A Symbolic-Numeric Validation Algorithm for Linear ODEs with Newton-Picard Method

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1 Introduction

Efficient and reliable evaluation of solutions to differential equations is a major challenge for a wide range of applications in critical engineering as well as computer-assisted proofs involving dynamical systems. Most of the time, one lacks closed form solution, and *validated numerics* [7] aims at providing numerical algorithms, yet with guaranteed bounds encompassing all sources of errors.

Among the vast literature dedicated to the design of such methods – even in the simpler case of ordinary differential equations (ODE) – *a posteriori Newton-Galerkin* methods have proven to efficiently compute afterwards tight error bounds ε for a candidate approximation, e.g. a polynomial p (see e.g. [8, 6]). The pair (p, ε) is called a *rigorous polynomial approximation* (RPA) and denotes an ε-ball containing the solution, in a suitable function space. In [3], we provided a thorough algorithmic analysis of such methods for linear ODEs in Chebyshev basis. This notably enhances the symbolic machinery of *D-finite functions* with efficient *symbolic-numeric* representations, namely RPAs in Chebyshev basis.

Problem 1. Given a polynomial y° approximating the exact solution y^* of the Initial Value Problem (IVP):

$$\begin{aligned} y^{(r)}(x) + a_{r-1}(x)y^{(r-1)}(x) + \cdots + a_0(x)y(x) = h(x), \quad x \in [x_l, x_r], \\ y(x_0) = v_0, \ldots, y^{(r-1)}(x_0) = v_{r-1}, \quad a_0, \ldots, a_{r-1}, h \in \mathbb{R}[x],\ x_0 \in [x_l, x_r], \end{aligned} \tag{1}$$

compute a bound $\varepsilon \geqslant \|y^\circ - y^*\| := \sup_{x\in[x_l,x_r]} |y^\circ(x) - y^*(x)|$.

The motivation of the present work is to overcome the limitations of Newton-Galerkin methods by designing a new family of a posteriori validation algorithms called *Newton-Picard*. As pointed out in [3], Newton-Galerkin methods suffer from an exponential complexity, making intractable the validation of harder instances, e.g. rapidly growing or oscillating functions. By contrast, the complexity of Newton-Picard validation algorithm remains polynomial with the magnitude of the input equation. Moreover, this new algorithm is mostly independent from the working basis (it is even possible to validate piecewise constant approximations, for example). This in particular makes it suitable to be implemented in a formal proof assistant, which we plan to do in the future, using a previously developed framework [4] for RPAs and a posteriori validation in Coq [2].

2 A Posteriori Validation and Newton-Galerkin Method

Let y° be a polynomial approximating the exact solution y^*. To validate it, we first automatically restate the IVP (1) as a Volterra integral equation:

$$\mathbf{F}\{y\} := y + \mathbf{K}\{y\} - g = 0, \quad \text{where} \quad \mathbf{K}\{y\}(x) := \int_{x_0}^{x} \mathfrak{K}(x,t)y(t)\mathrm{d}t, \qquad (2)$$

with a bivariate polynomial kernel $\mathfrak{K}(x,t) = \sum_{k=0}^{r-1} \beta_k(x)\alpha_k(t)$. The main steps of *a posteriori Newton validation* are:

1. Transform Equation (2) into an equivalent fixed-point equation:
$$\mathbf{T}\{y\} = y, \quad \text{where} \quad \mathbf{T}\{y\} := y - \mathbf{A}\{\mathbf{F}\{y\}\} = y - \mathbf{A}\{y + \mathbf{K}\{y\} - g\},$$
with $\mathbf{A}$ a linear operator approximating $(\mathbf{1}+\mathbf{K})^{-1}$.
2. Prove that $\mathbf{T}$ is contracting by computing $\lambda < 1$ s.t.:
$$\lambda \geqslant \|\mathbf{E}\|, \quad \text{where} \quad \mathbf{E} := \mathbf{I} - \mathbf{A}(\mathbf{I}+\mathbf{K}).$$
3. Apply the Banach fixed-point theorem to provide an error enclosure:
$$\frac{\|y^\circ - \mathbf{T}\{y^\circ\}\|}{1+\lambda} \leqslant \|y^\circ - y^*\| \leqslant \frac{\|y^\circ - \mathbf{T}\{y^\circ\}\|}{1-\lambda}.$$

The main challenge to make Newton validation effective is to find sufficiently accurate, yet explicitly computable operator $\mathbf{A}$ for the infinite-dimensional inverse of $\mathbf{1}+\mathbf{K}$. In Newton-Galerkin validation methods, this is achieved by projecting the integral operator $\mathbf{K}$ onto a finite subspace of a well-chosen coefficient space, yielding the truncated Galerkin operator $\mathbf{K}^{[N_\mathcal{G}]}$. Estimating an appropriate value for the truncation index $N_\mathcal{G}$ and rigorously bounding the operator norm of $\mathbf{E}$ are performed by the algorithms detailed in [3].

3 An Efficient Newton-Picard Validation Algorithm

3.1 Principle of the Method

The motivation of this new work is that $(\mathbf{1}+\mathbf{K})^{-1}$ is poorly approximated by inverse truncated operators $(\mathbf{1}+\mathbf{K}^{[N_\mathcal{G}]})^{-1}$, in $O(1/N_\mathcal{G})$ only, leading to exponential worst-case bounds for $N_\mathcal{G}$ (see [3, Sec. 5.2.2]). Instead, we make use of the following convergent series, historically known as Picard iterations [5]:

$$(\mathbf{1}+\mathbf{K})^{-1} = \mathbf{1}-\mathbf{K}+\mathbf{K}^2-\cdots = \mathbf{1}+\mathbf{R}, \quad \text{with} \quad \mathbf{R}\{y\}(x) = \int_{x_0}^{x} \mathfrak{R}(x,t)y(t)\mathrm{d}t, \quad (3)$$

with analytic $\mathfrak{R}(x,t)$ called the *resolvent kernel*. This simply comes from the property that the composition $\mathbf{KL}$ of two integral operators $\mathbf{K}$ and $\mathbf{L}$ of respective kernels $\mathfrak{K}$ and $\mathfrak{L}$ is again an integral operator:

$$\mathbf{K}\{\mathbf{L}\{y\}\}(x) = \int_{x_0}^{x} (\mathfrak{K}*\mathfrak{L})(x,t)y(t)\mathrm{d}t, \quad \text{with} \quad (\mathfrak{K}*\mathfrak{L})(x,t) := \int_{t}^{x} \mathfrak{K}(x,s)\mathfrak{L}(s,t)\mathrm{d}s.$$

Our new method consists in defining the linear operator $\mathbf{A}$ for step 1 of a posteriori Newton validation as $\mathbf{1} + \mathbf{R}^\circ$, by approximating the resolvent kernel $\mathfrak{R}$ with a polynomial kernel $\mathfrak{R}^\circ$, rather than projecting onto a finite-dimensional subspace – whence the name *Newton-Picard*. An efficient approximation method for it is described in the next section. In the following, we assume that $\mathfrak{R}^\circ$ is given and we implement steps 2 and 3 listed above.

2. The linear part $\mathbf{E}$ of $\mathbf{T}$ is again an integral operator:
$$\mathbf{E} = \mathbf{I} - \mathbf{A}(\mathbf{I} + \mathbf{K}) = \mathbf{I} - (\mathbf{I} + \mathbf{R}^\circ)(\mathbf{I} + \mathbf{K}) = -\mathbf{R}^\circ - \mathbf{K} - \mathbf{R}^\circ\mathbf{K},$$
with a polynomial kernel $\mathfrak{E} := -\mathfrak{R}^\circ - \mathfrak{K} - \mathfrak{R}^\circ * \mathfrak{K}$, explicitly computable as a finite sum $\sum_i \mu_i(x)\nu_i(t)$. Compute an upper bound $\lambda \geqslant \|\mathbf{E}\|$.
3. If $\lambda < 1$, then compute and return $\varepsilon := \|y^\circ - \mathbf{T}\{y^\circ\}\|/(1-\lambda)$.

3.2 Approximating the Resolvent Kernel

Approximating the resolvent kernel $\mathfrak{R}$ with a polynomial kernel $\mathfrak{R}^\circ$ can be achieved by truncating the series (3) and computing the iterated kernels $\mathfrak{K}^{*n}$. This is equivalent in disguise to the validation algorithm of [1]. For practical efficiency however, we propose an alternative way, based on the *transition matrix* $\Phi(x)$ associated to the homogeneous linear ODE.

Definition 1. *$\Phi(x) \in \mathbb{R}^{r\times r}$ is the unique solution of:*
$$\Phi'(x) = A(x)\Phi(x), \quad \text{with } A(x) := \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \\ \text{-}a_0(x) & \text{-}a_1(x) & \text{-}a_2(x) & \cdots & \text{-}a_{r-1}(x) \end{pmatrix} \text{ and } \Phi(x_0) = I_r.$$

We proceed as follows, using this key formula.

Proposition 1.
$$\mathfrak{R}(x,t) = (-1)^r \begin{pmatrix} 1 & 0 & \cdots & 0 \end{pmatrix} \Phi(x) \left(\Phi(t)^{-1}\right)^{(r)} \begin{pmatrix} 0 \\ \vdots \\ 1 \end{pmatrix} =: \sum_{k=0}^{r-1} \varphi_k(x)\psi_k(t).$$

- We compute a degree $N_{\mathfrak{R}}$ polynomial approximation $\Phi^\circ(x)$ of the transition matrix $\Phi(x)$ by numerically solving IVP (1) r times with corresponding initial conditions.
- $\Psi(t) := \left(\Phi(t)^{-1}\right)^T$ satisfies $\Psi(x_0) = I_r$ and $\Psi'(t) = A(t)^T\Psi(t)$. Hence, we compute a degree $N_{\mathfrak{R}}$ polynomial approximation $\Psi^\circ(t)$ and differentiate it r times.
- This gives a polynomial approximation of the resolvent kernel of the form:
$$\mathfrak{R}^\circ(x,t) := \sum_{k=0}^{r-1} \varphi_k^\circ(x)\psi_k^\circ(t) \approx \sum_{k=0}^{r-1} \varphi_k(x)\psi_k(t) = \mathfrak{R}(x,t).$$

3.3 Complexity Analysis

While spectral-Galerkin methods compute Chebyshev polynomial approximations that converge exponentially fast to the solution of the IVP problem, the Lipschitz constant of the Newton-Galerkin fixed-point operator converges to 0 in $O(1/N_{\mathcal{G}})$ only, where $N_{\mathcal{G}}$ is the truncation degree, yielding an exponential complexity for the validation method. This phenomenon is illustrated in [3, Sec. 7.1] with the Airy function over intervals $[0, a]$ for $a > 0$, for which the minimum value of n resulting in a contracting operator grows exponentially fast with a.

On the contrary, Theorem 1 below shows that the Lipschitz constant of the Newton-Picard validation operator converges exponentially fast w.r.t. the degree $N_{\mathfrak{R}}$ used in the inverse kernel approximation method described above. To simplify the picture, suppose we can compute exact degree $N_{\mathfrak{R}}$ truncated Chebyshev series φ_k°, ψ_k° for φ_k, ψ_k, so that $\|\varphi_k^\circ - \varphi_k\|_{\mathcal{E}_\rho} \leqslant 2\|\varphi_k\|_{\mathcal{E}_\rho}\rho^{-N_{\mathfrak{R}}}/(\rho-1)$ and $\|\psi_k^\circ - \psi_k\|_{\mathcal{E}_\rho} \leqslant 2\|\psi_k\|_{\mathcal{E}_\rho}\rho^{-N_{\mathfrak{R}}}/(\rho-1)$, where $\|\cdot\|_{\mathcal{E}_\rho}$ is the supremum norm over an ellipse $\mathcal{E}_\rho$ (for $\rho > 1$) of foci x_l and x_r and eccentricity $2/(\rho + \rho^{-1})$.

Theorem 1. *The operator norm of the linear part* $\mathbf{E}$ *of* $\mathbf{T}$ *is bounded by:*

$$\|\mathbf{E}\| \leqslant 4T\left(\frac{\rho^{-N_{\mathfrak{R}}}}{\rho-1} + \frac{\rho^{-2N_{\mathfrak{R}}}}{(\rho-1)^2}\right)\left(\sum_{k=0}^{r-1}\|\varphi_k\|_{\mathcal{E}_\rho}\|\psi_k\|_{\mathcal{E}_\rho}\right)\left(1 + T\sum_{k=0}^{r-1}\|\alpha_k\|\|\beta_k\|\right),$$

where $T = \max(x_r - x_0, x_0 - x_l)$ *is the maximum elapsed time. The* $\|\varphi_k\|_{\mathcal{E}_\rho}$, $\|\psi_k\|_{\mathcal{E}_\rho}$ *being exponentially bounded by the* $\|\alpha_k\|_{\mathcal{E}_\rho}, \|\beta_k\|_{\mathcal{E}_\rho}$*, the minimum* $N_{\mathfrak{R}}$ *for which* $\|\mathbf{E}\| < 1$ *depends linearly on the* $\|\alpha_k\|_{\mathcal{E}_\rho}$, $\|\beta_k\|_{\mathcal{E}_\rho}$.

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