A symbolic-numeric validation algorithm for linear ODEs with Newton-Picard method

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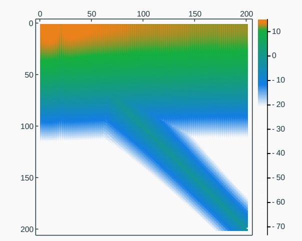
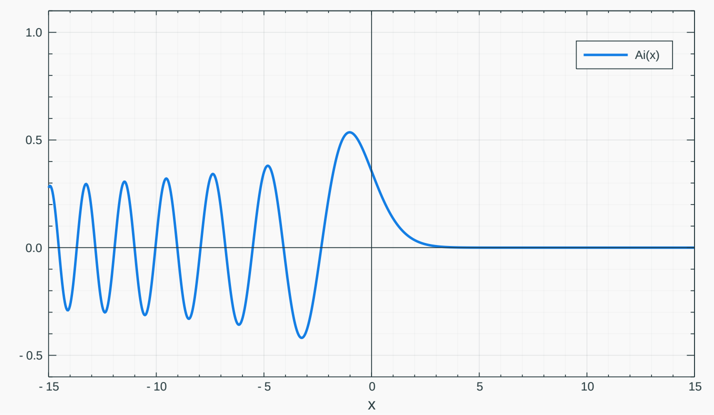


Introduction

An Example: Airy Function

- $\text{Ai}(x) = \frac{1}{\pi} \int_{0}^{+\infty} \cos\left(\frac{t^3}{3} + xt\right) dt$
- Linear Initial Value Problem: $y''(x) - xy(x) = 0, \quad \begin{cases} y(0) = \dfrac{1}{3^{\frac{2}{3}} \Gamma\left(\frac{2}{3}\right)} \\ y'(0) = -\dfrac{1}{3^{\frac{1}{3}} \Gamma\left(\frac{1}{3}\right)} \end{cases}$



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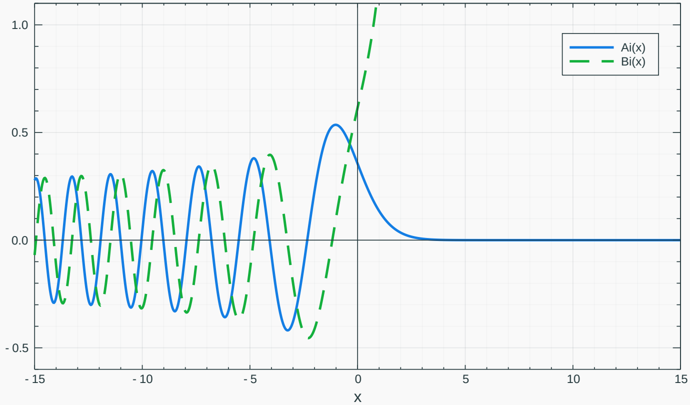

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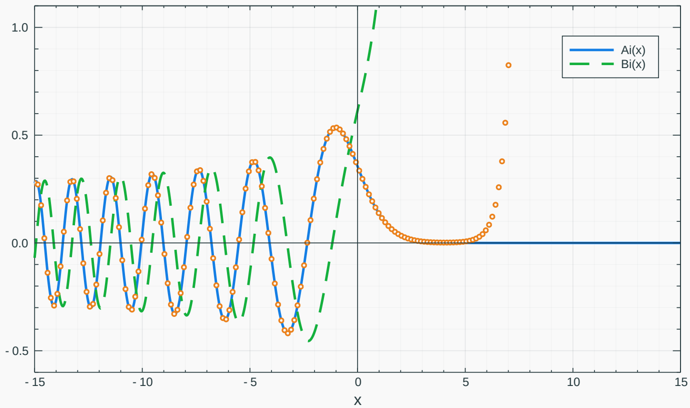

A Brief Review of Functional Analytic Validation Methods for ODEs

- Higher order methods proposed in the literature:
  - *Makino & Berz (1998–), CAPD, VNODE-LP:* Taylor methods
  - *Ultra-arithmetic (1982–), Benoit & Joldes & Mezzarobba (2017), Dzetkulič (2015) :* Picard iterations
  - *Zgliczynski (2002), Wilczak & Zgliczynski (2011):* Lohner methods
  - *Kedem (1981), Plum (1991):* Resolvent kernel/Green function based methods
  - *Mezzarobba (2011):* Majorant series (for D-finite functions)
  - *Yamamoto (1998), Lessard & Mireles James & van den Berg & al. (2014–), Bréhard & Brisebarre & Joldes (2018):* Newton-like a posteriori validated spectral methods
    $\rightarrow$ a.k.a. Newton-Galerkin

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- Comparison of Newton-Picard and Newton-Galerkin:
  - Newton-Galerkin: truncate integral operators (Galerkin projections) to design Newton operators
  - Newton-Picard: inspired by Picard iterations to design Newton operators

A Posteriori Validation Paradigm

$Ly = 0,\ \{y^{(i)}(0) = v_i\}_{i=0}^{r-1}$ linear IVP

Step 1 — Numerical approximation method: Spectral method

- *Polynomial approximations in Chebyshev basis*
- *Floating-point operations*

$\widetilde{y}$

Step 2 — A posteriori validation: Newton-Galerkin vs Newton-Picard

- *Interval operations + RPAs*
- *Newton-like fixed-point operator*

ε

Rigorous Polynomial Approximation (RPA) for y
= pair $(\widetilde{y}, \varepsilon)$ s.t. $\|\widetilde{y} - y\| \leqslant \varepsilon$

Chebyshev Approximations using Spectral Methods

From Differential Equations to Integral Equations (1)

- $L\{y\} \quad = \quad y^{(r)} + a_{r-1}(x)y^{(r-1)} + \cdots + a_1(x)y' + a_0(x)y \quad = \quad h(x),$

  with initial conditions: $\quad y^{(i)}(0) = v_i \quad$ for $\quad 0 \leqslant i < r, \quad \deg a_i \leqslant s$

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  - $f = y^{(r)} \quad \Rightarrow \quad y^{(i)}(x) = \int_0^x \int_0^{t_1} \cdots \int_0^{t_{r-1-i}} f(t_{r-i}) dt_{r-i} \ldots t_1 \; + \sum_{j=i}^{r-1} \frac{x^{j-i}}{(j-i)!} v_j$

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$$\mathfrak{K}(x,t) = \sum_{i=0}^{r-1} a_i(x) \frac{(x-t)^{r-1-i}}{(r-1-i)!} \qquad g(x) = h(x) - \sum_{i=0}^{r-1} a_i(x) \sum_{j=i}^{r-1} \frac{x^{j-i}}{(j-i)!} v_j$$

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Example (Airy)

$$y'' - xy = 0 \quad \Rightarrow \quad f + \int_0^x (xt - x^2) f(t)dt = v_0 x + v_1 x^2 \qquad f = \mathrm{Ai}''$$

From Differential Equations to Integral Equations (2)

- $L\{y\} = (-1)^r y^{(r)} + (-1)^{r-1}(b_{r-1}(x)y)^{(r-1)} + \cdots - (b_1(x)y)' + b_0(x)y = h(x)$,
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Spectral Method for Airy Function

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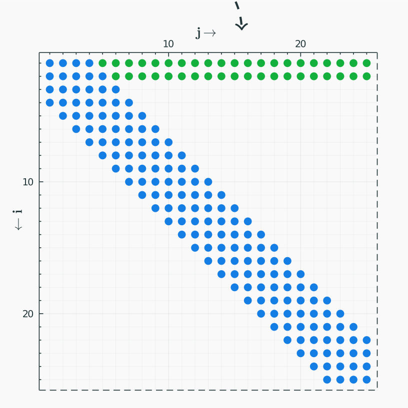

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$\mathbf{K}$: almost-banded, compact

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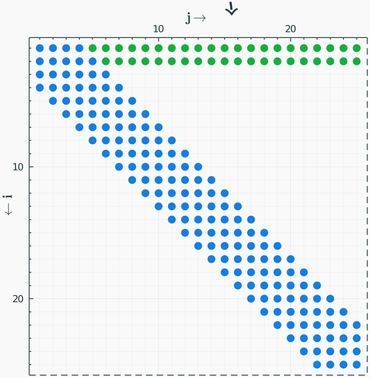

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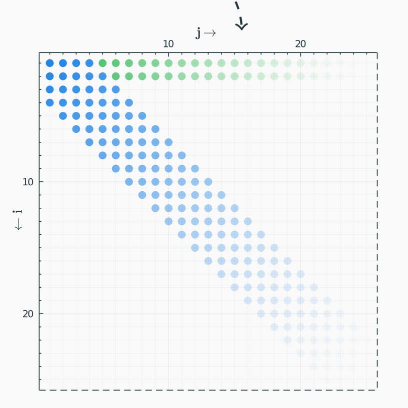

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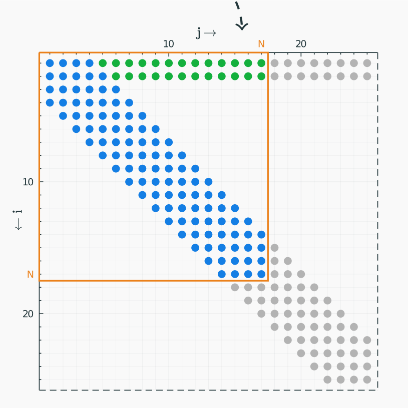

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$K^{[N]}$: truncated operator

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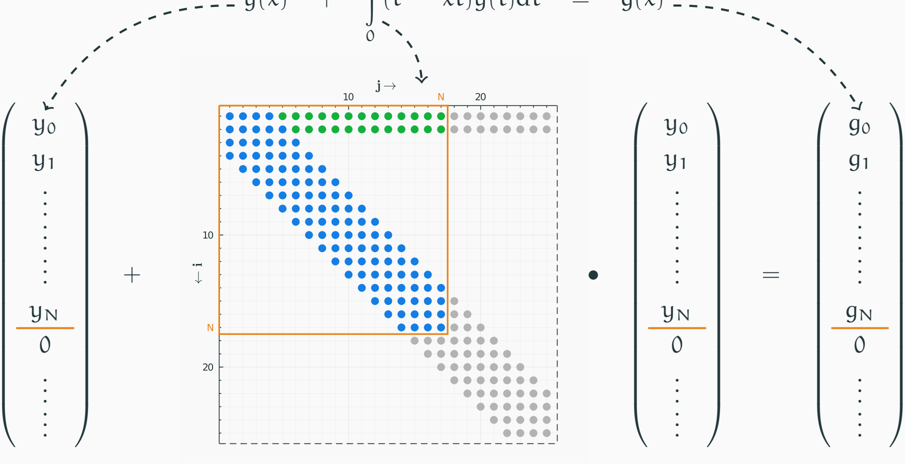
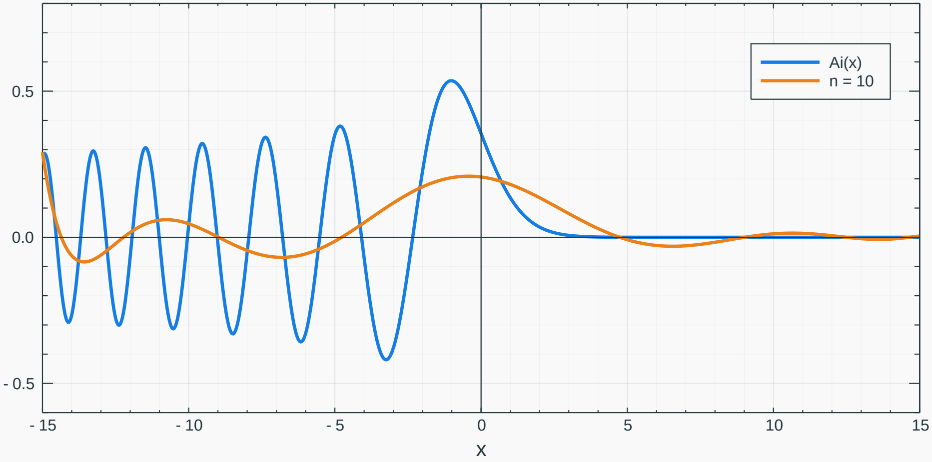


$\mathbf{K}^{[N]}$: truncated operator

- Solution in $\mathcal{O}((r+s)^2 N)$ arith. op. with Olver and Townsend's QR algorithm

Spectral Method for Airy Function



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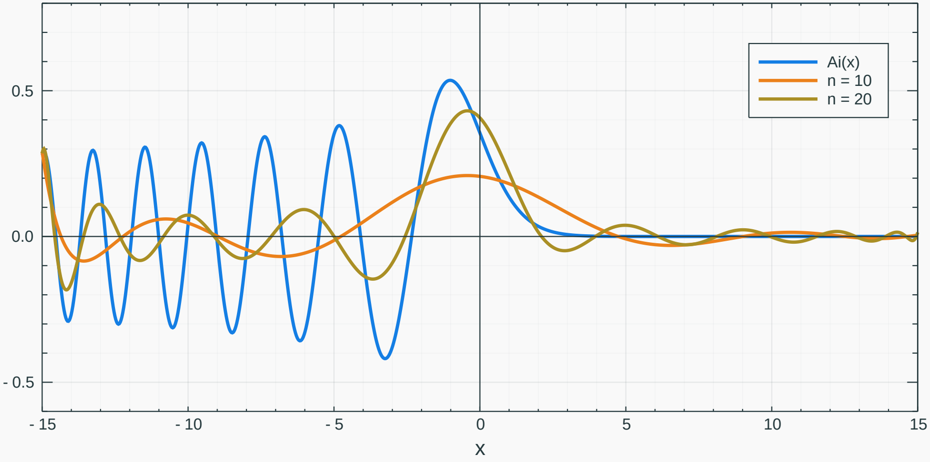

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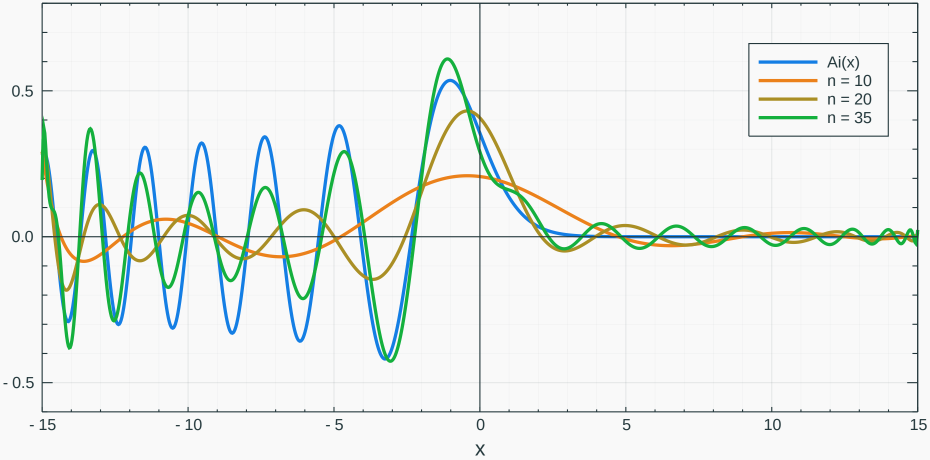

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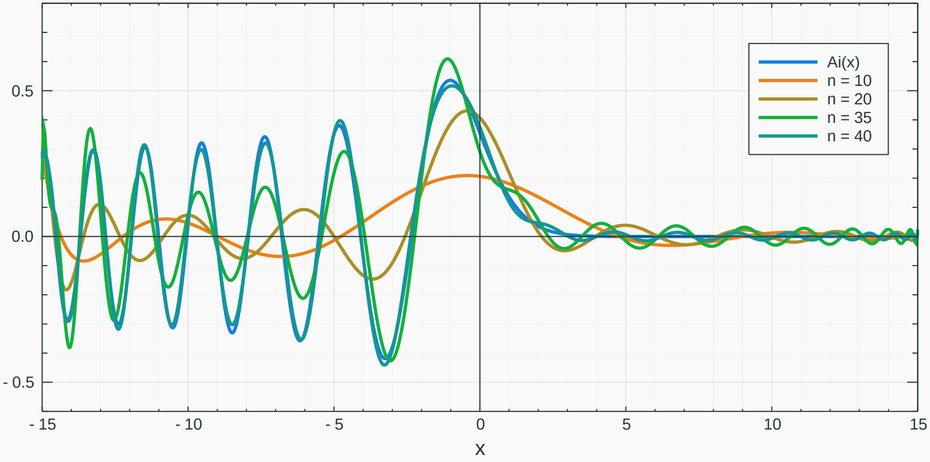

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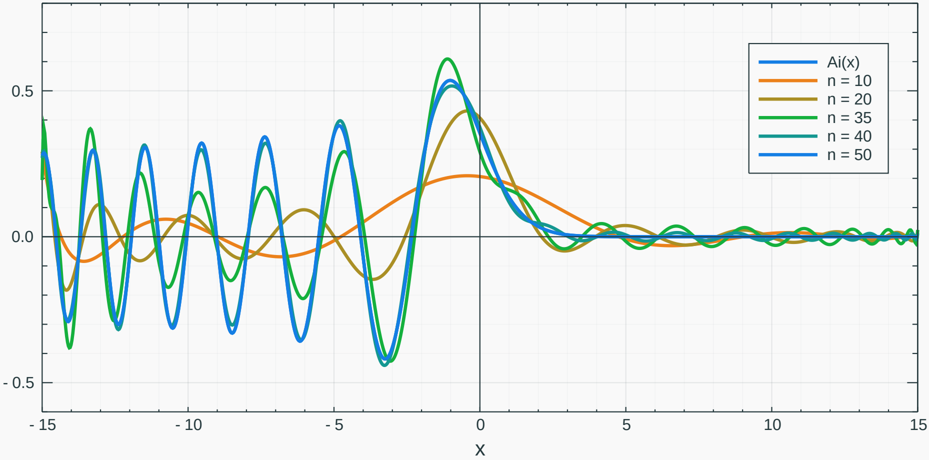
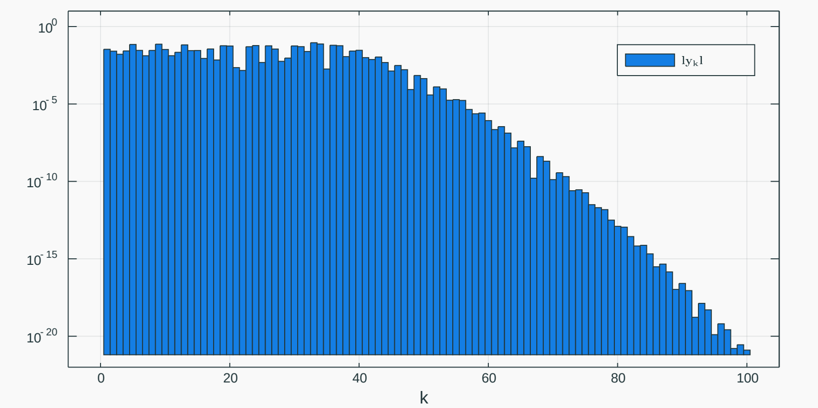


Chebyshev Coefficients of Airy Function

- Super-algebraic decay of Chebyshev coefficients for analytic functions



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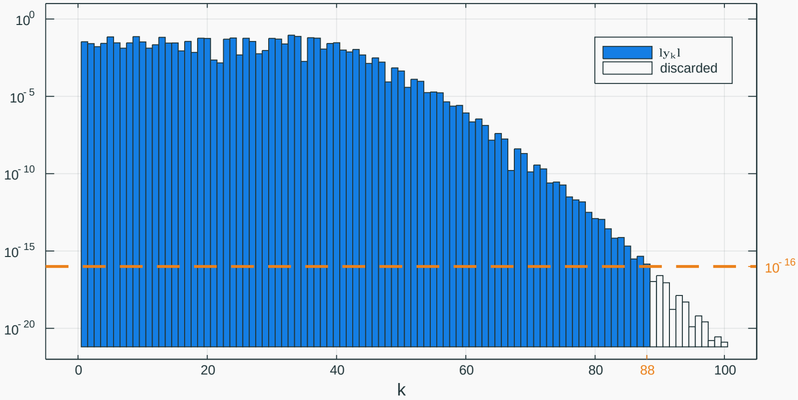


- Heuristic truncation methods in Chebfun, ...
- Need for validation algorithms

Fixed-Point Based Validation

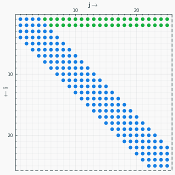
A Posteriori Validation Paradigm

Step 1 ∘ Numerical approximation method

- complexity
- numerical stability
- asymptotic convergence

$\widetilde{y}$

Step 2 ∘ A posteriori validation algorithm



Rigorous Polynomial Approximation (RPA) for y

$= \text{ pair } (\widetilde{y}, \varepsilon) \text{ s.t. } \|\widetilde{y} - y\| \leqslant \varepsilon$

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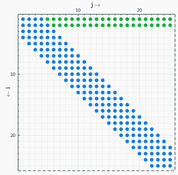
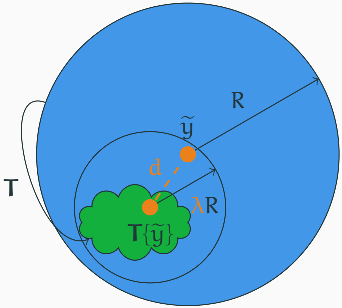


$\widetilde{y}$

Step 2 A posteriori validation algorithm

ε



Banach Fixed-Point Theorem

$$\frac{d}{1+\lambda} \leqslant \|\widetilde{y} - y\| \leqslant \frac{d}{1-\lambda}$$

$$d = \|T\{\widetilde{y}\} - \widetilde{y}\|$$

Rigorous Polynomial Approximation (RPA) for y

$$= \text{pair } (\widetilde{y}, \varepsilon) \text{ s.t. } \|\widetilde{y} - y\| \leqslant \varepsilon$$

Fixed-Point Based Validation

Newton-Galerkin Algorithm

Newton-Galerkin Validation Algorithm

- Newton: $y + \mathbf{K}\{y\} = g \qquad \Leftrightarrow \qquad \mathbf{T}\{y\} = y \quad \begin{cases} \mathbf{T}\{y\} := y - \mathbf{A}\{\, y + \mathbf{K}\{y\} - g \,\} \\ \mathbf{A} \approx (\mathbf{I} + \mathbf{K})^{-1} \end{cases}$

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Define approx inverse $\boldsymbol{A}$

- choose $N_{\mathcal{G}}$
- compute numerical
- $\boldsymbol{A} \approx (\mathbf{I} + \mathbf{K}^{[N_{\mathcal{G}}]})^{-1}$

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Bound the operator norm of T

$$\lambda := \|D\mathsf{T}\| = \|\mathbf{I} - \mathbf{A}\,(\mathbf{I} + \mathbf{K})\|$$
$$\leqslant \underbrace{\|\mathbf{I} - \mathbf{A}\,(\mathbf{I} + \mathbf{K}^{[N_{\mathcal{G}}]})\|}_{\text{approximation error}} + \underbrace{\|\mathbf{A}\,(\mathbf{K} - \mathbf{K}^{[N_{\mathcal{G}}]})\|}_{\text{truncation error}}$$

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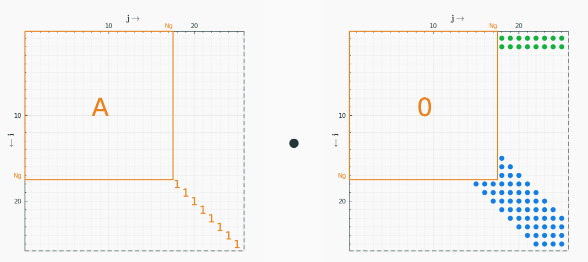

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$$\lambda := \|D\mathbf{T}\| = \|\mathbf{I} - \mathbf{A}(\mathbf{I} + \mathbf{K})\| \leqslant \underbrace{\|\mathbf{I} - \mathbf{A}(\mathbf{I} + \mathbf{K}^{[N_{\mathcal{G}}]})\|}_{\text{approximation error}} + \underbrace{\|\mathbf{A}(\mathbf{K} - \mathbf{K}^{[N_{\mathcal{G}}]})\|}_{\text{truncation error}}$$

- $\|\tilde{y} - y\| \leqslant \|\mathbf{T}\{\tilde{y}\} - \tilde{y}\| / (1 - \lambda)$

Theorem (Bréhard, Brisebarre, Joldes) — ACM Trans. Math. Softw.
Validating a degree N approximation $\tilde{y}$ requires:

$$\mathcal{O}(\, N_{\mathcal{G}}^2 (r + s) + (N_{\mathcal{G}} + r + s) N \,) \qquad \text{arithmetic operations}$$

Newton-Galerkin Validation Algorithm

- Newton: $y + \mathbf{K}\{y\} = g \quad \Leftrightarrow \quad \mathbf{T}\{y\} = y \quad \begin{cases} \mathbf{T}\{y\} := y - \mathbf{A}\{ y + \mathbf{K}\{y\} - g \} \\ \mathbf{A} \approx (\mathbf{I} + \mathbf{K})^{-1} \end{cases}$

Define approx inverse $\boldsymbol{A}$

- choose $N_{\mathcal{G}}$
- compute numerical
  $\mathbf{A} \approx (\mathbf{I} + \mathbf{K}^{[N_{\mathcal{G}}]})^{-1}$

Bound the operator norm of $\mathbf{T}$

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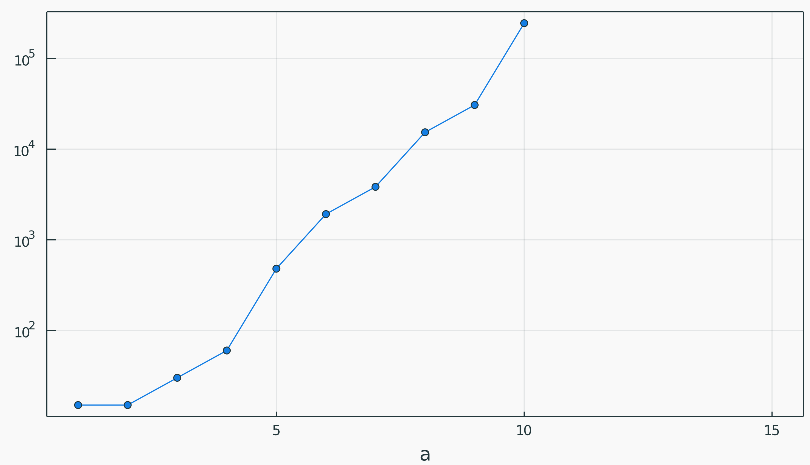
…but $N_{\mathcal{G}}$ may be exponential w.r.t. the $\|a_i\|$!

Newton-Galerkin Validation on Airy Example

- Newton-Galerkin method for Airy function over $[-a, a]$

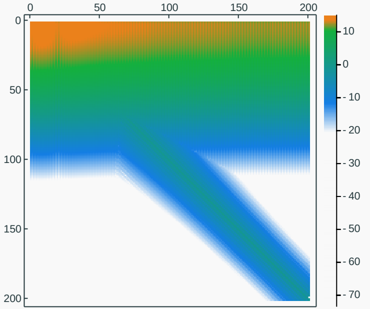


$\Rightarrow$ Truncation index $N_{\mathcal{G}}$ grows exponentially fast!

Fixed-Point Based Validation

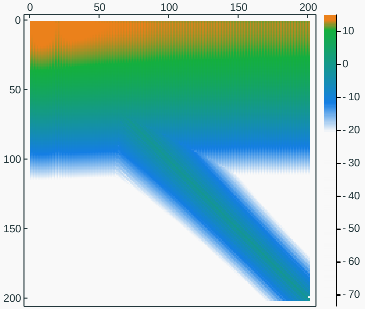
Newton-Picard Algorithm

Almost Banded Approximate Inverses



- $(\mathbf{I}+\mathbf{K})^{-1}$ is "asymptotically almost-banded"

Almost Banded Approximate Inverses



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… because of Picard iterations:

$$(\mathbf{I}+\mathbf{K})^{-1} = \mathbf{I} - \mathbf{K} + \mathbf{K}^2 - \cdots + (-1)^n \mathbf{K}^n + \ldots$$

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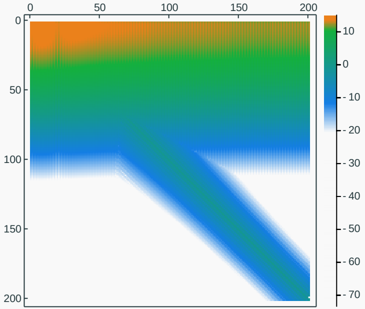

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$$\left.\begin{aligned} \mathbf{K} &\rightsquigarrow \mathfrak{K}(x,t) \\ \mathbf{L} &\rightsquigarrow \mathfrak{L}(x,t) \end{aligned}\right\} \quad \Rightarrow \quad \mathbf{K}\,\mathbf{L} \rightsquigarrow \mathfrak{K} * \mathfrak{L} \quad \text{where} \quad (\mathfrak{K} * \mathfrak{L})(x,t) := \int_t^x \mathfrak{K}(x,s)\mathfrak{L}(s,t)ds$$

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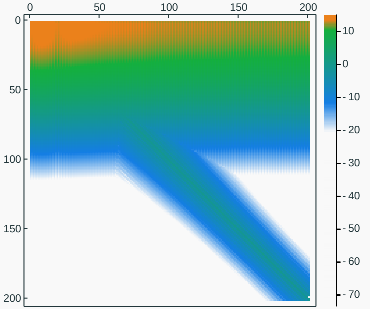

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Iterated Kernels and Resolvent Kernel

$$\left.\begin{aligned} |\mathfrak{K}^{*n}(x,t)| &\leqslant \frac{(x-t)^{n-1}}{(n-1)!} M^n \\ M &:= \sup_{0 \leqslant t \leqslant x \leqslant T} |\mathfrak{K}(x,t)| \end{aligned}\right\}$$

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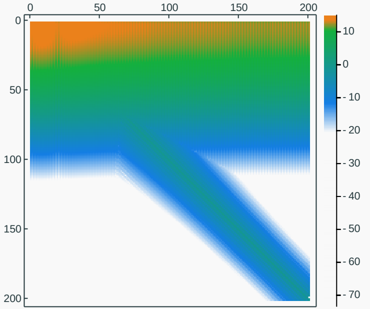

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$$= \mathbf{I} + \mathbf{R} \quad \text{where} \quad \mathbf{R} \rightsquigarrow \mathfrak{R}(x,t)$$

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Newton-Picard Validation Algorithm

Validating a candidate approximation $\widetilde{y}$:

1. Compute $\mathbf{I} + \widetilde{\mathbf{R}} \approx (\mathbf{I} + \mathbf{K})^{-1}$ with $\widetilde{\mathbf{R}} \rightsquigarrow \widetilde{\mathfrak{R}}(x, t) \approx \mathfrak{R}(x, t)$ polynomial

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2. Bound the operator norm:

   $$-D\mathbf{T} \;=\; (\mathbf{I} + \widetilde{\mathbf{R}})(\mathbf{I} + \mathbf{K}) - \mathbf{I} \;=\; \mathbf{K} + \widetilde{\mathbf{R}} + \widetilde{\mathbf{R}}\mathbf{K} \quad \rightsquigarrow \quad \mathfrak{K} + \widetilde{\mathfrak{R}} + \widetilde{\mathfrak{R}} * \mathfrak{K} \;=:\; \mathfrak{E}$$

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   $$\frac{d}{1+\lambda} \leqslant \|\widetilde{y} - y\| \leqslant \frac{d}{1-\lambda}$$

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> How to efficiently approximate $\mathfrak{R}(x,t)$?

Formulas for Resolvent Kernel Approximation

- $\mathbf{L} = \partial^r + a_{r-1}(x)\partial^{r-1} + \cdots + a_0(x) \quad \rightsquigarrow \quad$ $\mathbf{K}$ acting on $f = y^{(r)}$

$$\mathfrak{R}(x,t) = \sum_{i=0}^{r-1} \varphi_i^{(r)}(x)\psi_i(t)$$

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- Approximations using spectral methods to some degree $N_{\mathfrak{R}}$
- The idea is very close to the fast algorithm for power series solutions to ODEs, but in a symbolic-numeric setting
  (*Bostan, Chyzak, Ollivier, Salvy, Schost, Sedoglavic – 2006*)

Complexity Analysis of Newton-Picard Validation Algorithm

Validating a candidate approximation $\widetilde{y}$ of degree N:

1. Choose a validation degree $N_{\mathfrak{R}}$ and

   compute $\quad \widetilde{\mathfrak{R}}(x,t) := \sum_{i=0}^{r-1} \widetilde{\varphi}_i^{(r)}(x)\widetilde{\psi}_i(t) \approx \sum_{i=0}^{r-1} \varphi_i^{(r)}(x)\psi_i(t) =: \mathfrak{R}(x,t)$

2. Bound the norm of $\quad \mathfrak{E} := \mathfrak{K} + \widetilde{\mathfrak{R}} + +\widetilde{\mathfrak{R}} * \mathfrak{K}$

3. Compute defect $\quad \|\mathbf{T}\{\widetilde{y}\} - \widetilde{y}\| = \|(\mathbf{I} + \widetilde{\mathbf{R}})\{\,\widetilde{y} + \mathbf{K}\{\widetilde{y}\} - g\,\}\|$

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   complexity: $\quad \mathcal{O}((r+s)^2 N_{\mathfrak{R}})$

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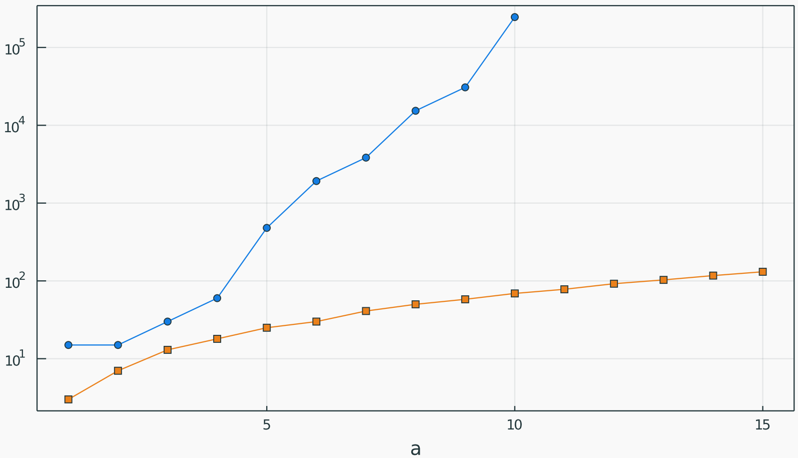
Newton-Galerkin's $N_{\mathcal{G}}$ *vs* Newton-Picard's $N_{\mathfrak{R}}$?

- $N_{\mathcal{G}} = \mathcal{O}\left(\sum_i \|\varphi_i^{(r)}\|\|\psi_i\|\right) \quad \rightsquigarrow \quad$ exponential in the $\|a_i\|$
- $N_{\mathfrak{R}} = \mathcal{O}\left(\log\left(\sum_i \|\varphi_i^{(r)}\|\|\psi_i\|\right)\right) \rightsquigarrow$ polynomial in the $\|a_i\|$

Newton-Galerkin vs Newton-Picard on Airy Example

- Validation for Airy function over $[-a, a]$



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- $N_{\mathfrak{R}}$ $\rightsquigarrow$ polynomial in the $\|a_i\|$