Computing Complex Singularities of Differential Equations with Chebfun

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- The singularities may have physical significance. E.g. complex singularities of Painlevé equations determine the oscillations and asymptotics along the real line.
- It can inform the mathematical analysis of the ODE. E.g. if all singularities lie outside the strip $|\mathrm{Im}(t)| \leq \tau$, then the transformation

$$\zeta = \frac{\exp(\pi t/2\tau) - 1}{\exp(\pi t/2\tau) + 1}$$

maps the strip to the unit disc. The solution must have a convergent expansion in powers of ζ.

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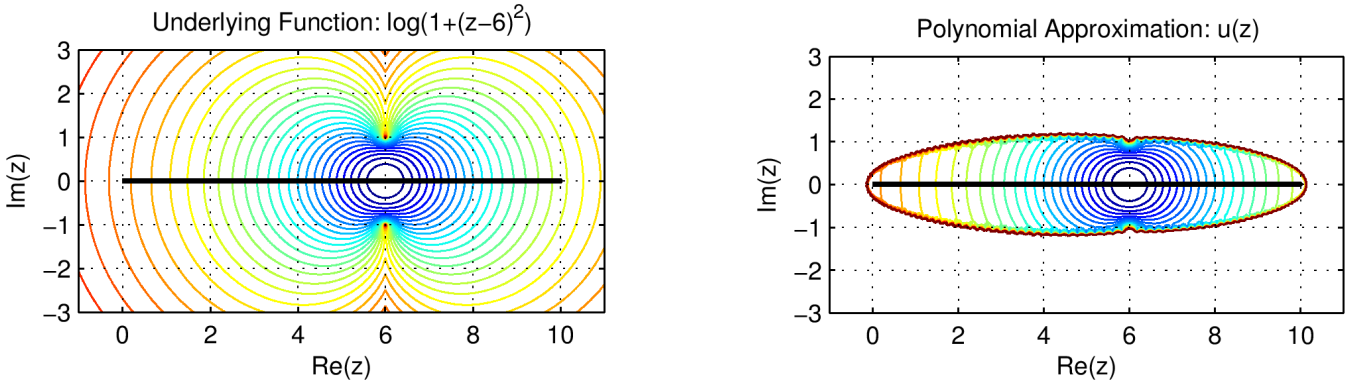

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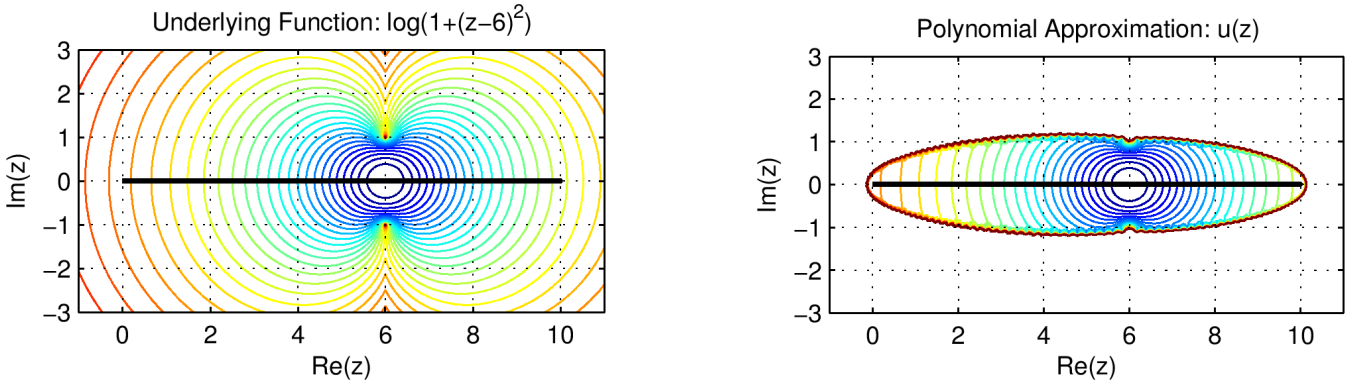

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- A better idea is to use rational functions, because they can have singularities in the complex plane.

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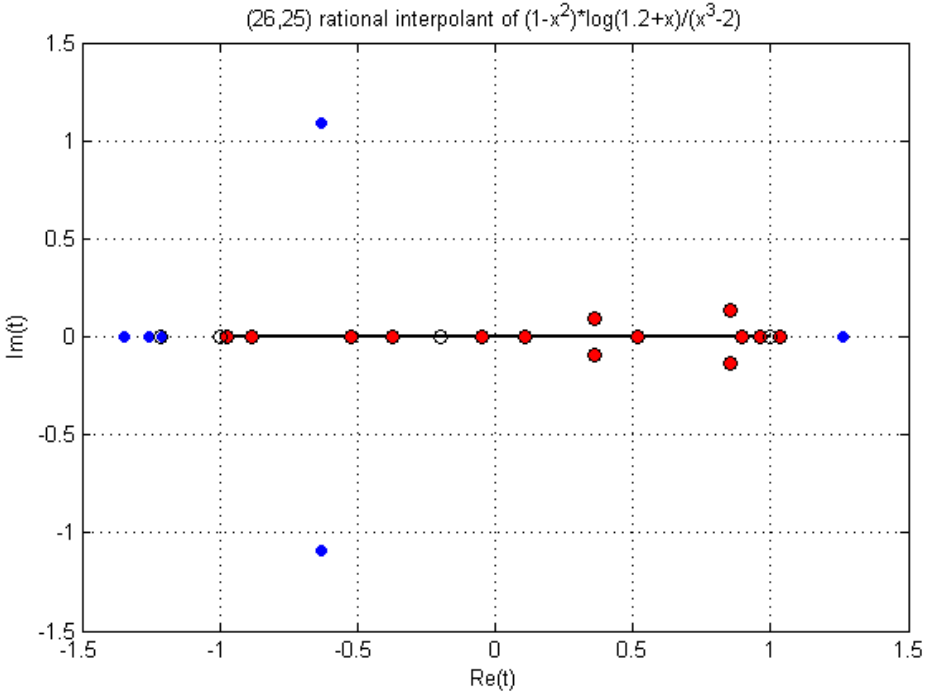

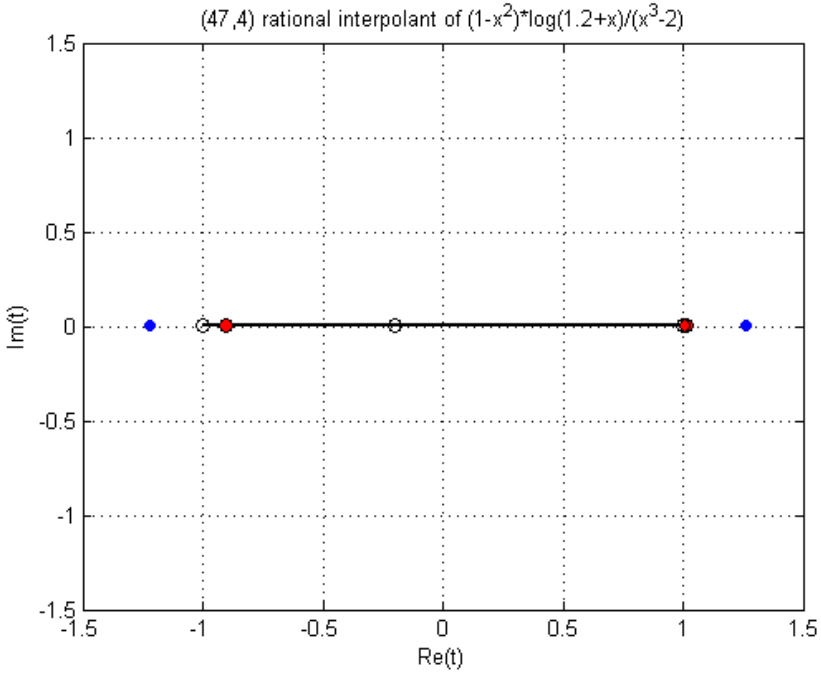

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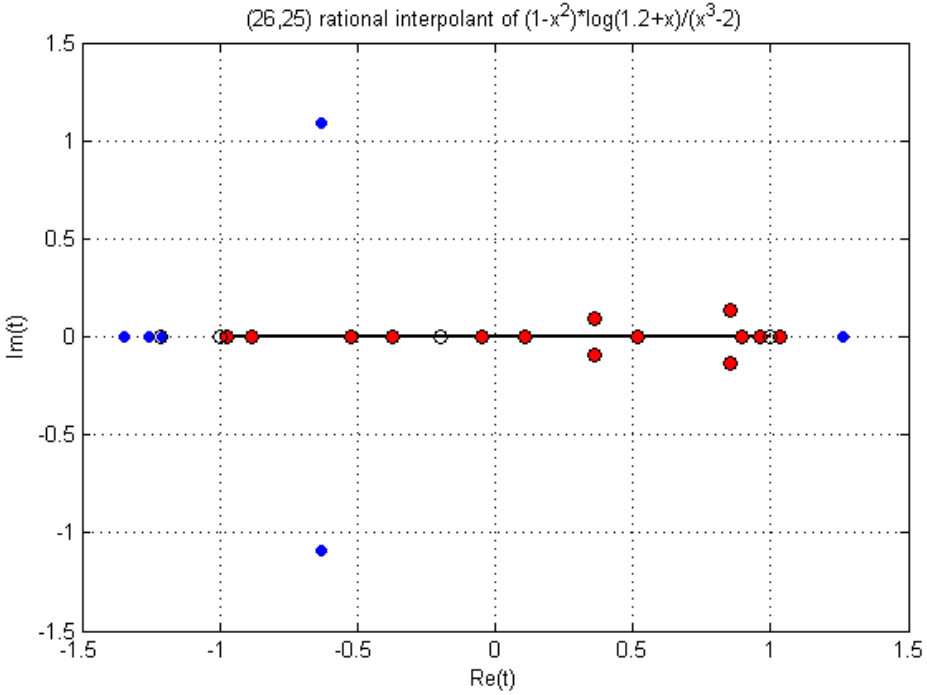

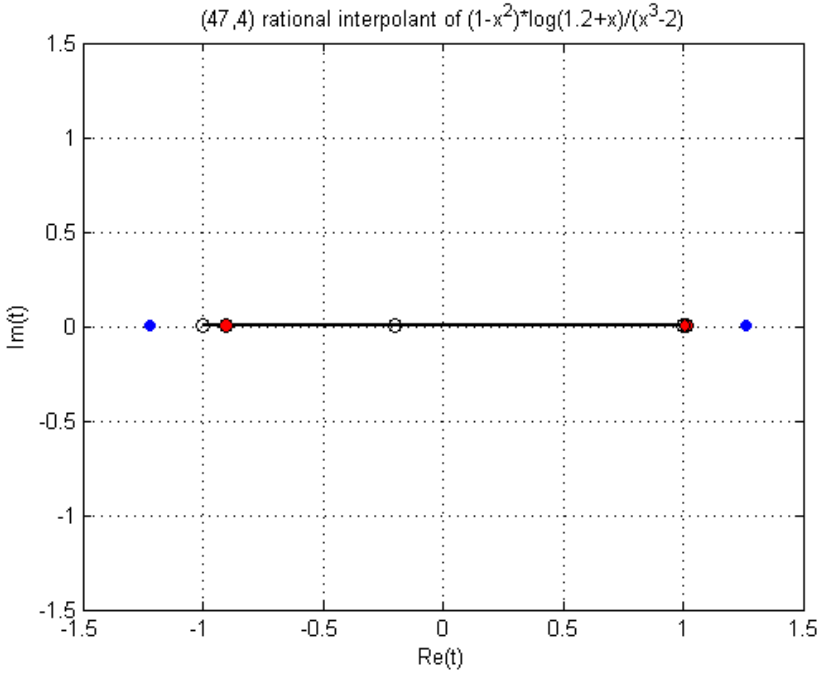

- We want a *robust* rational approximation.

Rational interpolation and least squares

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- To deal with this, consider the more general approach: Define

$$\langle f, g \rangle_N = \sum_{i=0}^{N} \lambda_i f(x_i) \overline{g(x_i)},$$

where $\lambda_i > 0$, and find $p \in \mathcal{P}_m$, $q \in \mathcal{P}_n$ (and take $r = p/q$) to

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- To this aim, we find orthogonal polynomials $(P_j)_{j=0}^N$ with respect to the discrete inner product $\langle \cdot, \cdot \rangle_N$.
- Simplest example: if **x** are roots of unity, take $\lambda_i = 1$ and $P_j(x) = x^j$. Merely orthogonality of the discrete Fourier basis.

Rational interpolation and least squares

- If $\mathbf{x}$ are Chebyshev points $x_i = \cos(i\pi/N)$, take $\lambda_0 = \lambda_N = \frac{1}{2N}$, $\lambda_i = \frac{2}{N}$, so that

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- The $''$ indicates halving the first and last enties. Then we have

$$\langle T_j, T_k \rangle_N = \begin{cases} 2 & \text{if } j = k = 0, N, \\ 1 & \text{if } j = k \neq 0, N, \\ 0 & \text{if } j \neq k. \end{cases}$$

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- Assume we have **normalised** T_0 and T_N.

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$$p = \sum_{j=0}^{N} a_j T_j, \quad q = \sum_{j=0}^{N} b_j T_j, \quad \hat{p} = \sum_{j=0}^{N} \hat{a}_j T_j.$$

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- Interpretation: coeff. space $\mathbf{a}$, $\mathbf{b} \leftarrow$ DCT $\rightarrow p(\mathbf{x})$, $q(\mathbf{x})$ value space

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- Repeat this until we have a unique $\mathbf{b}$. The resulting r should have no spurious poles!

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- We remove trailing coefficients of $\mathbf{a}$ and $\mathbf{b}$ that are smaller than *tol*, further reducing the degrees of p and q.
- Key point: if we ask for $r \in \mathcal{R}_{m,n}$, we will in fact get $r \in \mathcal{R}_{\mu,\nu}$ with $\mu \leq m$, $\nu \leq n$. This is the *exact type* of the interpolant.

Rational interpolation and least squares: Literature

- We call this the PGVT approach after Pachón, Gonnet, Van Deun, and Trefethen
- PGV 2011 introduces the novel approach for interpolation in arbitrary points
- GPT 2011 extends to least squares approximation, enabling robustness, but only for roots of unity
- Covered nicely in Trefethen's book Approximation Theory and Approximation Practice
- W 2013 discusses least squares for Chebyshev points, gives some heuristics for parameters and its usage, and demonstrates with some interesting ODE examples.

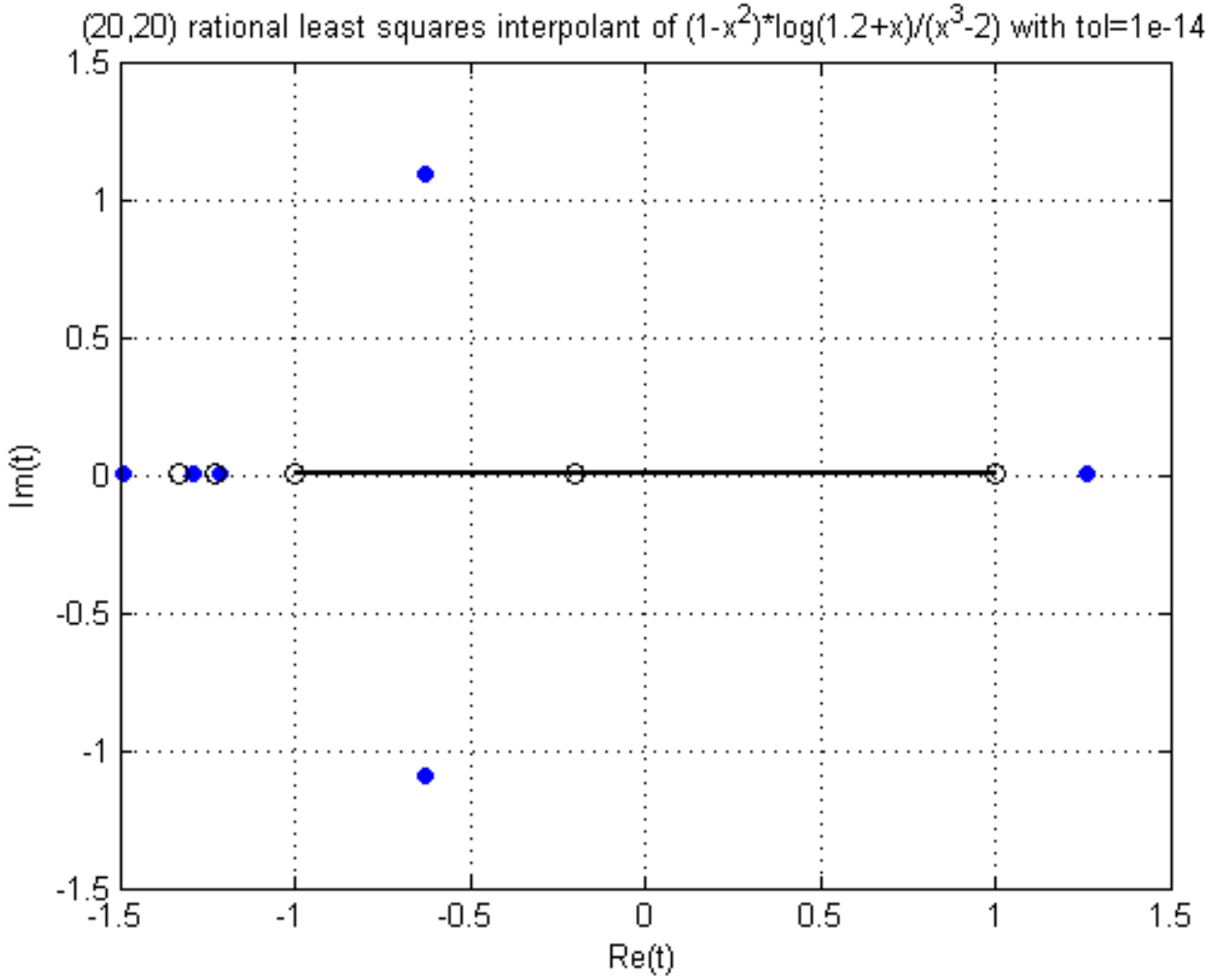


Figure : Ratinterp returns an $(20, 6)$ exact type rational least squares approximant with appropriate singularity structure.

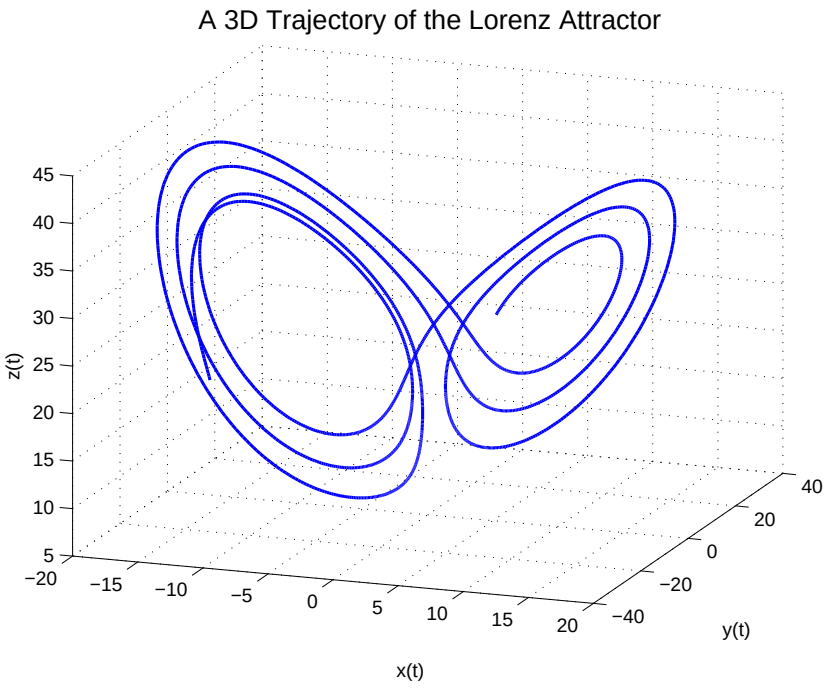
Lorenz Attractor

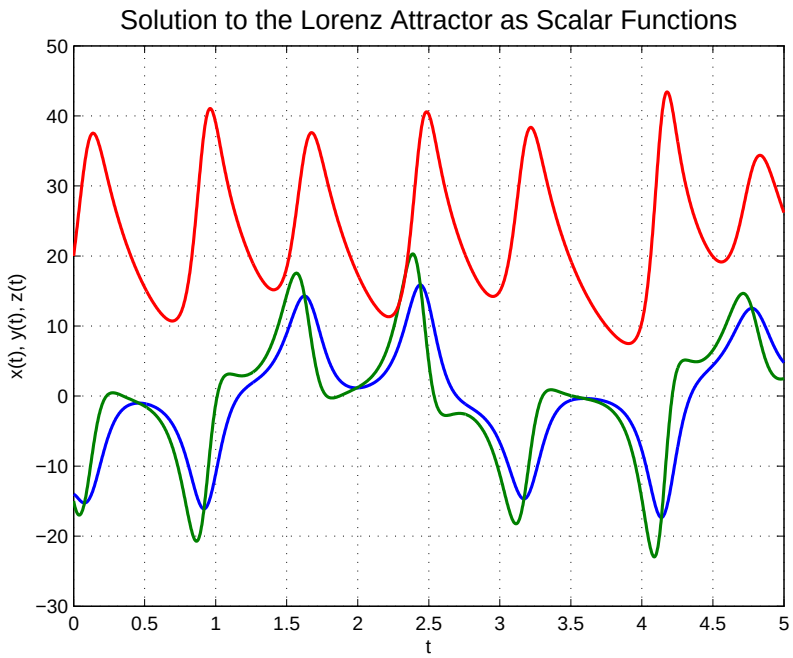
- The Lorenz system is a system of ODEs first studied by Edward Lorenz in the 1960s as a simplified model of convection rolls in the upper atmosphere.

$$\begin{aligned}\frac{\mathrm{d}x}{\mathrm{d}t} &= 10(y-x)\\ \frac{\mathrm{d}y}{\mathrm{d}t} &= 28x - y - xz\\ \frac{\mathrm{d}z}{\mathrm{d}t} &= -8z/3 + xy.\end{aligned}$$

- It is an example of a chaotic system.

Lorenz Attractor: Numerical Solution





- The two straightforward viewpoints for the solution are as a trajectory in 3 dimensions, or as three scalar functions.

Lorenz Attractor: Analytical Solution

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Lorenz Attractor: Analytical Solution

- However, a natural way to see the analytical solution is as a function of a complex variable (see "Complex Singularities of the Lorenz Attractor", Viswanath and Sahutoglu 2010)
- The analytical solution can be expressed **locally** as a Psi-series:

$$
\begin{aligned}
x(t) &= \frac{P_{-1}(\eta)}{t-t_0} + P_0(\eta) + P_1(\eta)(t-t_0) + P_2(\eta)(t-t_0)^2 + \dots, \\
y(t) &= \frac{Q_{-2}(\eta)}{(t-t_0)^2} + \frac{Q_{-1}(\eta)}{t-t_0} + Q_0(\eta) + Q_1(\eta)(t-t_0) + Q_2(\eta)(t-t_0)^2 + \dots, \\
z(t) &= \frac{R_{-2}(\eta)}{(t-t_0)^2} + \frac{R_{-1}(\eta)}{t-t_0} + R_0(\eta) + R_1(\eta)(t-t_0) + R_2(\eta)(t-t_0)^2 + \dots.
\end{aligned}
$$

- Here $\eta = \log(b(t-t_0))$ where $b = \pm i$, and the P_js, Q_js and R_js are polynomials. x has order 1 pseudo-pole at t_0; y and z have order 2 pseudo-poles.

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- Similarly, we get type $(227, 10)$ and $(221, 10)$ rational approximants for the other two components.

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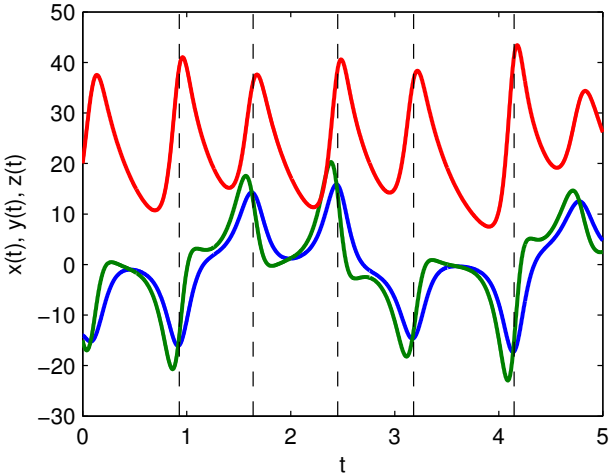

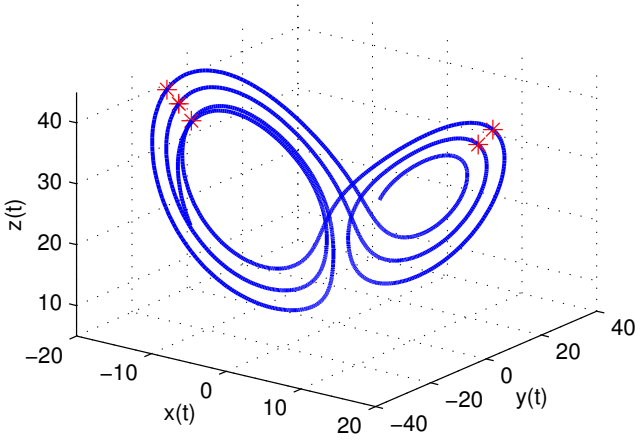

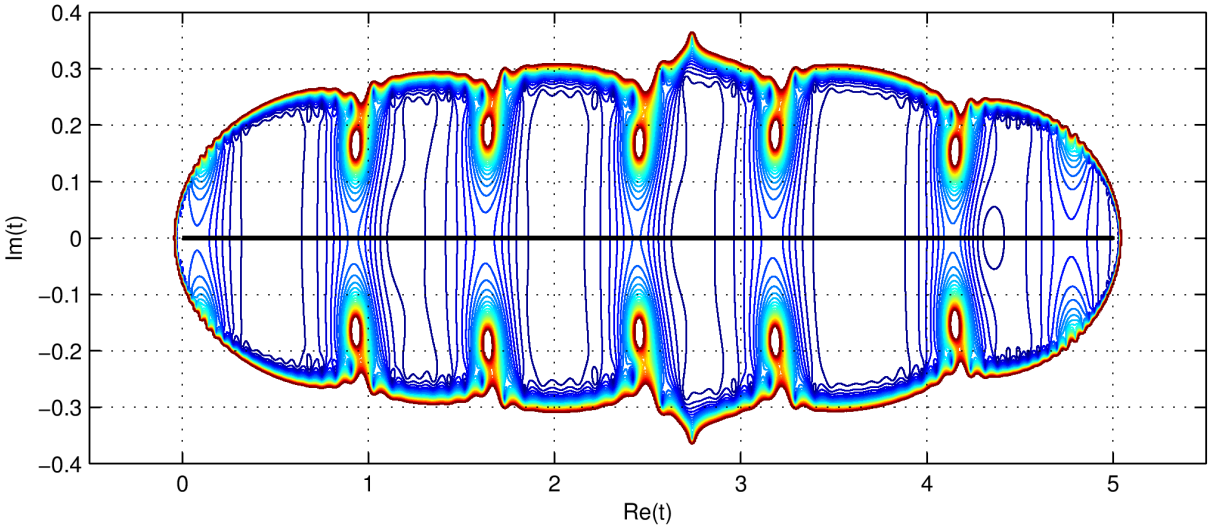

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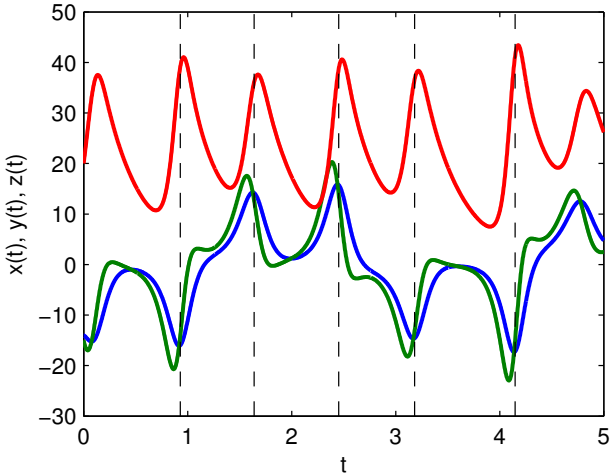

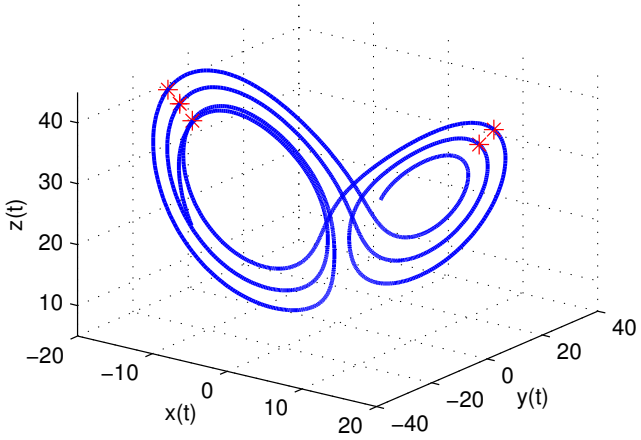

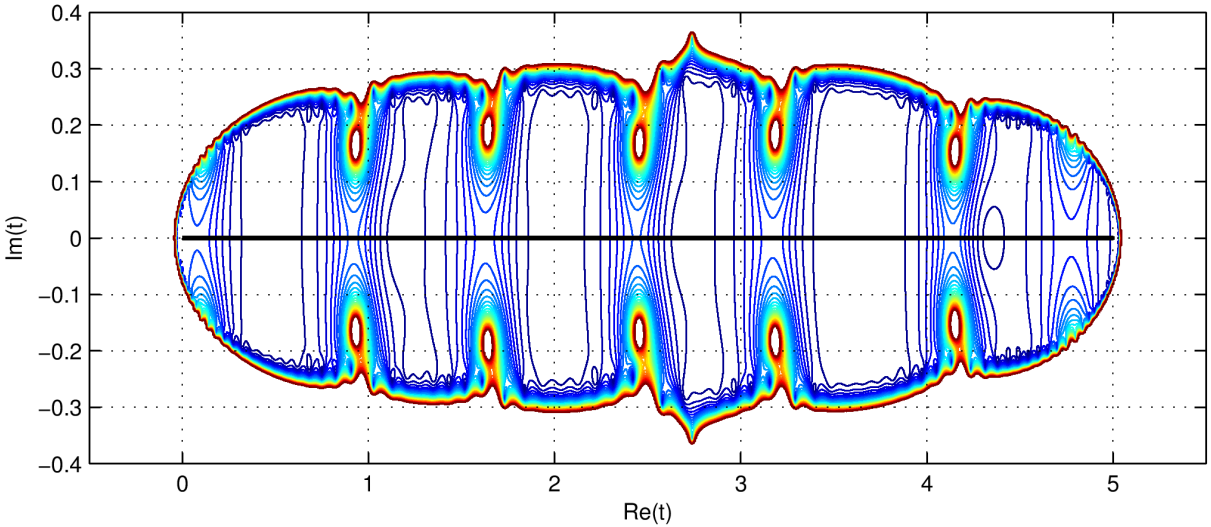

There are still open questions related to the analysis of the Lorenz system!

Lotka–Volterra

- The Lotka–Volterra system is a simple model for the population of predators (y) and their prey (x).

$$\frac{dx}{dt} = \alpha x - \beta xy, \quad \frac{dy}{dt} = -\gamma y + \delta xy.$$

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- The analysis is quite well understood compared to 3D systems. E.g. we know that there are **always** Psi-series singularities in the complex plane.

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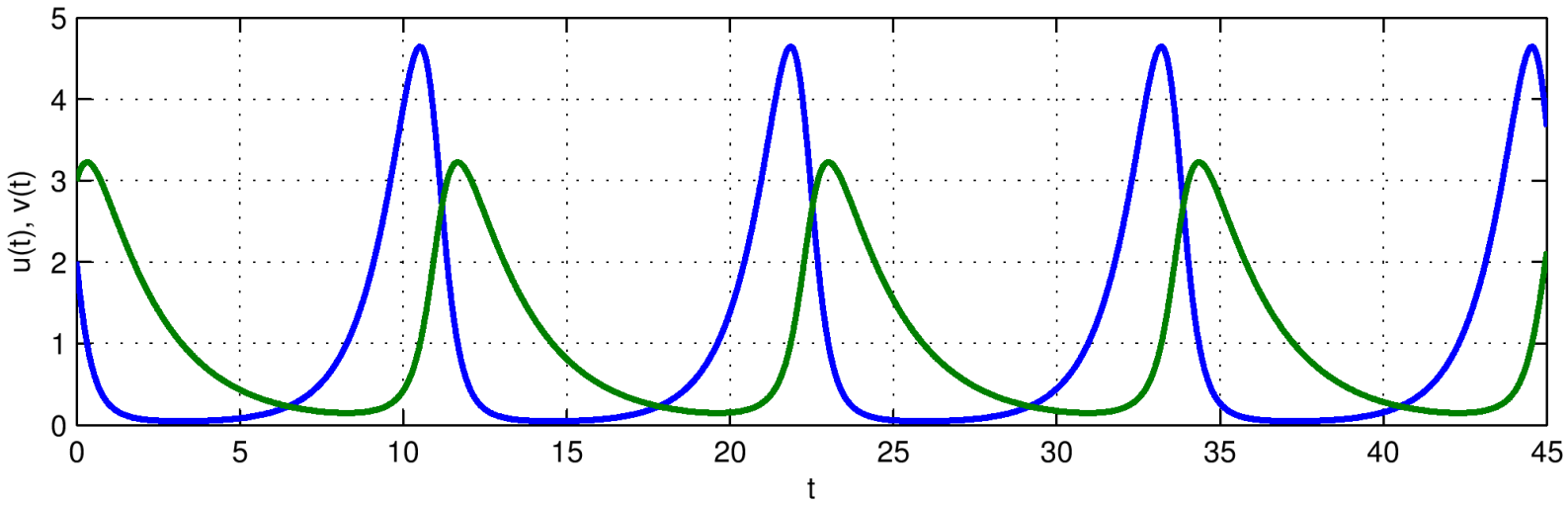
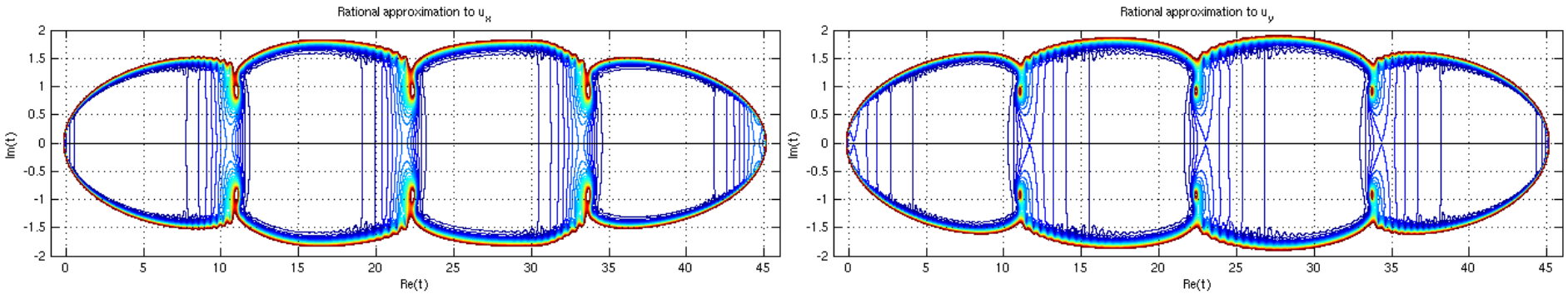


- The Chebfuns are of degrees 743 and 737. We compute $(371, 20)$ and $(366, 20)$ `ratinterp` least squares approximants on 743 and 737 Chebyshev points.
- `ratinterp` returns type $(297, 6)$ and $(287, 6)$ exact type approximants.



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- This makes it good for automated singularity location in parabolic PDEs, parametrised ODEs etc. (see Weideman 2003).

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- Then $\mathbf{a}_1 = Z_1\mathbf{b}$, $\mathbf{a}_2 = Z_2\mathbf{b}$, $\mathbf{a}_3 = Z_3\mathbf{b}$.

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- Thank you for your attention!