Identifying the non-trivial zeros of the Riemann zeta function for prime counting function approximation in the Loewner framework

Curves and Surfaces 2022 (Arcachon, France)

C. Poussot-Vassal, I.V. Gosea, P. Vuillemin and A.C. Antoulas

[Onera / Max Planck Institute / Rice University]
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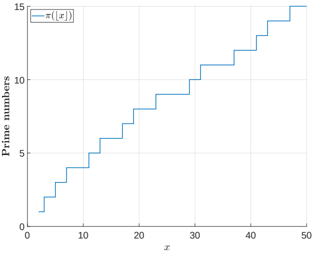
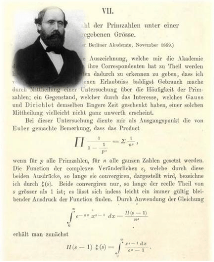
B. Riemann made an important (and unexpected) connection between number theory and complex functions analysis

$$\pi(\lfloor x \rfloor)$$





VII.

…hl der Primzahlen unter einer …gegebenen Grösse.

(…r Berliner Akademie, November 1859.)

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Bei dieser Untersuchung diente mir als Ausgangspunkt die von Euler gemachte Bemerkung, dass das Product

$$\Pi \frac{1}{1-\frac{1}{p^s}} = \Sigma \frac{1}{n^s},$$

wenn für p alle Primzahlen, für n alle ganzen Zahlen gesetzt werden. Die Function der complexen Veränderlichen s, welche durch diese beiden Ausdrücke, so lange sie convergiren, dargestellt wird, bezeichne ich durch $\zeta(s)$. Beide convergiren nur, so lange der reelle Theil von s grösser als 1 ist; es lässt sich indess leicht ein immer gültig bleibender Ausdruck der Function finden. Durch Anwendung der Gleichung

$$\int_0^\infty e^{-nx} x^{s-1}\, dx = \frac{\Pi(s-1)}{n^s}$$

erhält man zunächst

$$\Pi(s-1)\,\zeta(s) = \int_0^\infty \frac{x^{s-1}\,dx}{e^x - 1}.$$

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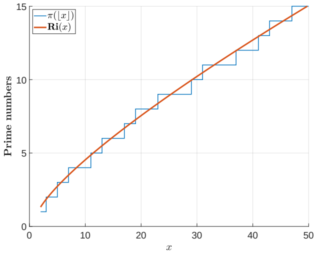
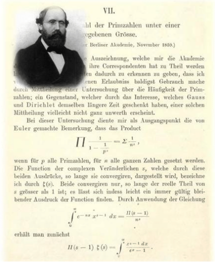
$$\pi(\lfloor x \rfloor) \approx \mathbf{Ri}(x)$$





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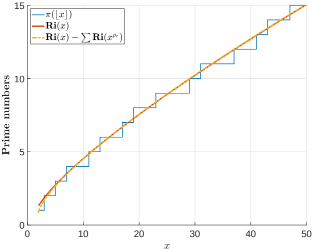
$\mathbf{Ri}(x) = \sum_{n=1}^{\infty} \frac{\mu(n)}{n} \mathbf{Li}(x^{1/n})$, $\mu(n)$ is the Mobius function and $\mathbf{Li}(x) = \int_2^x \frac{dt}{\mathbf{ln}(t)}$

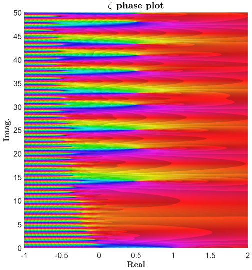
Introduction

Glimpse of the Riemann conjecture idea

B. Riemann made an important (and unexpected) connection between number theory and complex functions analysis

$$\pi(\lfloor x \rfloor) \approx \mathbf{Ri}(x) - \sum_{\rho_r} \mathbf{Ri}(x^{\rho_r}) \text{ (trivial zeros)}$$





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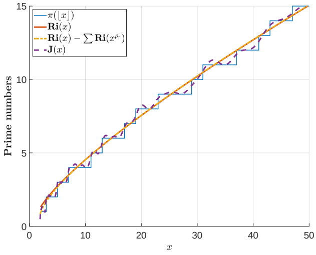
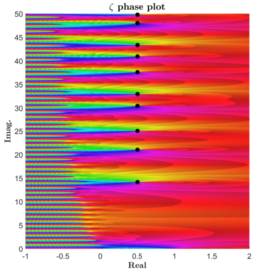
B. Riemann made an important (and unexpected) connection between number theory and complex functions analysis

$$\pi(\lfloor x \rfloor) \approx \mathbf{Ri}(x) - \sum_{\rho_r} \mathbf{Ri}(x^{\rho_r}) - \sum_{\rho_i} \mathbf{Ri}(x^{\rho_i}) = \mathbf{J}(x)$$ (trivial and non-trivial zeros)





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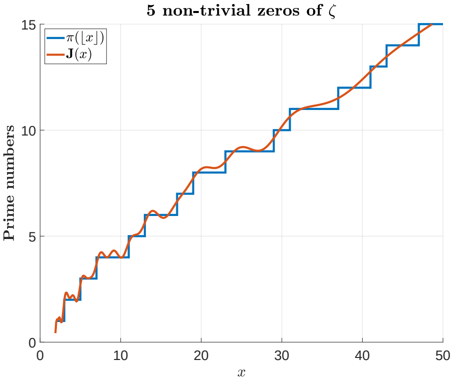
Glimpse of the Riemann conjecture idea[1]

$$\mathbf{J}(x) = \mathbf{Ri}(x) - \sum_{\rho_r} \mathbf{Ri}(x^{\rho_r}) - \sum_{\rho_i} \mathbf{Ri}(x^{\rho_i})$$



[1] Authors warmly thank **David Louapre** (`https://scienceetonnante.com/`) for providing the Python code allowing to compute the Riemann prime counting function.

Introduction

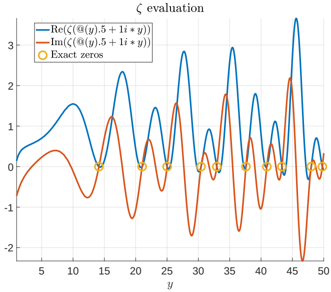
The ζ function... a central element

Initially defined as $(z \in \mathbb{C}_{\Re(z)>1})$

$$\zeta(z) = \sum_{n=1}^{\infty} \frac{1}{n^z}$$

A continuation is used $(z \in \mathbb{C}_{\Re(z)\neq 1})$

$$\zeta(z) = \frac{1}{1-2^{1-z}} \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n^z}$$



Evalutation of ζ along

$$z = \frac{1}{2} + \imath y$$

J-P. Berrut and L.N. Trefethen, *"Barycentric Lagrange interpolation"*, SIAM review, 2004.

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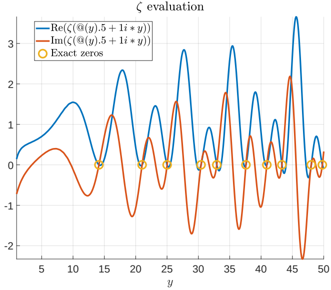

Barycentric form

$$\hat{\zeta}(z) = \frac{\sum_i \beta_i/(z-\lambda_i)}{\sum_i \alpha_i/(z-\lambda_i)} \approx \zeta(z)$$

J-P. Berrut and L.N. Trefethen, *"Barycentric Lagrange interpolation"*, SIAM review, 2004.

Loewner and AAA to approximate ζ zeros

- Interpolatory **Loewner** method [Mayo/Antoulas]
- Interpolatory **AAA** method [Anderson/Antoulas] & [Trefethen]

We consider transfer function

$$\mathbf{H}(z) = \frac{\sum_i \beta_i/(z-\lambda_i)}{\sum_i \alpha_i/(z-\lambda_i)}$$

Realizations

$$\mathcal{S} : (E, A, B, C, \mathbf{0})$$

and Loewner pencil

$$(\mathbb{L}, \mathbb{M})$$

A.C. Antoulas, C. Beattie and S. Gugercin, *"Interpolatory methods for model reduction"*, SIAM Computational Science and Engineering, Philadelphia, 2020.

A.J. Mayo and A.C. Antoulas, *"A framework for the solution of the generalized realization problem"*, Linear Algebra and its Applications, 2007.

Y. Nakatsukasa, O. Sete and L.N. Trefethen, *"The AAA algorithm for rational approximation"*, SIAM Journal on Scientific Computing, 2018.

L.N. Trefethen, *"Rational functions (von Neumann Prize lecture)"*, SIAM Annual Meeting, 2020.

Interpolatory framework

Loewner model-based approximation (rational interpolation)

Given model $\mathbf{H}$ and μ_j, λ_i, seek $\hat{\mathbf{H}}$ s.t.

$$\begin{aligned}\hat{\mathbf{H}}(\mu_j) &= \mathbf{H}(\mu_j)\\ \hat{\mathbf{H}}(\lambda_i) &= \mathbf{H}(\lambda_i)\end{aligned}$$

$i = 1, \ldots, k$; $j = 1, \ldots, q$.

A.J. Mayo and A.C. Antoulas, *"A framework for the solution of the generalized realization problem"*, Linear Algebra and its Applications, 425(2-3), 2007, pp 634-662.

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$$\mathbb{L} = \begin{bmatrix} \frac{\mathbf{H}(\mu_1)-\mathbf{H}(\lambda_1)}{\mu_1-\lambda_1} & \cdots & \frac{\mathbf{H}(\mu_1)-\mathbf{H}(\lambda_k)}{\mu_1-\lambda_k} \\ \vdots & \ddots & \vdots \\ \frac{\mathbf{H}(\mu_q)-\mathbf{H}(\lambda_1)}{\mu_q-\lambda_1} & \cdots & \frac{\mathbf{H}(\mu_q)-\mathbf{H}(\lambda_k)}{\mu_q-\lambda_k} \end{bmatrix}$$

$$\mathbb{M} = \begin{bmatrix} \frac{\mu_1\mathbf{H}(\mu_1)-\mathbf{H}(\lambda_1)\lambda_1}{\mu_1-\lambda_1} & \cdots & \frac{\mu_1\mathbf{H}(\mu_1)-\mathbf{H}(\lambda_k)\lambda_k}{\mu_1-\lambda_k} \\ \vdots & \ddots & \vdots \\ \frac{\mu_q\mathbf{H}(\mu_q)-\mathbf{H}(\lambda_1)\lambda_1}{\mu_q-\lambda_1} & \cdots & \frac{\mu_q\mathbf{H}(\mu_q)-\mathbf{H}(\lambda_k)\lambda_k}{\mu_q-\lambda_k} \end{bmatrix}$$

$$\mathbf{W} = \begin{bmatrix} \mathbf{H}(\lambda_1) & \ldots & \mathbf{H}(\lambda_k) \end{bmatrix}$$

$$\mathbf{V}^T = \begin{bmatrix} \mathbf{H}(\mu_1) & \ldots & \mathbf{H}(\mu_q) \end{bmatrix}$$

$\hat{\mathbf{H}}(z) = \mathbf{W}(-z\mathbb{L} + \mathbb{M})^{-1}\mathbf{V}$ $\Rightarrow$ Rational interpolation

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Loewner data-driven approximation (rational interpolation)

Given $\{\mu_j, \mathbf{v}_j\}$, $\{\lambda_i, \mathbf{w}_i\}$ data, seek $\hat{\mathbf{H}}$, s.t.

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$\hat{\mathbf{H}}(z) = \mathbf{W}(-z\mathbb{L} + \mathbb{M})^{-1}\mathbf{V}$ $\Rightarrow$ Rational interpolation (data-driven)

A.J. Mayo and A.C. Antoulas, *"A framework for the solution of the generalized realization problem"*, Linear Algebra and its Applications, 425(2-3), 2007, pp 634-662.

Interpolatory framework

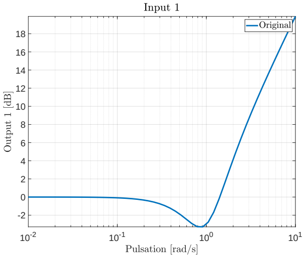
Some features of the Loewner landmark

Rational function satisfies

$$\hat{\mathbf{H}}(\lambda_i) = \mathbf{H}(\lambda_i) \text{ and } \hat{\mathbf{H}}(\mu_j) = \mathbf{H}(\mu_j)$$

$$\mathbf{H}(s) = \frac{s^2 + s + 1}{s + 1}$$

Sampled with $\lambda_i = [1, 2, \ldots, 20]$ and $\mu_j = [1.5, 2.5, \ldots, 20.5]$, leads to realization of dimension



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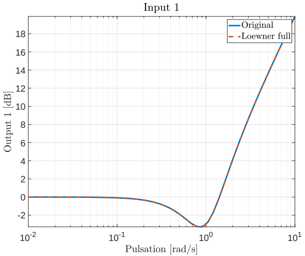

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$$\mathbf{rank}([\mathbb{L}, \mathbb{M}]) = r$$

$$\mathbf{rank}(\mathbb{L}) = \nu$$

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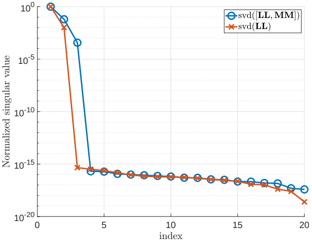

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Minimal realization

$$\hat{\mathbf{H}}_r(s) = \mathbf{W} X(-sY^T \mathbb{L} X + Y^T \mathbb{M} X)^{-1} Y^T \mathbf{V}$$

$$\mathbf{H}(s) = \frac{s^2 + s + 1}{s + 1}$$

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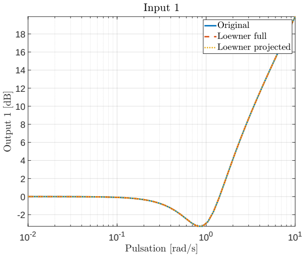

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Interpolatory framework

AAA model-based approximation (rational interpolation)

Given $\{\nu_j, h_j\}$, $\{\eta_i, g_i\}$ data, seek $\hat{\mathbf{H}}$, s.t.

$$\hat{\mathbf{H}}_\ell(\xi) = \frac{\sum_{j=1}^{\ell} \frac{\alpha_j^{(\ell)} h_j}{\xi - \nu_j}}{\sum_{j=1}^{\ell} \frac{\alpha_j^{(\ell)}}{\xi - \nu_j}}$$

$i = 1, \ldots, \ell$ and $j = 1, \ldots, 2n - \ell$.

Mixes **Least Squares** with **Loewner** in an **iteration**

- Find $\nu_\ell \in \Omega^{(\ell-1)}$, where $\nu_\ell = \arg\max_{1 \le k \le 2M} \left\| f_k - \hat{\mathbf{H}}_{\ell-1}(z_k) \right\|$
- Set $\Omega^{(\ell)} := \Omega^{(\ell-1)} \setminus \{\nu_\ell\}$, where , $h^\ell := \mathbf{H}(\nu_\ell)$
- Compute $\alpha^{(\ell)} = -\mathbb{L}^{\#}\mathbf{f}$
- Set

$$\begin{aligned}
\hat{E} &= \mathbf{diag}(1, \ldots, 1, 0) \\
\hat{A} &= \mathbf{diag}(\nu_1, \ldots, \nu_r, 1) - \hat{B}\mathbf{e}_{r+1}^T \\
\hat{B} &= [\alpha_1^{(r)}, \ldots, \alpha_r^{(r)}, 1]^T \\
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- Compute $\alpha^{(\ell)} = -\mathbb{L}^\# \mathbf{f}$
- Set

$$\begin{aligned}
\hat{E} &= \mathbf{diag}(1, \ldots, 1, 0) \\
\hat{A} &= \mathbf{diag}(\nu_1, \ldots, \nu_r, 1) - \hat{B}\mathbf{e}_{r+1}^T \\
\hat{B} &= [\alpha_1^{(r)}, \ldots, \alpha_r^{(r)}, 1]^T \\
\hat{C} &= [h_1, \ldots, h_r, 0]
\end{aligned}$$

Y. Nakatsukasa, O. Sete and L.N. Trefethen, *"The AAA algorithm for rational approximation"*, SIAM Journal on Scientific Computing, 2018.

Chebfun Developers, *"http://www.chebfun.org/"*, University of Oxford.

Interpolatory framework

AAA model-based approximation (rational interpolation)

Given $\{\nu_j, h_j\}$, $\{\eta_i, g_i\}$ data, seek $\hat{\mathbf{H}}$, s.t.

$$\hat{\mathbf{H}}_\ell(\xi) = \frac{\sum_{j=1}^{\ell} \frac{\alpha_j^{(\ell)} h_j}{\xi - \nu_j}}{\sum_{j=1}^{\ell} \frac{\alpha_j^{(\ell)}}{\xi - \nu_j}}$$

$i = 1, \ldots, \ell$ and $j = 1, \ldots, 2n - \ell$.

Mixes **Least Squares** with **Loewner** in an **iteration**

- Find $\nu_\ell \in \Omega^{(\ell-1)}$, where $\nu_\ell = \arg\max_{1 \le k \le 2M} \left\| f_k - \hat{\mathbf{H}}_{\ell-1}(z_k) \right\|$
- Set $\Omega^{(\ell)} := \Omega^{(\ell-1)} \setminus \{\nu_\ell\}$, where , $h^\ell := \mathbf{H}(\nu_\ell)$
- Compute $\boldsymbol{\alpha}^{(\ell)} = -\mathbb{L}^{\#}\mathbf{f}$
- Set

$$\begin{aligned} \hat{E} &= \mathbf{diag}(1, \ldots, 1, 0) \\ \hat{A} &= \mathbf{diag}(\nu_1, \ldots, \nu_r, 1) - \hat{B}\mathbf{e}_{r+1}^T \\ \hat{B} &= [\alpha_1^{(r)}, \ldots, \alpha_r^{(r)}, 1]^T \\ \hat{C} &= [h_1, \ldots, h_r, 0] \end{aligned}$$

$\hat{\mathbf{H}}_\ell(z) = \hat{C}(z\hat{E} - \hat{A})^{-1}\hat{B}$ $\Rightarrow$ best average fitting of the data (data-driven)

Y. Nakatsukasa, O. Sete and L.N. Trefethen, *"The AAA algorithm for rational approximation"*, SIAM Journal on Scientific Computing, 2018.

Chebfun Developers, *"http://www.chebfun.org/"*, University of Oxford.

Numerical illustration

Process

A continuation of ζ is used ($z \in \mathbb{C}_{\Re(z)\neq 1}$)

$$\frac{1}{1-2^{1-z}}\sum_{n=1}^{\infty}\frac{(-1)^{n-1}}{n^z}$$

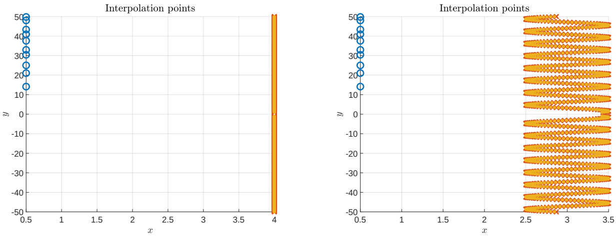
$\Rightarrow$

Rational approximation

ROM

- Rational function
- r state variables

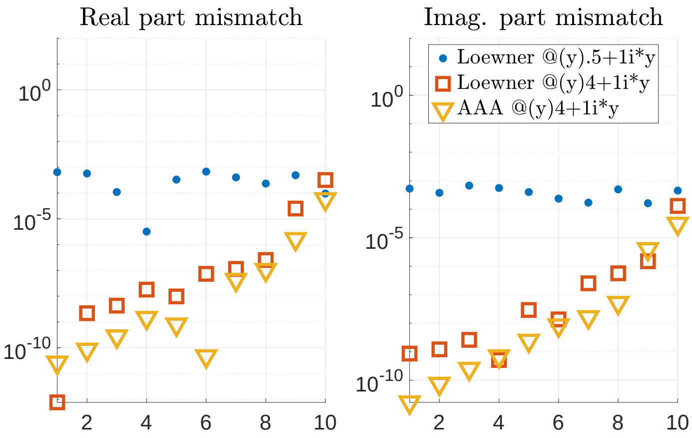
μ_j and λ_i (Loewner case) & ν_j and η_i (AAA case)
As chosen by Trefethen et al. (left) & Random case (right)



Numerical illustration

Zeros computation on the rational interpolant

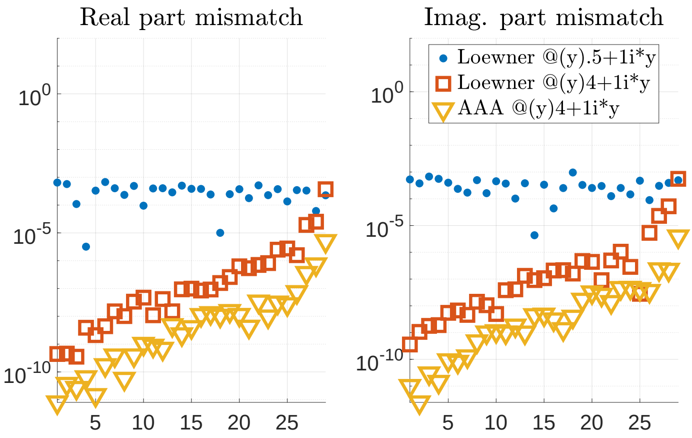
Interval $[0, 50]$, $n = 1000$, $\zeta(4 + \imath y)$



Numerical illustration

Zeros computation on the rational interpolant

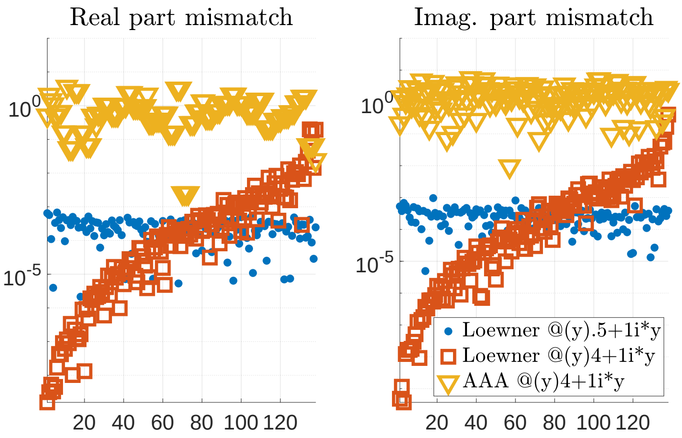
Interval $[0, 100]$, $n = 1000$, $\zeta(4 + \imath y)$



Numerical illustration

Zeros computation on the rational interpolant

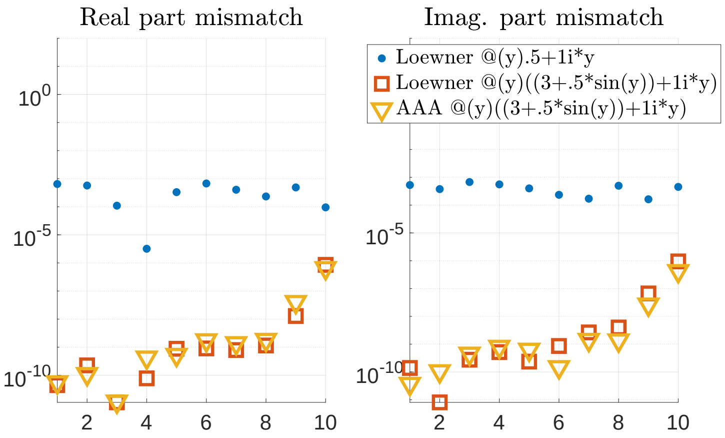
Interval $[0, 300]$, $n = 1000$, $\zeta(4 + \imath y)$



Numerical illustration

Zeros computation on the rational interpolant

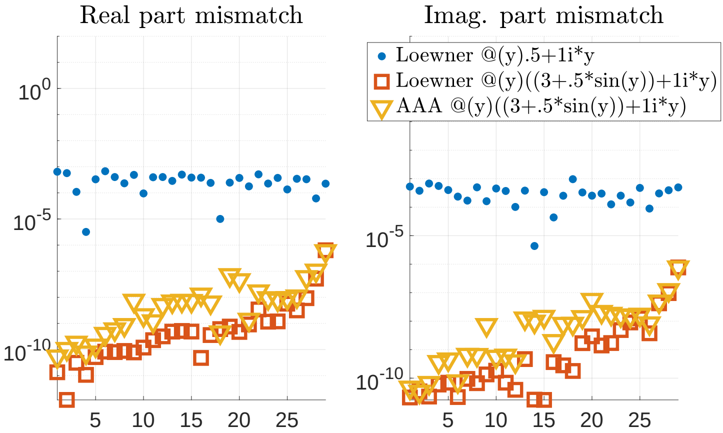
Interval $[0, 50]$, $n = 1000$, $\zeta(3 + 0.5\sin(y) + \imath y)$



Numerical illustration

Zeros computation on the rational interpolant

Interval $[0, 100]$, $n = 1000$, $\zeta(3 + 0.5\sin(y) + \imath y)$



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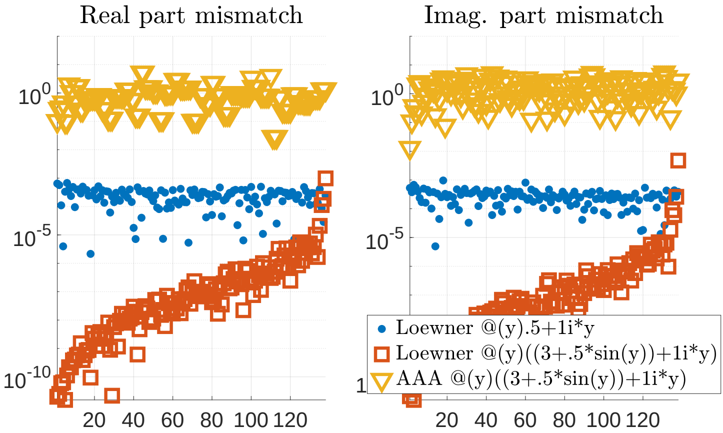
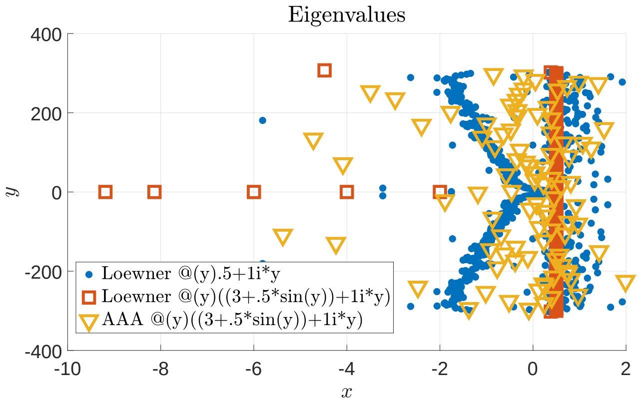


Numerical illustration

Zeros computation on the rational interpolant

Interval $[0, 300]$, $n = 1000$, $\zeta(3 + 0.5\sin(y) + \imath y)$

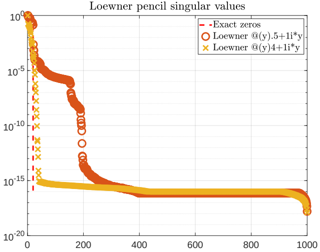


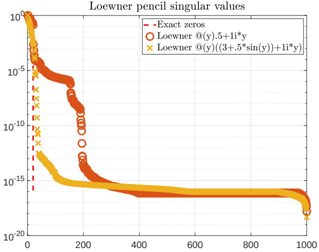
Loewner pencil finds trivial and non-trivial zeros, whatever the choice of interpolation points

Numerical illustration

Pencil singular values

Interval $[0, 50]$, $n = 1000$, $\zeta(4 + \imath y)$ & $\zeta(3 + 0.5\sin(y) + \imath y)$



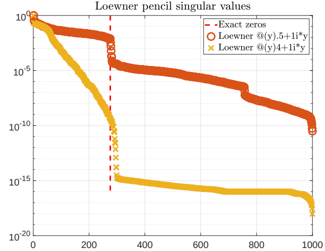


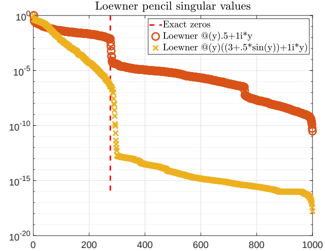
Loewner pencil detects the number of non-trivial zeros

Numerical illustration

Pencil singular values

Interval $[0, 300]$, $n = 1000$, $\zeta(4 + \imath y)$ & $\zeta(3 + 0.5sin(y) + \imath y)$



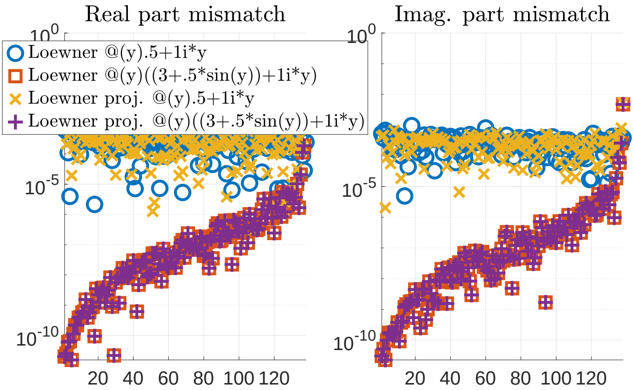


Loewner pencil detects the number of non-trivial zeros

Numerical illustration

Zeros computation with projected rational model

Interval $[0, 300]$, $n = 1000$, $\zeta(4 + \imath y)$ & $\zeta(3 + 0.5sin(y) + \imath y)$



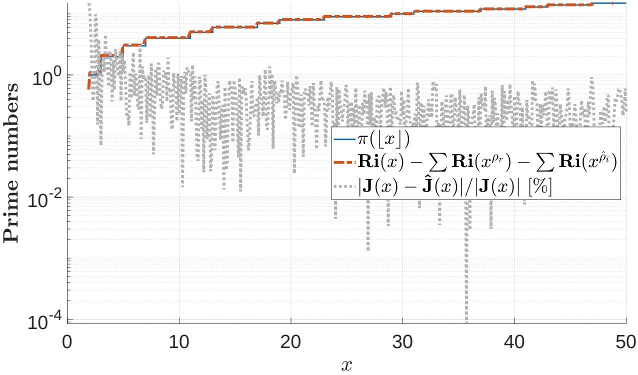
$$\hat{\mathbf{H}}_r(s) = \mathbf{W}X(-sY^T\mathbb{L}X + Y^T\mathbb{M}X)^{-1}Y^T\mathbf{V}$$

Minimal rational function catches the zeros as accurately as full realization!

Conclusions

Back to $\mathbf{J}(x)$... $\hat{\mathbf{J}}(x)$

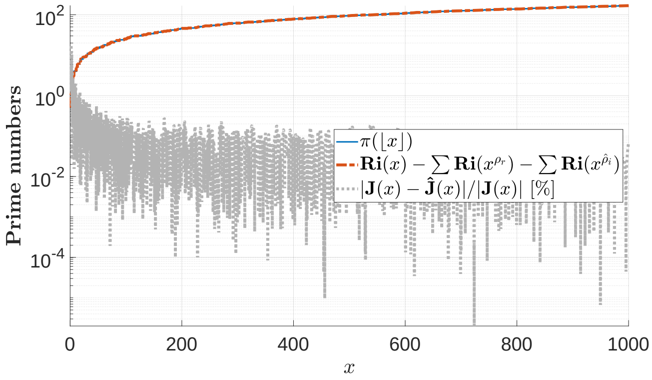
$$\hat{\mathbf{J}}(x) = \mathbf{Ri}(x) - \sum_{\rho_r} \mathbf{Ri}(x^{\rho_r}) - \sum_{\rho_i i=1\ldots500} \mathbf{Ri}(x^{\hat{\rho}_i})$$



Conclusions

Back to $\mathbf{J}(x)$... $\hat{\mathbf{J}}(x)$

$$\hat{\mathbf{J}}(x) = \mathbf{Ri}(x) - \sum_{\rho_r} \mathbf{Ri}(x^{\rho_r}) - \sum_{\rho_i i=1\ldots 200} \mathbf{Ri}(x^{\hat{\rho}_i})$$



Conclusions

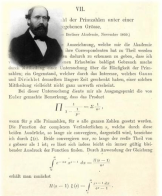
Take home message[2]

Loewner and **AAA** enforce rational approximation of complex functions,

- **Loewner** and **AAA** find "accurate" rational models
- **Loewner pencil** catches the exact number of ζ zeros at low cost
- **Loewner** seems more robust to the interpolation points selection

$\rightarrow$ **How to select interpolation points?**
$\rightarrow$ **Any idea? Please contact us!**

Bernhard Riemann (1826 - 1866)



VII.

…hl der Primzahlen unter einer …gegebenen Grösse.

(… Berliner Akademie, November 1859.)

… Auszeichnung, welche mir die Akademie … ihre Correspondenten hat zu Theil werden …en dadurch zu erkennen zu geben, dass ich …enen Erlaubniss baldigst Gebrauch mache durch Mittheilung einer Untersuchung über die Häufigkeit der Primzahlen; ein Gegenstand, welcher durch das Interesse, welches Gauss und Dirichlet demselben längere Zeit geschenkt haben, einer solchen Mittheilung vielleicht nicht ganz unwerth erscheint.

Bei dieser Untersuchung diente mir als Ausgangspunkt die von Euler gemachte Bemerkung, dass das Product

$$\Pi \frac{1}{1-\frac{1}{p^s}} = \Sigma \frac{1}{n^s},$$

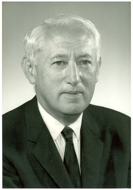
wenn für p alle Primzahlen, für n alle ganzen Zahlen gesetzt werden. Die Function der complexen Veränderlichen s, welche durch diese beiden Ausdrücke, so lange sie convergiren, dargestellt wird, bezeichne ich durch $\zeta(s)$. Beide convergiren nur, so lange der reelle Theil von s grösser als 1 ist; es lässt sich indess leicht ein immer gültig bleibender Ausdruck der Function finden. Durch Anwendung der Gleichung

$$\int_0^\infty e^{-nx} x^{s-1}\, dx = \frac{\Pi(s-1)}{n^s}$$

erhält man zunächst

$$\Pi(s-1)\,\zeta(s) = \int_0^\infty \frac{x^{s-1}\, dx}{e^x - 1}.$$

Karl Loewner (1893 - 1968)



[2] Ack. to **David Louapre** (`https://scienceetonnante.com/`) for inspiration and help.

Identifying the non-trivial zeros of the Riemann zeta function for prime counting function approximation in the Loewner framework

Curves and Surfaces 2022 (Arcachon, France)

C. Poussot-Vassal, I.V. Gosea, P. Vuillemin and A.C. Antoulas

[Onera / Max Planck Institute / Rice University]

June, 2022

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Appendix

Interpolation points?

Interval $[0, 100]$, $n = 1000$, $\zeta(4 + \imath y)$ & $\zeta(3 + 0.5\sin(y) + \imath y)$
Alternate vs. Random shift