Uniform and unitary rational approximations of the matrix exponential

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29th Biennial Numerical Analysis Conference
Strathclyde

Overview

Based on joint work with

Tobias Jawecki (TU Wien)

[JS 23] *Unitarity of some barycentric rational approximants*, Jawecki & S, arXiv:2205.10606 [math.NA]

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Lead to geometric numerical integrators.

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Wave, KdV, NLS, Dirac, Liouville–von Neumann, Linblad, Pauli, MCTDHF, CCSD, TDDFT, ...

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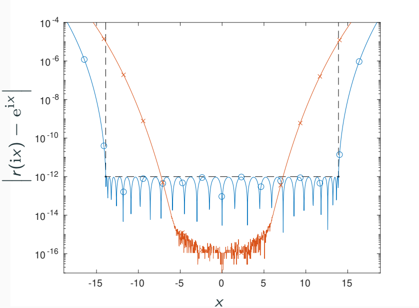
$(13, 13)$ Padé and AAA–Lawson approximants.



Padé methods are rational methods,

$$r_{m,n}(z) = \frac{p_m(z)}{q_n(z)} \approx e^z, \qquad p_m \in \mathcal{P}_m, q_n \in \mathcal{P}_n,$$

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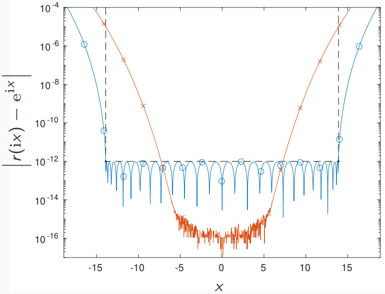

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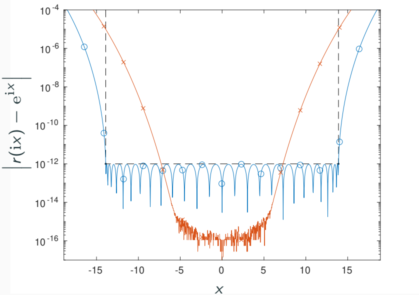

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AAA and AAA–Lawson methods are adaptive algorithms that can produce rational approximants with uniform accuracy over a specified interval or test nodes x_k.

Padé vs AAA

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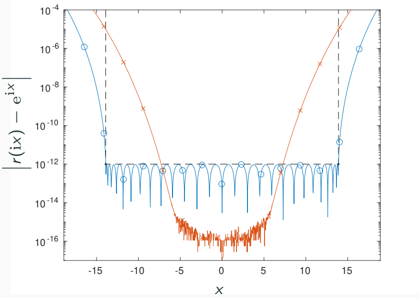

Padé methods are rational methods,

$$r_{m,n}(z) = \frac{p_m(z)}{q_n(z)} \approx e^z, \qquad p_m \in \mathcal{P}_m, q_n \in \mathcal{P}_n,$$

which approximate the Taylor expansion of e^z to the highest degree possible. These are asymptotic in accuracy, i.e. under $z \to 0$, and need to focus most effort near the origin.

AAA and AAA–Lawson methods are adaptive algorithms that can produce rational approximants with uniform accuracy over a specified interval or test nodes x_k.

$$r(x) = \underbrace{\sum_{j=1}^{m} \frac{e^{iy_j} w_j}{x - y_j}}_{n(x)} \Big/ \underbrace{\sum_{j=1}^{m} \frac{w_j}{x - y_j}}_{d(x)},$$

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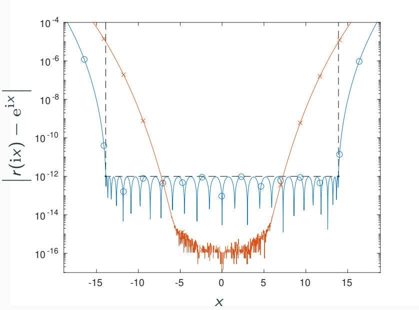

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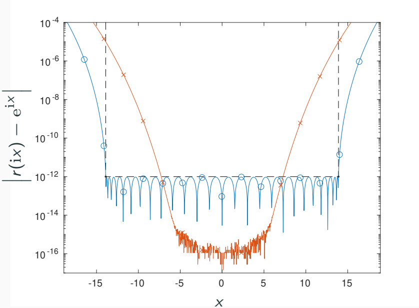

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linearize & minimize $\quad \operatorname{argmin}_w \left(\sum_{k=1}^{n} \mu_k \left| n(x_k) - \mathrm{e}^{\mathrm{i}x_k} d(x_k) \right|^2 \right)^{1/2}.$

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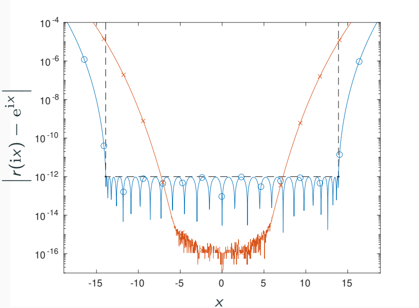

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Linear (weighted) least squares $\Rightarrow$ SVD

Loewner matrix (NST 18)

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Loewner matrix (NST 18)

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Modified AAA via a rotated Loewner matrix (JS 23)

$$K = \mathrm{diag}\Big((1 - \mathrm{e}^{-\mathrm{i}y_j})/|1 - \mathrm{e}^{-\mathrm{i}y_j}|\Big) \quad \text{and} \quad R = \mathrm{diag}\Big((1 - \mathrm{e}^{-\mathrm{i}x_k})/|1 - \mathrm{e}^{-\mathrm{i}x_k}|\Big)$$

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$$S_f K = -K^*, \quad \text{and} \quad R S_F = -R^*.$$

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$$\widehat{L} = -\mathrm{i}RS_F MK + \mathrm{i}RMS_f K$$

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$$\widehat{L} = -\mathrm{i}RS_F MK + \mathrm{i}RMS_f K = \mathrm{i}(R^* MK - RMK^*) = 2\operatorname{Im}(RMK^*) \in \mathbb{R}^{n\times m},$$

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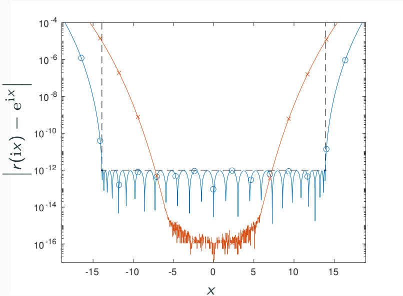
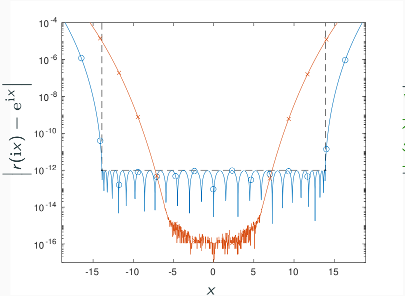
Unitarity to machine precision

Error in approximation of e^{ix}
(Padé vs AAA–Lawson)

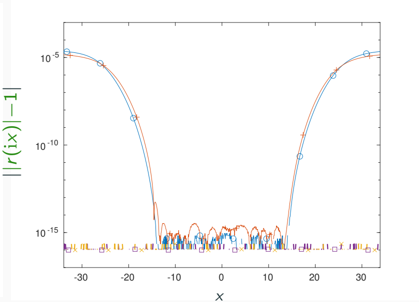


Unitarity to machine precision

Error in approximation of $\mathrm{e}^{\mathrm{i}x}$
(Padé vs AAA–Lawson)



Error in unitarity of approximant r
(original and modified AAA/AAA–Lawson)



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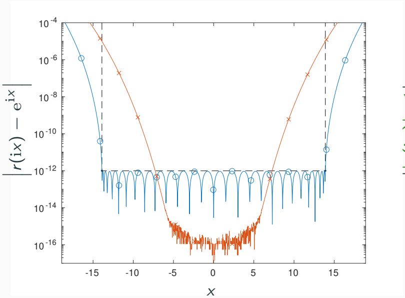

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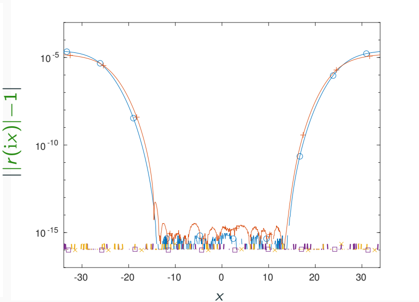

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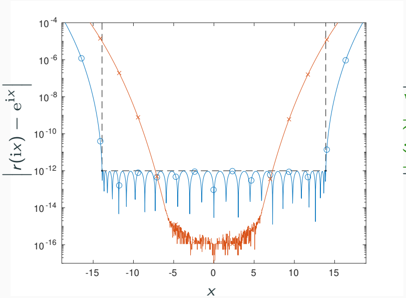

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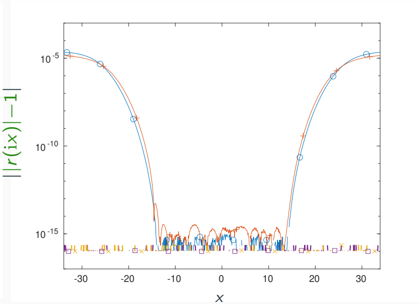

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$$\widetilde{r}(x) = \xi(x)^* \xi(x)^{-1}$$

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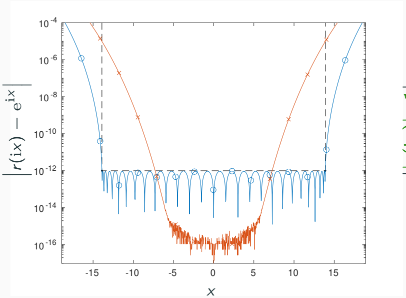

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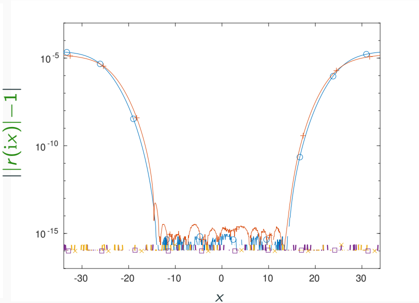

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[JS 23] *Unitarity of some barycentric rational approximants*, Jawecki & S, arXiv:2205.10606