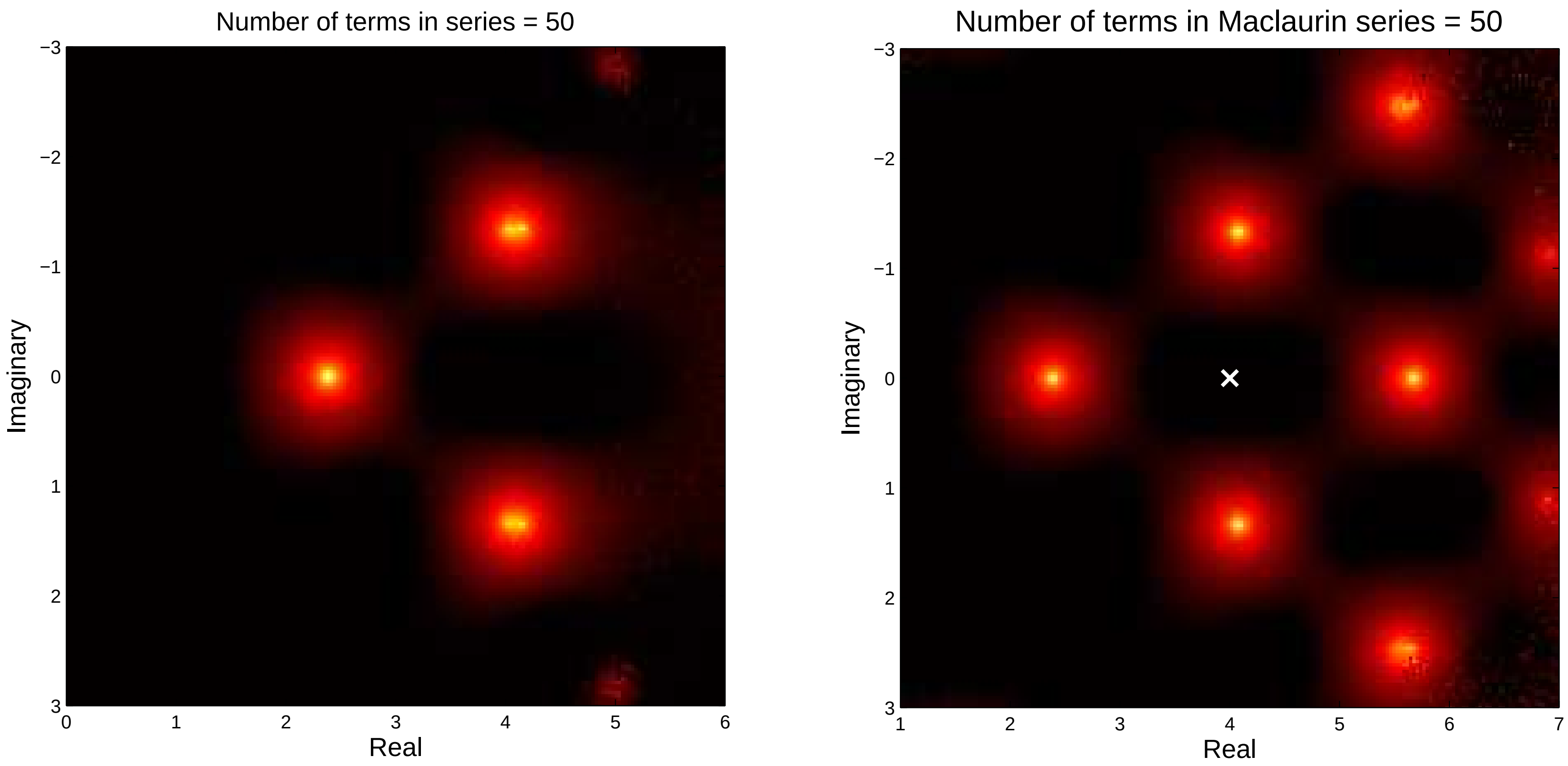
Step B: Continue into complex plane by Padé approximation

Try to compute poles of titronquée solution of P1. Corresponding values of y_0, y_1 can be computed by solving a two-point boundary value problem Novokshenov [2009]. These values were confirmed by chebfun.





“Pole vaulting” Corliss [1980]



Location of poles can be computed by minimizing $\log \frac{1}{|y|}$.

For example, pole of P1 nearest to the orgin is found to be located at

$$z_p = \underline{2.38416877}38895$$

Order of poles can be estimated by the principle of the argument

$$\frac{1}{2\pi i} \int_C \frac{y'(z)}{y(z)}\, dz = \#\text{zeros} - \#\text{poles}$$

Use circle around computed pole z_p as contour

$$z = z_p + r\, e^{i\theta}, \qquad \theta \in [0, 2\pi].$$

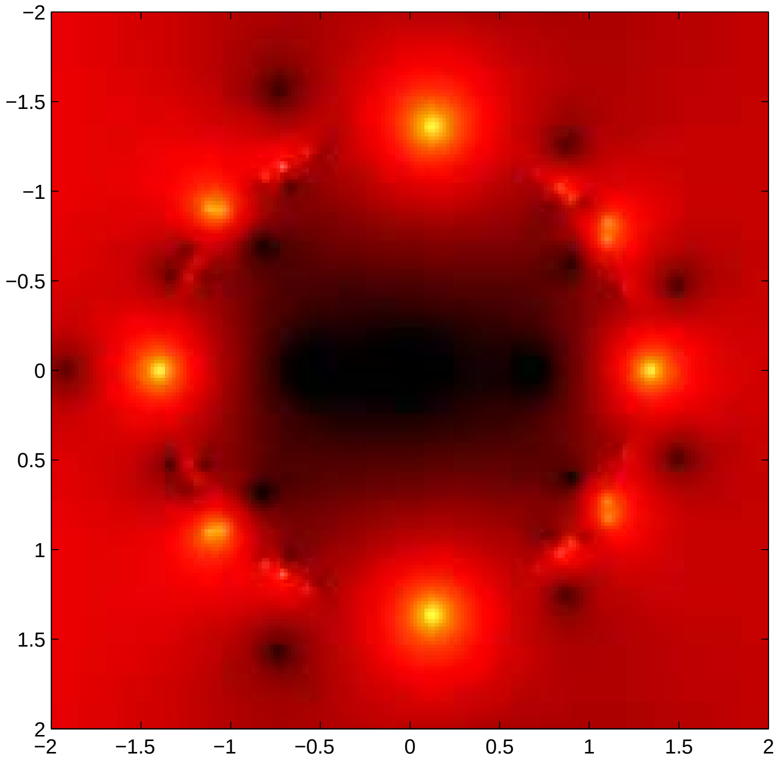
Approximate

- $y'(z)$ by Fourier differentiation
- contour integral by trapezoidal rule.

With 128 terms in trapezoidal rule and $r = 0.1$ this yields order of pole of P1 as 1.99999999999999

Chazy equation

$$y''' = 2\,y\,y'' - 3(y')^2, \quad y(0) = 0, \quad y'(0) = 5, \quad y''(0) = 5$$



Improvements:

- Optimal way to implement “Pole vaulting”: step size vs. degree of rational function?
- Quadratic Padé Approximation
- Reliable error estimates

Quadratic Padé: Consider $[M, M]$ Padé approximation

$$r_M(z) = \frac{p_M(z)}{q_M(z)} \approx f(z)$$

.

Express it as

$$q_M(z)f(z) - p_M(z) = O(z^{2M+1})$$

Generalize to quadratic Padé

$$s_M(z)(f(z))^2 + q_M(z)f(z) + p_M(z) = O(z^{3M+2})$$

Solve by quadratic formula, thereby introducing branch-points.
Not easy to interpret results.