A Newton-like Validation Method for Chebyshev Approximate Solutions of Linear Ordinary Differential Systems

Florent Bréhard

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Florent Bréhard[1]

[1]École Normale Supérieure de Lyon and LAAS-CNRS, France

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Abstract

We provide a new framework for *a posteriori* validation of vector-valued problems with componentwise tight error enclosures, and use it to design a symbolic-numeric Newton-like validation algorithm for Chebyshev approximate solutions of coupled systems of linear ordinary differential equations. More precisely, given a coupled differential system of dimension p with polynomial coefficients over a compact interval (or continuous coefficients rigorously approximated by polynomials) and polynomial approximate solutions Φ_i° in Chebyshev basis ($1 \leqslant i \leqslant p$), the algorithm outputs rigorous upper bounds ε_i for the approximation error of Φ_i° to the exact solution $\Phi_i^\star$, with respect to the uniform norm over the interval under consideration.

A complexity analysis shows that the number of arithmetic operations needed by this algorithm (in floating-point or interval arithmetics) is proportional to the approximation degree when the differential equation is considered fixed. Finally, we illustrate the efficiency of this fully automated validation method on an example of a coupled Airy-like system.

1 Introduction

Notations. Let p be a positive integer for the ambient space $\mathbb{R}^p$, whose canonical basis is denoted by $(e_1, \ldots, e_p)$. For a ring $\mathbb{A}$, $\mathcal{M}_p(\mathbb{A})$ denotes the set of order p square matrices, with $\mathbf{1}$ and $\mathbf{0}$ the identity and zero matrices.

The order $\leqslant$ over $\mathbb{R}$ is componentwise extended to a (partial) order over $\mathbb{R}^p$ and $\mathcal{M}_p(\mathbb{R})$: for all $u, v \in \mathbb{R}^p$ (resp. A, B in $\mathcal{M}_p(\mathbb{R})$), $u \leqslant v$ if and only if $u_i \leqslant v_i$ for all $i \in [\![1, p]\!]$ (resp. $A \leqslant B$ iff $A_{ij} \leqslant B_{ij}$ for all $i, j \in [\![1, p]\!]$).

Unless otherwise specified, a function f is defined over the interval $[-1, 1]$, with $\|f\|_\infty = \sup_{x\in[-1,1]} |f(x)|$ denoting the uniform norm over $[-1, 1]$.

Problem statement and contributions. We present a symbolic-numeric *a posteriori* fixed-point validation algorithm for Chebyshev approximations to solutions of coupled linear ordinary differential equations (LODEs), that provides *componentwise* and *tight* error enclosures. Coefficients of the system must be continuous functions, given as polynomials with rigorous error bounds. However, for the sake of simplicity, we mainly focus on the polynomial case, and refer to the solutions as *vector-valued D-finite functions*. Although such functions can be seen as vectors of (scalar) D-finite functions, the decoupling of the system followed by a possible desingularization step may produce hard to validate scalar LODEs (see Section 4). Moreover, in the nonpolynomial case, such techniques do not apply.

Using an appropriate integral transform of the linear differential system, we obtain a Volterra integral equation of the second kind with polynomial kernel, whence the following problem statement:

Problem 1. *For a given integral equation of unknown $\Phi : [-1, 1] \to \mathbb{R}^p$:*

$$\Phi(t) + \int_{-1}^{t} K(t, s) \cdot \Phi(s)\mathrm{d}s = \Psi(t),$$

with a p-dimensional polynomial kernel $K(t, s) \in \mathcal{M}_p(\mathbb{R}[t, s])$ and $\Psi \in \mathbb{R}[t]^p$, assuming we are given for each component $\Phi_i^\star$ of the exact solution $\Phi^\star$ a polynomial approximation Φ_i° in Chebyshev basis, compute componentwise error bounds ε_i, as tight as possible:

$$\|\Phi_i^\circ - \Phi_i^\star\| \leqslant \varepsilon_i, \qquad \textit{for all } i \in [\![1, p]\!].$$

Fixed-point methods are extensively used in the field of functional analysis and differential equations. They provide iterative approximation schemes, like Picard-Chebyshev which integrates nonlinear dynamical systems arising, for instance, in space flight mechanics problems [8, 4]. They also underlie numerous validation methods for function space problems [13, 23].

A wide range of fixed-point validation methods use Banach fixed-point theorem. Given an equation $x = \mathbf{T} \cdot x$ with $\mathbf{T}$ contracting of ratio $\lambda \in (0, 1)$ over a complete metric space, and an approximation x to the exact solution $x^\star$, it provides an enclosure of the error:

$$\frac{\|x - \mathbf{T} \cdot x\|}{1 + \lambda} \leqslant \|x - x^\star\| \leqslant \frac{\|x - \mathbf{T} \cdot x\|}{1 - \lambda}. \tag{1}$$

However, in the case we consider, x belongs to a product space, and the classical method consisting in endowing it with a global norm fails to produce componentwise tight error enclosures. This is particularly annoying when the components of the system are of different nature (e.g., position and speed) or magnitude.

Based on a new refinement with lower bounds for Perov fixed-point theorem (a vector-valued generalization of Banach fixed-point principle), we propose a validation algorithm to solve Problem 1. It is a generalization of the validation method presented in [7] to vectorial LODEs, within a new general framework for vector-valued fixed-point validation.

Theorem 1. *Algorithms 1 and 3 solve together Problem 1 by providing componentwise error enclosures.*

(i) Algorithm 1 only depends on the integral equation (not on the provided approximation). It produces and rigorously bounds a Newton-like validation operator and requires $O(p^3 {N_{\text{val}}}^2 d)$ arithmetic operations.

(ii) Algorithm 3 computes the error enclosures for the approximation and runs in linear time with respect to the maximum degree of the approximations Φ_i° and the right-hand sides Ψ_i. More precisely, its complexity is $O(p^2 d^2 N_{\text{app}} + pN_{\text{rhs}} + p^2 N_{\text{val}} \min(\max(N_{\text{app}} + d, N_{\text{rhs}}), N_{\text{val}}))$.

where:

- $N_{\text{app}} = \max_i \deg \Phi_i^\circ$ *and* $N_{\text{rhs}} = \max_i \deg \Psi_i$*;*
- $d = 1 + \max_{ij} \deg k_{ij}(t, s)$*;*
- N_{val} *is a truncation index used to rigorously approximate the problem in finite dimension.*

We assume a uniform complexity model, i.e., a unit cost for each arithmetic operation ($+, -, \times, /, \sqrt{}$), with, say, floating-point or interval operands.

The previous complexity estimates still involve a truncation index N_{val}, which is directly related to how tight the desired error enclosures have to be. As detailed in Theorem 4, its minimal value ensuring a contracting Newton-like operator is potentially exponential with respect to the magnitude of the coefficients of the integral equation, in the case of stiff LODEs for example. In practice however, this method works efficiently and fully automatically. An open source library implementing this validation method (and its extension to the nonpolynomial case) can be found here [1]. It was also recently used for a space flight dynamics application [3].

[1] http://perso.ens-lyon.fr/florent.brehard

Previous work. In this context, applications of Banach fixed-point theorem include early works [13, 23], where variations of Newton's method perform *a posteriori* validation in function spaces. More recent works developed techniques (e.g., *radii polynomials* [10]) to find a stable neighborhood of an approximation φ over which Banach fixed-point theorem applies. They have the advantage of dealing with nonlinear problems (examples can be found in [14, 22, 10]). However, the above mentioned methods were not fully automated and little emphasis was put on their algorithmic aspects.

By contrast, [5] is a pioneer work towards effective methods for validation of approximations of D-finite functions in Chebyshev basis. At the cost of a more restricted class of functions, namely, D-finite functions, this article introduces a fully automated algorithm together with complexity estimates, based on a Picard iteration scheme. In line with this work, [7] describes another algorithm based on a Newton-like method in an appropriate function space, which is easily extended to the case of continuous coefficients rigorously approximated by Chebyshev polynomials.

The above mentioned validation techniques are usually transposed to the vectorial case by fixing a norm over the vector-valued function space. However, this does not provide componentwise tight error enclosures. To overcome this limitation, we consider the notion of *vector-valued* (or *generalized*) metric spaces and *generalized contractions* (or *P-contractions*) [11, 21, 18]. Perov fixed-point theorem [11, 19] is a natural extension of Banach fixed-point theorem and provides componentwise upper bounds for the approximation error. Several works applied this theorem in various settings, for example [24] for the Newton method or [2, 20, 16] for ODEs with nonlocal conditions. To the best of our knowledge, however, none of these works investigate the existence of lower bounds, nor address validation problems.

Outline. Section 2 introduces a general framework for componentwise fixed-point validation in generalized metric spaces. In Section 3, we design the Newton-like validation algorithm for Chebyshev approximations of vector-valued D-finite functions. Finally, Section 4 details the validation of a two-dimensional highly oscillating system. For completeness, we also provide a comparison with a decoupling technique that boils down to solving scalar LODEs.

2 A Framework for Vector-Valued Validation Problems

We address the general problem of componentwise validating an approximation x to the exact solution $x^\star$ of a fixed-point equation $x = \mathbf{T} \cdot x$. Section 2.1 gives a rigorous definition of "several components and norms" with the notion of generalized metric spaces, leading to Perov fixed-point theorem. Section 2.2 presents a new result that complements Perov theorem with lower bounds on the componentwise approximation errors.

A toy example in the plane illustrates the vector-valued validation framework. Consider the trigonometric equation $\sin^3 \vartheta + \cos 3\vartheta = 0$ for $\vartheta \in \mathbb{R}$. By introducing $c = \cos x$ and $s = \sin x$, this is equivalent to finding the roots of the following polynomial system in the plane (c, s):

$$\mathbf{F} \cdot (c, s) = \begin{pmatrix} s^3 + 4c^3 - 3c \\ c^2 + s^2 - 1 \end{pmatrix} = 0. \tag{2}$$

Let $x^\star = (c^\star, s^\star)$ be an exact solution and $x^\circ := (c^\circ, s^\circ) = (0.84, 0.55)$ an approximation of it. In order to validate this solution with respect to a given norm $\|\cdot\|$ on $\mathbb{R}^2$, we define a Newton-like operator $\mathbf{T} \cdot (c, s) = (c, s) - \mathbf{A} \cdot \mathbf{F} \cdot (c, s)$ with $\mathbf{A} := \begin{pmatrix} 0.25 & -0.20 \\ -0.37 & 1.2 \end{pmatrix} \approx (\mathrm{D}\mathbf{F}_{x^\circ})^{-1} \in \mathcal{M}_2(\mathbb{R})$ an approximate inverse of the Fréchet derivative $\mathrm{D}\mathbf{F}_{x^\circ}$ of $\mathbf{F}$ at x°. Since $\mathbf{A}$ is injective, its fixed points are exactly the roots of $\mathbf{F}$. In this example, $\mathbf{F}$ is nonlinear, so one must find a *stable closed neighborhood* over which $\mathbf{T}$ is contracting, for Banach theorem to apply. It suffices to determine a radius $r > 0$ satisfying the following two conditions:

(i) $\lambda := \sup_{\|x - x^\circ\| \leqslant r} \|\mathbf{1} - \mathbf{A} \cdot \mathrm{D}\mathbf{F}_x\| < 1$;

(ii) $\|x^\circ - \mathbf{T} \cdot x^\circ\| + kr \leqslant r$.

If such a radius exists, then by Banach fixed-point theorem, we have $\|x^\circ - x^\star\| \leqslant \|\mathbf{A} \cdot \mathbf{F} \cdot x\|/(1 - \lambda)$. However, such a bound captures a "global" error, which may not be what we expect, if, for example, the two components are of different nature (e.g., position and velocity), or differ by several orders of magnitude.

2.1 Generalized Metric Spaces and Perov Fixed-Point Theorem

Definition 1. *Let X be a set (resp. E a linear space). A function $d : X \times X \to \mathbb{R}_+^p$ (resp. $\|\cdot\| : E \to \mathbb{R}_+^p$) is a* vector-valued *or* generalized *metric (resp. norm) if for all x, y, z in X or E and $\lambda \in \mathbb{R}$:*

- $d(x,y) = 0$ *iff* $x = y$, *resp.* $\|x\| = 0$ *iff* $x = 0$;
- $d(x,y) = d(y,x)$, *resp.* $\|\lambda x\| = |\lambda|\|x\|$;
- $d(x,y) \leqslant d(x,z) + d(z,y)$, *resp.* $\|x+y\| \leqslant \|x\| + \|y\|$.

Then (X,d) *(resp.* $(E, \|\cdot\|)$*) is a* vector-valued *or* generalized *metric space (resp. linear space).*

A straightforward example is the product of p metric spaces (X_i, d_i), $i \in [\![1,p]\!]$ (resp. p normed linear spaces $(E, \|\cdot\|_i)$) and the vector-valued metric $d(x,y) = (d_1(x_1,y_1), \ldots, d_p(x_p,y_p))$ (resp. the vector-valued norm $\|x\| = (\|x_1\|_1, \ldots, \|x_p\|_p)$).

Remark 1. *A vector-valued metric space (respectively a vector-valued normed linear space) can be trivially seen as a metric space (respectively a normed linear space) by taking the maximum of all the components of the vector-valued metric (respectively norm). We therefore recover all the useful topological notions of convergence, limit, neighborhood, completeness, etc.*

In the context of vector-valued metric spaces, the notion of contracting map needs to be generalized. Let $\mathcal{M}_p^{\to 0}(\mathbb{R}) \subseteq \mathcal{M}_p(\mathbb{R})$ denote the *convergent to zero matrices*, that is the matrices M such that $M^k \to 0$ as $k \to \infty$. Equivalently, these are matrices M with spectral radius $\rho(M) < 1$. Then, $\mathcal{M}_p^{\to 0}(\mathbb{R}_+) = \mathcal{M}_p^{\to 0}(\mathbb{R}) \cap \mathcal{M}_p(\mathbb{R}_+)$ denotes those among them with nonnegative coefficients.

Definition 2. *Let* (X,d) *be a vector-valued metric space and* $\mathbf{T} : X \to X$ *an operator.*

- $\mathbf{T}$ *is* Λ*-Lipschitz for some* $\Lambda \in \mathcal{M}_p(\mathbb{R}_+)$ *if:*

$$d(\mathbf{T} \cdot x, \mathbf{T} \cdot y) \leqslant \Lambda \cdot d(x,y), \qquad \text{for all } x, y \in X.$$

- *If moreover* Λ *is convergent to* 0 *(*$\Lambda \in \mathcal{M}_p^{\to 0}(\mathbb{R}_+)$*), then* $\mathbf{T}$ *is said to be a generalized contraction.*

Using these definitions, Perov fixed-point theorem[2] is a generalization of Banach fixed-point theorem.

Theorem 2 (Perov)**.** *Let* (X,d) *be a complete vector-valued metric space and* $\mathbf{T} : X \to X$ *a generalized contraction with a Lipschitz matrix* $\Lambda \in \mathcal{M}_p^{\to 0}(\mathbb{R}_+)$*. Then:*

[2]Although commonly attributed to Perov [19] (in Russian), the idea of generalizing Banach fixed-point theorem to generalized norms for investigating the componentwise errors in an iterative process first appeared in Kantorovich's work [11] (in Russian too).

(i) $\mathbf{T}$ *admits a unique fixed-point* $x^\star \in X$*;*

(ii) for every $x^\circ \in X$*, the iterated sequence defined by* $x_0 = x^\circ$ *and* $x_{n+1} = \mathbf{T} \cdot x_n$ *converges to* $x^\star$ *with the following upper bound on the approximation error:*

$$d(x_n, x^\star) \leqslant \Lambda^n \cdot (\mathbf{1} - \Lambda)^{-1} \cdot d(x^\circ, \mathbf{T} \cdot x^\circ), \qquad \textit{for all } n \in \mathbb{N}. \tag{3}$$

A proof of this theorem is given in Appendix A.1. Reference proofs may also be found in [18].

Perov theorem applied to the toy example. Endowing $\mathbb{R}^2$ with the vector-valued norm $\|(c, s)\| := (|c|, |s|)$ does not change the definition of $\mathbf{T}$. The two conditions needed to apply Banach fixed-point theorem are adapted to Perov theorem as follows. Choose a *multi-radius* $r = (r_1, r_2)$ such that:

(i) $\Lambda := (|(\mathrm{D}\mathbf{T})_{ij}|)_{1 \leqslant i,j \leqslant 2}$ satisfies $\rho(\Lambda) < 1$;

(ii) $\|x^\circ - \mathbf{T} \cdot x^\circ\| + \Lambda \cdot r \leqslant r$.

For $r = (0.005, 0.005)$, one obtains:

$$\Lambda = \begin{pmatrix} 5.81 & 1.31 \\ 5.63 & 3.40 \end{pmatrix} \cdot 10^{-2}, \qquad \rho(\Lambda) = 7.57 \cdot 10^{-2},$$

which satisfies (i) and (ii). Hence, Theorem 2 gives:

$$|c^\circ - c^\star| \leqslant 2.90 \cdot 10^{-3}, \qquad |s^\circ - s^\star| \leqslant 3.65 \cdot 10^{-3}.$$

To assess the tightness of these bounds, we provide lower bounds on the componentwise approximation errors.

2.2 Lower Bounds and Error Enclosures

Let $\varepsilon = d(x^\circ, x^\star) \in \mathbb{R}^p_+$ be the vector of unknown errors and $\eta = d(x^\circ, \mathbf{T} \cdot x^\circ) \in \mathbb{R}^p_+$. By the triangle inequality, ε is circumscribed into a polytope of $\mathbb{R}^p_+$:

$$\begin{aligned} (\mathbf{1} - \Lambda) \cdot \varepsilon &\leqslant \eta, \\ (\mathbf{1} + \Lambda) \cdot \varepsilon &\geqslant \eta, \\ \varepsilon &\geqslant 0. \end{aligned} \tag{4}$$

The first inequality gives the upper bounds $\varepsilon^+ = (\mathbf{1} - \Lambda)^{-1} \cdot \eta$, as stated by Theorem 2 (with $n = 0$). However, the second one does not directly give the desired lower bounds, say ε^-, because the inverse $(\mathbf{1} + \Lambda)^{-1} = \sum_{k \geqslant 0} (-\Lambda)^k$ is not nonnegative in general. It is clear that each ε_i^- is given by the i-th coordinate of some vertex of this polytope. Instead of testing its 2^p vertices, the following theorem identifies the correct vertex.

Theorem 3 (Lower bounds for Perov theorem)**.** *With the above notations, for each $i \in [\![1, p]\!]$, the lower bound ε_i^- on the i-th component ε_i of the approximation error of x° to $x^\star$ is given by the i-th component of the vertex defined by the intersection of the i-th lower-bound constraint together with all the j-th upper-bound constraints with $j \neq i$ from* (4)*. Formally:*

$$\varepsilon_i \geqslant \varepsilon_i^- \quad \text{with} \quad \varepsilon_i^- = e_i^T \cdot (\mathbf{1} - D_i \cdot \Lambda)^{-1} \cdot \eta,$$

where D_i is the order p diagonal matrix defined by $(D_i)_{ii} = -1$ and $(D_i)_{jj} = 1$ for $j \neq i$.

Remark 2. *Contrary to the one-dimensional case, the obtained lower bound ε_i^- may be negative, in which case we round it to* 0*, meaning that the overestimation factor of the upper bound provided by Theorem 2 is not controlled (see Appendix A.2).*

The proof of Theorem 3 relies on the following technical lemma, whose proof is given in Appendix A.1.

Lemma 1. *Let $\Lambda \in \mathcal{M}_p^{\to 0}(\mathbb{R}_+)$ be a convergent to zero nonnegative matrix. Then, for every $i \in [\![1, p]\!]$, $\Lambda - D_i$ is nonsingular and the entries on the i-th row of its inverse are nonnegative.*

Proof of Theorem 3. Among the Inequalities (4), take the p upper-bound constraints and replace the i-th one by the corresponding lower-bound constraint. Multiply these $p-1$ upper-bound constraints by -1 to obtain the following system of inequalities:

$$(\Lambda - D_i) \cdot \varepsilon \geqslant -D_i \cdot \eta. \tag{5}$$

From Lemma 1, $\Lambda - D_i$ is nonsingular and its inverse has nonnegative coefficients on its i-th row. Hence we can multiply (5) by $(\Lambda - D_i)^{-1}$ and only keep the resulting i-th constraint:

$$\begin{aligned}\varepsilon_i &= e_i^T \cdot (\Lambda - D_i)^{-1} \cdot (\Lambda - D_i) \cdot \varepsilon \\ &\geqslant e_i^T \cdot (\Lambda - D_i)^{-1} \cdot (-D_i) \cdot \eta = e_i^T \cdot (\mathbf{1} - D_i \cdot \Lambda)^{-1} \cdot \eta.\end{aligned}$$

□

Lower bounds for the toy example. The polytope given by the linear constraints (4) is depicted in Figure 1. The top right vertex corresponds to $(\varepsilon_1^+, \varepsilon_2^+)$. Also, the ε_1^- (resp. ε_2^-) is given by the top left (resp. bottom right) vertex, which is consistent with Theorem 3. This gives the following numerical enclosures:

$$\begin{aligned} \varepsilon_1^- &= 2.48 \cdot 10^{-3} \leqslant \varepsilon_1 = |c^\circ - c^\star| \leqslant \varepsilon_1^+ = 2.90 \cdot 10^{-3}, \\ \varepsilon_2^- &= 3.09 \cdot 10^{-3} \leqslant \varepsilon_2 = |s^\circ - s^\star| \leqslant \varepsilon_2^+ = 3.65 \cdot 10^{-3}. \end{aligned} \tag{6}$$

A discussion on the tightness of these enclosures is carried out in Appendix A.2. Roughly speaking, the ratio $\varepsilon_i^+/\varepsilon_i^-$ depends not only on Λ (like in the univariate case), but also on $\eta = d(x^\circ, \mathbf{T} \cdot x^\circ)$.

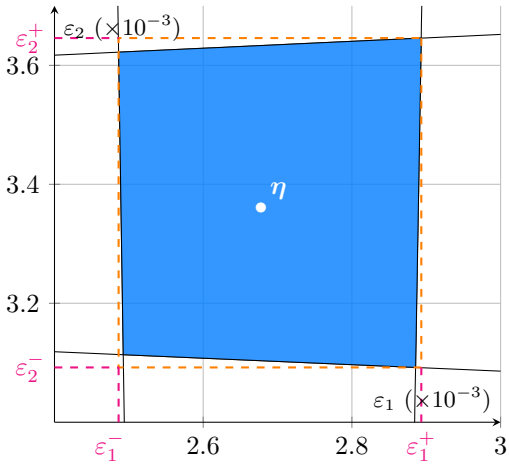


Figure 1: Error polytope for the toy example.

3 Componentwise Validation of Chebyshev Approximations to Vector-Valued D-finite Functions

We present the validation method to solve Problem 1. Section 3.1 contains reminders about Chebyshev approximation theory and LODEs. This leads to an efficient approximating procedure (Section 3.2). Section 3.3 presents **Algorithms 1** and **2** to create and bound a Newton-like operator associated to a given vectorial LODE, then **Algorithm 3** to compute componentwise error enclosures for any Chebyshev approximation $(\Phi_i^\circ)_{1 \leqslant i \leqslant p}$.

3.1 Some Reminders about Chebyshev Approximations to LODEs

Chebyshev series and Ч^1 ***space.*** The Chebyshev family of polynomials is defined by the three-term recurrence $T_{n+2} = 2XT_{n+1} - T_n$ with initial terms

$T_0 = 1$ and $T_1 = X$. They satisfy the fundamental trigonometric relation $T_n(\cos\vartheta) = \cos(n\vartheta)$, from which we deduce some of their basic algebraic properties:

$$T_n T_m = \frac{1}{2}(T_{n+m} + T_{|n-m|}), \quad \int T_n = \frac{T_{n+1}}{2(n+1)} - \frac{T_{n-1}}{2(n-1)} = T_n \ (n \geqslant 2), \quad (7)$$

and that $|T_n(t)| \leqslant 1$ for $x \in [-1, 1]$.

Let $L^2_{\text{Ч}} = L^2(1/\sqrt{1-t^2})$ denote the space of real-valued measurable functions f over $[-1, 1]$ such that $\int_{-1}^{1} f(t)^2/\sqrt{1-t^2}\mathrm{d}t < \infty$. The inner product :

$$\langle f, g\rangle = \int_{-1}^{1} f(t)g(t)/\sqrt{1-t^2}\mathrm{d}t = \int_0^{\pi} f(\cos\vartheta)g(\cos\vartheta)\mathrm{d}\vartheta,$$

defines a Hilbert space structure over $L^2_{\text{Ч}}$, for which the Chebyshev polynomials form a complete orthogonal system. To any continuous function f in this space we can associate its Chebyshev coefficients:

$$[f]_n = \begin{cases} \frac{1}{\pi}\int_0^{\pi} f(\cos\vartheta)\mathrm{d}\vartheta, & \text{if } n = 0, \\ \frac{2}{\pi}\int_0^{\pi} f(\cos\vartheta)\cos(n\vartheta)\mathrm{d}\vartheta, & \text{if } n > 0. \end{cases}$$

Hence, the truncated Chebyshev series $f^{[N]} = \text{п}_N \cdot f := \sum_{n=0}^{N}[f]_n T_n$ of f is simply the orthogonal projection of f onto the finite-dimensional subspace spanned by $T_0, \ldots, T_N$. In addition to the $L^2_{\text{Ч}}$ convergence, and analogously to Fourier series, Chebyshev series have excellent approximation properties [6]. For example, if f is of class $\mathcal{C}^r$ over $[-1, 1]$ with $r \geqslant 1$, then $f^{[N]}$ uniformly converges to f in $O(N^{-r})$, and the convergence is even exponential for analytic functions. Moreover, at fixed degree N, the N-th truncated Chebyshev series $f^{[N]}$ is a near-best approximation of f among degree N polynomials, with a factor growing relatively slowly, in $O(\log(N))$ [15].

We call Ч^1 the Banach space of continuous functions with absolutely summable Chebyshev series, and define the associated norm $\|f\|_{\text{Ч}^1} = \sum_{n\geqslant 0}|[f]_n|$. Note that Ч^1 is analogous to the Wiener algebra $A(\mathbb{T})$ of absolutely convergent Fourier series [12, §I.6]: for $f \in \text{Ч}^1$, we have $\|f\|_{\text{Ч}^1} = \|f(\cos)\|_{A(\mathbb{T})}$. We obtain a Banach algebra structure: $\|fg\|_{\text{Ч}^1} \leqslant \|f\|_{\text{Ч}^1}\|g\|_{\text{Ч}^1}$. Moreover, this norm is a safe overestimation of the supremum norm $\|\cdot\|_\infty$ over $[-1, 1]$:

$$\|f\|_{\text{Ч}^1} \geqslant \sup_{-1\leqslant t\leqslant 1}\sum_{n\geqslant 0}|[f]_n T_n(t)| \geqslant \sup_{-1\leqslant t\leqslant 1}|f(t)| = \|f\|_\infty.$$

Given an endomorphism $\mathbf{F} : \text{Ч}^1 \to \text{Ч}^1$, the operator norm induced by the Ч^1 norm is given by:

$$\|\mathbf{F}\|_{\text{Ч}^1} = \sup_{\|f\|_{\text{Ч}^1}\leqslant 1}\|\mathbf{F}\cdot f\|_{\text{Ч}^1} = \sup_{n\geqslant 0}\|\mathbf{F}\cdot T_n\|_{\text{Ч}^1}. \quad (8)$$

This corresponds to the maximum sum of the coefficients in absolute value over all columns of the matrix representation of $\mathbf{F}$.

D-finite equations and integral transforms. We consider a generic p-dimensional order r system of LODEs over the compact interval $[-1,1]$:

$$Y^{(r)} + A_{r-1}(t) \cdot Y^{(r-1)} + \cdots + A_1(t) \cdot Y' + A_0(t) \cdot Y = G(t), \tag{9}$$

of unknown $Y = (Y_1, \ldots, Y_p) : [-1,1] \to \mathbb{R}^p$, with polynomial coefficients $A_k = (a_{kij})_{1 \leqslant i,j \leqslant p} \in \mathcal{M}_p(\mathbb{R}[t])$ and right-hand side $G = (G_1, \ldots, G_p) \in \mathbb{R}[t]^p$. We also fix initial conditions at -1:

$$Y^{(i)}(-1) = v_i, \qquad v_i \in \mathbb{R}^p, \quad \text{for all } i \in [\![0, r-1]\!]. \tag{10}$$

Together, (9) and (10) form an *Initial Value Problem* (IVP).

Several barriers arise when working directly on a differential equation (9): the differentiation of Chebyshev polynomials does not admit a compact formula, whence a dense linear system to solve, and, from the theoretical point of view, the space Ч^1 is not stable under differentiation. A common way to circumvent these limitations is to apply an integral transform onto the IVP problem so as to obtain an equivalent *Volterra integral equation of the second kind* over $[-1,1]$:

$$\Phi + \mathbf{K} \cdot \Phi = \Psi, \quad \text{with} \quad \mathbf{K} \cdot \Phi(t) = \int_{-1}^{t} K(t,s) \cdot \Phi(s) \mathrm{d}s, \tag{11}$$

with a bivariate polynomial kernel $K = (k_{ij})_{1 \leqslant i,j \leqslant p} \in \mathcal{M}_p(\mathbb{R}[t,s])$ and right-hand side $\Psi = (\Psi_1, \ldots, \Psi_p) \in \mathbb{R}[t]^p$. Depending on the integral transform, the unknown function $\Phi = (\Phi_1, \ldots, \Phi_p) : [-1,1] \to \mathbb{R}^p$ can be either Y or one of its derivatives. For example, [5] acts over Y, whereas [7] considers the last derivative $Y^{(r)}$.

In any case, $\mathbf{K} : \Phi \mapsto \int_{-1}^{t} K(t,s) \cdot \Phi(s) \mathrm{d}s$ is a bounded linear operator from $(\text{Ч}^1)^p$ to itself. We may describe it by blocks $\mathbf{K} = (\mathbf{K}_{ij})_{1 \leqslant i,j \leqslant p}$, where each $\mathbf{K}_{ij}$ is a one-dimensional integral operator of kernel $k_{ij}(t,s)$. By decomposing $k_{ij}(t,s)$ in Chebyshev basis with respect to s, we obtain unique polynomials $b_{ijk}(t)$ such that:

$$k_{ij}(t,s) = \sum_{k=0}^{\kappa_{ij}} b_{ijk}(t) T_k(s), \quad \mathbf{K}_{ij} \cdot \varphi(t) = \sum_{k=0}^{\kappa_{ij}} b_{ijk}(t) \int_{-1}^{t} T_k(s) \varphi(s) \mathrm{d}s.$$

Consequently to the multiplication and integration formulas (7), the (infinite dimensional) matrix representation of $\mathbf{K}_{ij} : \text{Ч}^1 \to \text{Ч}^1$ has a so-called (h_{ij}, d_{ij}) *almost-banded* structure [17], meaning that the nonzero entries are

located on the h_{ij} first rows (*horizontal band* with *initial entries*) and the diagonal plus the first d_{ij} upper and lower diagonals (*diagonal band* with *diagonal entries*), with $h_{ij} = \max_{0\leqslant k\leqslant \kappa_{ij}} \deg b_{ijk}(t)$ and $d_{ij} = 1 + \deg k_{ij}(t,s) = 1 + \max_{0\leqslant k\leqslant \kappa_{ij}} k + \deg b_{ijk}(t)$ (see Figure 2(a)).

3.2 Efficient numerical solving

The integral equation (11) is an infinite-dimensional linear system over the Chebyshev coefficients of the unknown function Φ. The *projection method* (also sometimes called *Galerkin method* [9]) consists in truncating for a given index N_{app} and solving the obtained finite-dimensional linear system. In our case, this can be efficiently done by taking advantage of its sparse structure.

Define the N_{app}-th truncation of $\mathbf{K}$ as $\mathbf{K}^{[N_{\text{app}}]} = (\mathbf{K}_{ij}^{[N_{\text{app}}]})_{1\leqslant i,j\leqslant p}$, where $\pi_{N_{\text{app}}} \cdot \mathbf{K}_{ij} \cdot \pi_{N_{\text{app}}}$ (see Figure 2(b)). It is represented by the order $p(N_{\text{app}}+1)$ square matrix depicted by blocks in Figure 2(c). By permuting the natural basis $\mathcal{B}_{p,N_{\text{app}}}$ of $(\pi_{N_{\text{app}}} \cdot \text{Ч}^1)^p$ into $\mathcal{B}'_{p,N_{\text{app}}}$:

$$\begin{aligned} \mathcal{B}_{p,N_{\text{app}}} &= (T_0 e_1, \ldots, T_{N_{\text{app}}} e_1, \ldots\ldots, T_0 e_p, \ldots, T_{N_{\text{app}}} e_p), \\ \mathcal{B}'_{p,N_{\text{app}}} &= (T_0 e_1, \ldots, T_0 e_p, \ldots\ldots, T_{N_{\text{app}}} e_1, \ldots, T_{N_{\text{app}}} e_p), \end{aligned} \tag{12}$$

$\mathbf{K}^{[N_{\text{app}}]}$ recovers a (ph, pd) almost-banded structure, where $h = \max_{ij} h_{ij}$ and $d = \max_{ij} d_{ij}$ (see Figure 2(d)).

Hence, solving the approximate problem:

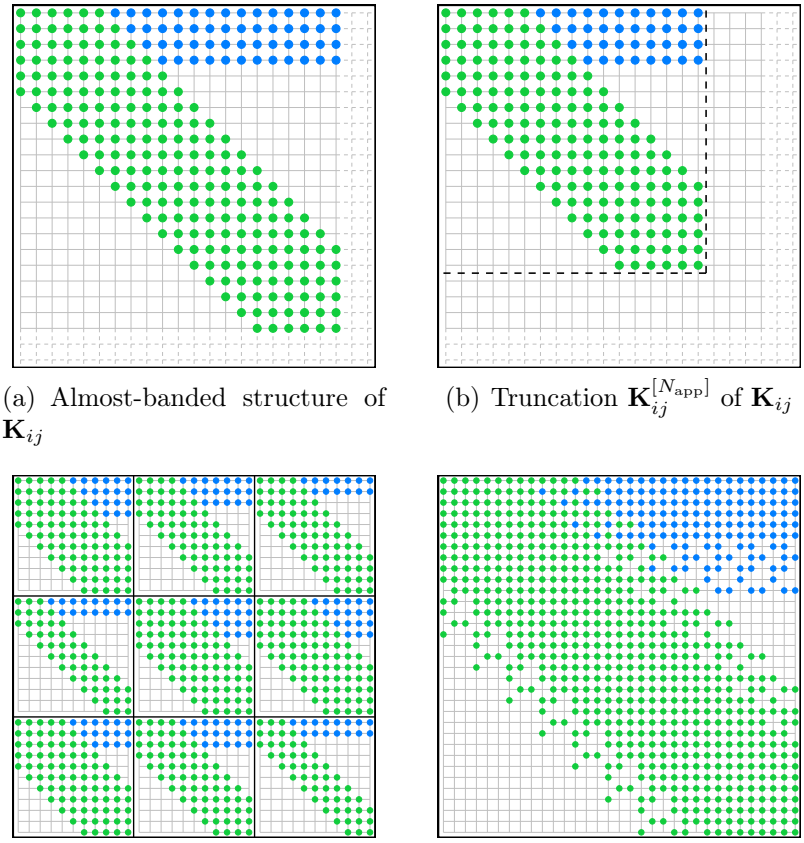
$$\Phi + \mathbf{K}^{[N_{\text{val}}]} \cdot \Phi = \Psi$$

requires $O(p^3 N_{\text{app}} d^2)$ operations, using the algorithm of [17] for solving almost-banded linear systems.

3.3 Validation Procedure

We extend the validation procedure of [7] to the vectorial case. We prove the main Theorem 1 in order to solve Problem 1 in two steps: (1) a Newton-like validation operator is created and bounded by **Algorithm 1**. This first step is independent of the approximation degree N_{app}. (2) The error enclosure of the given approximation is computed by **Algorithm 3**, following Theorems 2 and 3.

Newton-like validation operator. Following the idea of Newton's method and similar approaches, Equation (11) is transformed into the fixed-point



(a) Almost-banded structure of $\mathbf{K}_{ij}$

(b) Truncation $\mathbf{K}_{ij}^{[N_{\text{app}}]}$ of $\mathbf{K}_{ij}$

(c) $\mathbf{K}^{[N_{\text{app}}]}$ in $\mathcal{B}_{p,N_{\text{app}}}$, by blocks ($p = 3$)

(d) $\mathbf{K}^{[N_{\text{app}}]}$ in $\mathcal{B}'_{p,Napp}$ is almost-banded

Figure 2: Almost-banded structure of integral operators

equation:

$$\mathbf{T} \cdot \Phi = \Phi, \qquad \mathbf{T} \cdot \Phi := \Phi - \mathbf{A} \cdot (\Phi + \mathbf{K} \cdot \Phi - \Psi), \tag{13}$$

which is equivalent to (11) as soon as $\mathbf{A} : (\text{Ч}^1)^p \to (\text{Ч}^1)^p$ is injective. Moreover, $\mathbf{T}$ is an affine operator of linear part $\mathrm{D}\mathbf{T} = \mathbf{1} - \mathbf{A} \cdot (\mathbf{1} + \mathbf{K})$. The main challenge is to efficiently compute $\mathbf{A}$ and bound $\|\mathrm{D}\mathbf{T}\|_{(\text{Ч}^1)^p}$. This is handled by **Algorithm 1**. Similarly to numerical solving, $\mathbf{A}$ approximates $(\mathbf{1} + \mathbf{K}^{[N_{\text{val}}]})^{-1}$, for some truncation order N_{val}. Choosing N_{val} is a trade-off between proving $\mathbf{T}$ is contracting (N_{val} must be large enough so that $\|\mathbf{K} - \mathbf{K}^{[N_{\text{val}}]}\|_{(\text{Ч}^1)^p}$ is rigorously proved to be sufficiently small) and efficiency requirements (see [7] for heuristics to find N_{val}).

Once N_{val} is fixed, **Algorithm 1** first computes an approximate inverse A (lines 1-4). Since $\mathbf{1} + \mathbf{K}^{[N_{\text{val}}]}$ is almost-banded in $\mathcal{B}'_{p,N_{\text{val}}}$, its numerical inverse can be either computed with [17], or approximated by a (ph', pd') almost-banded matrix [7, **Algorithm 5**]. This requires $O(p^3 N_{\text{val}}(h' + d')(h + d))$ floating-point operations. The operator $\mathbf{A}$ is defined by extending A to the whole space $(\text{Ч}^1)^p$ by the identity.

Second, **Algorithm 1** bounds a Lipschitz matrix for $\mathbf{T}$, as $\|\mathrm{D}\mathbf{T}\|_{(\text{Ч}^1)^p} = (\|(\mathrm{D}\mathbf{T})_{ij}\|_{\text{Ч}^1})_{1 \leqslant i,j \leqslant p}$, block by block, using the triangle inequality:

$$\|\mathrm{D}\mathbf{T}\|_{\text{Ч}^1} \leqslant \|\mathbf{1} - \mathbf{A} \cdot (\mathbf{1} + \mathbf{K}^{[N_{\text{val}}]})\|_{\text{Ч}^1} + \|\mathbf{A} \cdot (\mathbf{K} - \mathbf{K}^{[N_{\text{val}}]})\|_{\text{Ч}^1}. \tag{14}$$

The first part of (14) is the *approximation error*, measuring how far $\mathbf{A}$ is from the inverse of $\mathbf{1} + \mathbf{K}^{[N_{\text{val}}]}$. This is straightforwardly bounded as Λ^A by **Algorithm 1** (lines 5-9) using $O(p^3 N_{\text{val}}(h' + d')(h + d))$ interval arithmetic operations.

The second part of (14) is the *truncation error*, because the truncated operator $\mathbf{K}^{[N_{\text{val}}]}$ only approximates $\mathbf{K}$. Let $\mathbf{E}_{ij}$ be the (i, j) block of $\mathbf{E} := \mathbf{A} \cdot (\mathbf{K} - \mathbf{K}^{[N_{\text{val}}]})$:

$$\mathbf{E}_{ij} = \sum_{k=1}^{p} \mathbf{A}_{ik} \cdot (\mathbf{K}_{kj} - \mathbf{K}_{kj}^{[N_{\text{val}}]}). \tag{15}$$

Algorithm 1 (lines 10-16) computes $\Lambda^T \geqslant \|\mathbf{E}\|_{(\text{Ч}^1)^p}$ by blocks, with the triangle inequality: each subterm of (15) is rigorously bounded by **Algorithm 2**. This algorithm, detailed below, requires $O((h' + d')(h + d)^2)$ interval arithmetic operations. Hence the computation of Λ^T is in $O(p^3(h' + d')(h + d)^2)$.

Finally, **Algorithm 1** computes $\Lambda = \Lambda^A + \Lambda^T$ and checks that this Lipschitz matrix is convergent to zero, in which case the constructed Newton-like operator $\mathbf{T}$ is contracting.

Proof of Theorem 1(i). The detailed description of **Algorithm 1** above proves its correctness, and the given complexity estimates for lines 1-4, 5-9 and 10-16 sum to a global complexity of $O(p^3 N_{\text{val}}(h' + d')(h + d))$ operations. In the worst case, when A is dense ($h' + d' \approx N_{\text{val}}$), we recover the estimate of Theorem 1*(i)*. □

Truncation error bounding. From Equation (15), one needs to bound $\|\mathbf{A}_{ik} \cdot (\mathbf{K}_{kj} - \mathbf{K}_{kj}^{[N_{\text{val}}]})\|_{\text{Ч}^1}$, where $\mathbf{A}_{ik}$ is the extension to Ч^1 of the order $N_{\text{val}}+1$ matrix A_{ik} by the identity if $i = k$, and zero otherwise. This computation is handled by **Algorithm 2**, which is a modification of [7, **Algorithm 6**], that only treats the case $i = k$.

Specifically, let $\mathbf{K}$ denote here a *one-dimensional* (h, d) almost-banded integral operator, and $\mathbf{A} : \text{Ч}^1 \to \text{Ч}^1$ the extension of an order $N_{\text{val}} + 1$ matrix A by the identity or zero. We have:

$$\|\mathbf{A} \cdot (\mathbf{K} - \mathbf{K}^{[N_{\text{val}}]})\|_{\text{Ч}^1} = \sup_{\ell \geqslant 0} B(\ell), \quad \text{with } B(\ell) = \|\mathbf{A} \cdot (\mathbf{K} - \mathbf{K}^{[N_{\text{val}}]}) \cdot T_\ell\|_{\text{Ч}^1}.$$

Indices ℓ are divided into four groups, reflecting how the initial and diagonal coefficients are impacted by the action of $\mathbf{A}$: $[\![0, N_{\text{val}} - d]\!]$, $[\![N_{\text{val}} - d + 1, N_{\text{val}}]\!]$, $[\![N_{\text{val}} + 1, N_{\text{val}} + d]\!]$ and $[\![N_{\text{val}} + d + 1, +\infty]\!]$. The T_ℓ in the first group lie in the kernel. The second and third ones are explicitly computed, yielding bounds $\delta^{(1)}$ and $\delta^{(2)}$ in **Algorithm 2** (lines 1-7 and 8-13). For the infinite last group, $B(\ell)$ is decomposed as $B_I(\ell) + B_D(\ell)$, the contribution of the initial and diagonal coefficients. **Algorithm 2** uses the efficient bounding strategy of [7]. First, it computes the image of $T_{N_{\text{val}}+d+1}$ for the initial and diagonal coefficients (lines 16 and 22). Then, it bounds the difference between the images of $T_{N_{\text{val}}+d+1}$ and the remaining T_ℓ for $\ell > N_{\text{val}} + d + 1$ to finally deduce bounds $\delta^{(3)}$ and $\delta^{(4)}$ (lines 17 and 23).

Error enclosures. Finally, **Algorithm 3** implements the validation procedure of Theorems 2 and 3 by applying the operator $\mathbf{T}$ to the candidate approximation Φ°, bounding the distance of the resulting polynomial to Φ° and producing componentwise error enclosures to $\Phi^\star$ with respect to the Ч^1 norm.

Proof of Theorem 1(ii). **Algorithm 3** computes $\Phi^\circ - \mathbf{T} \cdot \Phi^\circ = \mathbf{A} \cdot (\Phi^\circ + \mathbf{K} \cdot \Phi^\circ - \Psi)$. Each P_k (line 1) is a polynomial of degree at most $\max(N_{\text{app}} + d, N_{\text{rhs}})$, and computing its Chebyshev coefficients is in $O(pd^2 N_{\text{app}} + N_{\text{rhs}})$. Then, the computation of the coefficients of each $A_{ik} \cdot \text{п}_{N_{\text{val}}} \cdot P_k$ (line 3) is in $O((h' + d') \deg(\text{п}_{N_{\text{val}}} \cdot P_k)) = O((h' + d') \min(\max(N_{\text{app}} + d, N_{\text{rhs}}), N_{\text{val}}))$. Finally, the complexity of computing the enclosures (lines 6-7) only depends

Algorithm 1 Create and bound a Newton-like operator $\mathbf{T}$

Require: A polynomial integral operator $\mathbf{K} = (\mathbf{K}_{ij})_{1\leqslant i,j\leqslant p}$ given by the $(b_{ijk})_{0\leqslant k\leqslant \kappa_{ij}}^{1\leqslant i,j\leqslant p}$, and a truncation order N_{val}.

Ensure: An approximate inverse $\mathbf{A}$ of $\mathbf{1} + \mathbf{K}^{[N_{\text{val}}]}$ and a certified Lipschitz matrix Λ for $\mathbf{1} - \mathbf{A} \cdot (\mathbf{1} + \mathbf{K})$, or fail if N_{val} not large enough.

▷ *Compute an approximate inverse matrix A.*

$M = (M_{ij})_{1\leqslant i,j\leqslant p} \leftarrow \mathbf{1} + \mathbf{K}^{[N_{\text{val}}]}$, by blocks

$M' \leftarrow M$ in basis $\mathcal{B}'_{p,N_{\text{val}}}$

$A' \leftarrow$ a numerical approximate inverse of M', either dense or almost-banded.

$A = (A_{ij})_{1\leqslant i,j\leqslant p} \leftarrow A'$ in basis $\mathcal{B}_{p,N_{\text{val}}}$, by blocks

▷ *Compute the approx error $\Lambda^A = (\lambda^A_{ij})$ in interval arith.*

for $i = 1$ **to** p and $j = 1$ **to** p **do**

  $C \leftarrow \sum_{1\leqslant k\leqslant p} A_{ik} \cdot M_{kj}$

  if $i = j$ **then** $C \leftarrow C - \mathbf{1}_{N_{\text{val}}+1}$

  $\lambda^A_{ij} \leftarrow \|C\|_{\text{Ч}^1}$

end for

▷ *Compute the trunc error $\Lambda^T = (\lambda^T_{ij})$ in interval arith.*

for $i = 1$ **to** p and $j = 1$ **to** p **do**

  $\lambda^T_{ij} \leftarrow 0$

  for $k = 1$ **to** p **do**

    $\delta \leftarrow$ **Algorithm 2** on $\mathbf{K}_{jk}$, A_{ik} and $diag := (i = k)$.

    $\lambda^T_{ij} \leftarrow \lambda^T_{ij} + \delta$

  end for

end for

▷ *Compute Λ and check if $\mathbf{T}$ contracting.*

$\Lambda \leftarrow \Lambda^A + \Lambda^T$

if $\rho(\Lambda) < 1$ **then**

  return A, Λ

else

  print "Fail, Λ is not convergent to 0"

end if

Algorithm 2 Bound the truncation error

Require: A polynomial (one-dimensional) integral operator $\mathbf{K}$ given by the $(b_k)_{0\leqslant k\leqslant \kappa}$, a truncation order N_{val}, a $N_{\text{val}}+1$ order square matrix A, and a Boolean *diag*.

Ensure: An upper bound δ for $\|\mathbf{A}\cdot(\mathbf{K}-\mathbf{K}^{[N_{\text{val}}]})\|_{\text{Ч}^1}$, where $\mathbf{A}$ is the extension of A to the whole space Ч^1 by the identity if $diag = true$, and by zero otherwise.

$\triangleright$ ***All operations are performed in interval arithmetics***

$\triangleright$ *Compute* $\delta^{(1)} \geqslant \sup_{\ell\in[\![N_{\text{val}}-d+1,N_{\text{val}}]\!]} B(\ell)$

$\delta^{(1)} \leftarrow 0$
if *diag* **then**
  for $\ell = N_{\text{val}} - d + 1$ **to** N_{val} **do**
    $P \leftarrow (\mathbf{1} - \Pi_{N_{\text{val}}}) \cdot \mathbf{K} \cdot T_\ell$
    if $\|P\|_{\text{Ч}^1} > \delta^{(1)}$ **then** $\delta^{(1)} \leftarrow \|P\|_{\text{Ч}^1}$
  end for
end if

$\triangleright$ *Compute* $\delta^{(2)} \geqslant \sup_{\ell\in[\![N_{\text{val}}+1,N_{\text{val}}+d]\!]} B(\ell)$

$\delta^{(2)} \leftarrow 0$
for $\ell = N_{\text{val}} + 1$ **to** $N_{\text{val}} + d$ **do**
  $P \leftarrow A \cdot \Pi_{N_{\text{val}}} \cdot \mathbf{K} \cdot T_\ell$
  if *diag* **then** $P \leftarrow P + (\mathbf{1} - \Pi_{N_{\text{val}}}) \cdot \mathbf{K} \cdot T_\ell$
  if $\|P\|_{\text{Ч}^1} > \delta^{(2)}$ **then** $\delta^{(2)} \leftarrow \|P\|_{\text{Ч}^1}$
end for

$\triangleright$ *Compute* $\delta^{(3)} \geqslant \sup_{\ell\geqslant N_{\text{val}}+d+1} B_D(\ell)$

$\ell_0 \leftarrow N_{\text{val}} + d + 1$ **and** $B \leftarrow \sum_{k=0}^{\kappa} \|b_k\|_{\text{Ч}^1}$
if *diag* **then**
  $P \leftarrow (\mathbf{1} - \Pi_{N_{\text{val}}}) \cdot \mathbf{K} \cdot T_{\ell_0}$
  $\delta^{(3)} \leftarrow \|P\|_{\text{Ч}^1} + \frac{(\kappa+1)B}{(\ell_0-(\kappa-1))^2}$
else
  $\delta^{(3)} \leftarrow 0$
end if

$\triangleright$ *Compute* $\delta^{(4)} \geqslant \sup_{\ell\geqslant N_{\text{val}}+d+1} B_I(\ell)$

$B' \leftarrow \sum_{k=0}^{\kappa} \|A \cdot b_k\|_{\text{Ч}^1}$
$P \leftarrow A \cdot \Pi_{N_{\text{val}}} \cdot \mathbf{K} \cdot T_{\ell_0}$
$\delta^{(4)} \leftarrow \|P\|_{\text{Ч}^1} + \frac{(\kappa+1)^3 B'}{(\ell_0^2-(\kappa+1)^2)^2}$
$\delta \leftarrow \max(\delta^{(1)}, \delta^{(2)}, \delta^{(3)} + \delta^{(4)})$
return δ

on p, and is therefore negligible. The overall complexity is:

$$O(p^2 d^2 N_{\text{app}} + p N_{\text{rhs}} + p^2 (h' + d') \min(\max(N_{\text{app}} + d, N_{\text{rhs}}), N_{\text{val}})),$$

which gives the estimate of Theorem 1*(ii)* when $h', d' \approx N_{\text{val}}$. □

Algorithm 3 Validate a candidate solution of an integral equation

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Require: A polynomial integral operator $\mathbf{K} = (\mathbf{K}_{ij})_{1 \leqslant i,j \leqslant p}$ given by the $(b_{ijk})_{0 \leqslant k \leqslant \kappa_{ij}}^{1 \leqslant i,j \leqslant p}$, a polynomial right-hand side $\Psi = (\Psi_1, \ldots, \Psi_p)$, a truncation order N_{val}, (A, Λ) obtained from Algorithm 1 with Λ convergent to 0, and a candidate solution $\Phi^\circ = (\Phi_1^\circ, \ldots, \Phi_p^\circ)$.

Ensure: Two vectors of upper and lower bounds ε^+ and ε^- such that $\|\Phi_i^\circ - \Phi_i^\star\|_{\text{Ч}^1} \in [\varepsilon_i^-, \varepsilon_i^+]$ for $1 \leqslant i \leqslant p$.

▷ ***All operations are performed in interval arithmetics***

for $k = 1$ **to** p **do** $P_k \leftarrow \Phi_k + \sum_{j=1}^p \mathbf{K}_{kj} \cdot \Phi_j^\circ - \Psi_k$
for $i = 1$ **to** p **do**
  $Q_i \leftarrow \sum_{k=1}^p A_{ik} \cdot \text{П}_{N_{\text{val}}} \cdot P_k + (\mathbf{1} - \text{П}_n) \cdot P_i$
  $\eta_i \leftarrow \|Q_i\|_{\text{Ч}^1}$
end for
$\varepsilon^+ \leftarrow (\mathbf{1} - \Lambda)^{-1} \cdot \eta$
for $i = 1$ **to** p **do** $\varepsilon_i^- \leftarrow ((\mathbf{1} - D_i \cdot \Lambda)^{-1} \cdot \eta)_i$
return ε^+ and ε^-

Estimating N_{val}. The following theorem provides a worst-case estimate for the minimal value of N_{val}.

Theorem 4. *Let $B_{ij} = \sum_{k=0}^{\kappa_{ij}} \|b_{ijk}\|_{\text{Ч}^1}$ and $B = (B_{ij})_{1 \leqslant i,j \leqslant p}$. The following bound estimates the minimal possible value for N_{val} making **Algorithm 1** produce a contracting Newton-like operator:*

$$N_{\text{val}} = O\left(d\rho(B)^2 \exp(2\rho(B))\right), \tag{16}$$

where $\rho(B)$ denotes the spectral radius of B.

The proof is an adaptation of the argument given in [7] to the vectorial case, and is given in Appendix A.3. Note that although theoretically interesting, this exponential bound is overpessimistic for a wide range of examples.

4 Example and Discussion

Consider the following order 1, two-dimensional system, for $x \in [0, a]$ with $a > 0$, whose solutions (depicted in Figure 3) are highly oscillating functions.

Rescale it over $[-1,1]$ with the change of variable $x = \frac{a}{2}(1+t)$:

$$\begin{cases} y_1' = -x^n y_2 \\ y_2' = x^m y_1 \\ y_1(0) = 1, y_2(0) = 0 \end{cases} \Rightarrow \begin{cases} Y_1' = -\left(\frac{a}{2}\right)^{n+1}(1+t)^n Y_2 \\ Y_2' = \left(\frac{a}{2}\right)^{m+1}(1+t)^m Y_1 \\ Y_1(-1) = 1, Y_2(-1) = 0 \end{cases}. \tag{17}$$

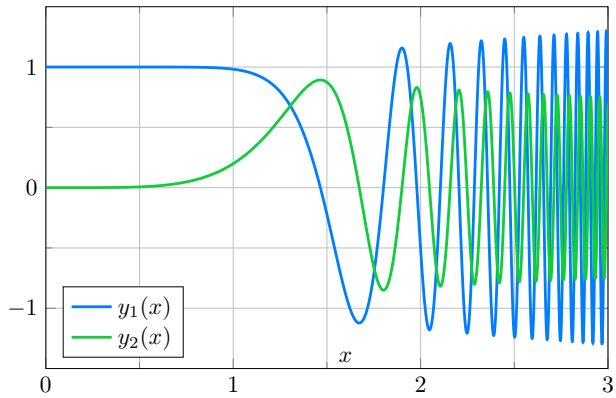

Figure 3: Solution of (17) with $n = 5$, $m = 4$ and $a = 3$

We give two different integral transforms associated to this equation. The integral transform described in [5] consists in integrating Equation (17) once, resulting into an integral equation for Y with polynomial kernel and right-hand side given by:

$$K(t,s) = \begin{pmatrix} 0 & \left(\frac{a}{2}\right)^{n+1}(1+s)^n \\ -\left(\frac{a}{2}\right)^{m+1}(1+s)^m & 0 \end{pmatrix}, \qquad \Psi(t) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

$K(t,s)$, which is of degree 0 in t, is decomposed over the Chebyshev basis with respect to s into constant polynomials $b_{001}, b_{101}, \ldots, b_{n01}$ and $b_{010}, b_{110}, \ldots, b_{m10}$.

On the other side, the integral transform used in [7] allows us to validate the derivative $\Phi = Y'$. The polynomial kernel and right-hand side are:

$$K(t,s) = \begin{pmatrix} 0 & \left(\frac{a}{2}\right)^{n+1}(1+t)^n \\ -\left(\frac{a}{2}\right)^{m+1}(1+t)^m & 0 \end{pmatrix}, \qquad \Psi(t) = \begin{pmatrix} \left(\frac{a}{2}\right)^{n+1}(1+t)^n \\ 0 \end{pmatrix}.$$

Now, $K(t,s)$ is of degree 0 with respect to s, giving two polynomials b_{001} and b_{010} of respective degrees n and m.

Let's now focus on the first integral transform, with $n = 5$, $m = 4$, $a = 3$. Using the spectral method explained in Section 3.1 and implemented in our C library, we fix an approximation degree $N_{\text{app}} = 100$ and obtain numerical approximations Y_1° and Y_2°, that must now be validated. The whole implemented procedure automatically computes and bounds for increasing values

of N_{val} the Newton-like operator $\mathbf{T}$ associated to the truncated operator $\mathbf{K}^{[N_{\text{val}}]}$. The approximate inverse is computed as an $(2h', 2d')$ almost-banded order $2(N_{\text{val}}+1)$ matrix. This process stops as soon as the total Lipschitz matrix returned by **Algorithm 1** has a spectral radius less than 1. In case of failure of **Algorithm 1**, the procedure is relaunched with $N_{\text{val}} \leftarrow 2N_{\text{val}}$. For this example, we obtain $N_{\text{val}} = 1664$, $h' = 48$ and $d' = 304$, giving the following Lipschitz matrix:

$$\Lambda = \begin{pmatrix} 9.73 \cdot 10^{-4} & 9.89 \cdot 10^{-2} \\ 3.60 \cdot 10^{-2} & 9.92 \cdot 10^{-2} \end{pmatrix}, \qquad \rho(\Lambda) = 6.06 \cdot 10^{-2}.$$

The last step is performed by **Algorithm 3**. Given the numerical approximations Y_1° and Y_2°, it computes $\eta = \|Y^\circ - \mathbf{T} \cdot Y^\circ\|_{(\mathfrak{l}^1)^2}$ (the examples gives $\eta_1 = 3.20 \cdot 10^{-3}$ and $\eta_2 = 1.91 \cdot 10^{-3}$) and outputs the error enclosures given by Theorems 2 and 3:

$$\begin{aligned} \varepsilon_1^- &= 2.99 \cdot 10^{-3}, & \varepsilon_1^+ &= 3.41 \cdot 10^{-3}, \\ \varepsilon_2^- &= 1.78 \cdot 10^{-3}, & \varepsilon_2^+ &= 2.04 \cdot 10^{-3}. \end{aligned}$$

This whole process for this example takes about 30 seconds on a modern computer.

Comparison with decoupling/desingularization. In the case of polynomial coefficients, an alternative to our method consists in decoupling the system to obtain p scalar LODEs of order p, at the cost of introducing singularities in the equations. As an example, the first component y_1 in the system (17) satisfies the following differential equation:

$$xy_1'' - ny_1' + x^{n+m+1}y_1 = 0. \tag{18}$$

This equation is *singular*, as its leading coefficient vanishes at 0 (that is, at -1 in the corresponding rescaled equation). This prevents us from directly applying the validation method in the scalar case. However, one can use *desingularization* techniques [1] to obtain a higher order but nonsingular equation, whose set of solutions (strictly) contains the ones of the singular equation. In our example, it is possible to differentiate Equation (18) n times and divide the result by x:

$$y_1^{(n+2)} + \frac{1}{x}\frac{\mathrm{d}^n}{\mathrm{d}x^n}(x^{n+m+1}y_1) = 0. \tag{19}$$

By inverting the roles of n and m, a similar equation can be deduced for the second component y_2. Hence, validating the approximation y of System (17) can be entirely realized with the validation algorithm for the scalar

case, presented in [7]. Several caveats must therefore be raised. Applying the integral operator of [7] results into a totally intractable problem, since the minimal value for proving that $\mathbf{T}$ is contracting is far too large (in practice, we stopped at $N_{\text{val}} \simeq 10^6$). This is due to the fact that this transform is used to validate the last derivative $y_1^{(n+2)}$, which increases very rapidly due to the highly oscillating behaviour of y_1. On the other hand, the integral transform of [5] yields a far more tractable problem: a truncation order $N_{\text{val}} = 750$ is sufficient for our example. However, Equation (19) is very ill-conditioned because of the factorial terms created by the n differentiations. For instance, with classical double precision (53 bits), the scalar validation procedure is able to produce and bound a contracting Newton-like operator $\mathbf{T}$ (**Algorithm 1**), but **Algorithm 3** outputs an upper bound $\varepsilon_1^+ = 2.57$, which is 3 orders of magnitude larger than what was found with the vector-valued validation method.

The non D-finite case. In the case of nonpolynomial coefficients $a_i(t)$, there is no general method to decouple and desingularize the system. Moreover, these coefficients may not be known exactly, but only given as polynomial approximations together with rigorous error bounds. We do believe that in such a general case, the vector-valued approach presented in this article is essential to approximate and validate the solution. Detailing such a "realistic" example is beyond the scope of this article, but a successful application of our method is given in [3] for a station keeping problem of a satellite.

Future extensions include: validated expansions in other orthogonal polynomial bases for LODEs; automation and complexity analysis for some classes of nonlinear ODEs; formally proving this method in a proof assistant.

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Appendix

A.1 Complementary Proofs for Section 2

Proof of Theorem 2. (i) Endow X with the metric $d_\infty(x,y) = \|d(x,y)\|_\infty = \max_{1\leqslant i\leqslant p} d_i(x)$, so that (X, d_∞) is a complete metric space. For an order p square matrix A, define:

$$\|A\|_\infty = \max_{1\leqslant i\leqslant p} \sum_{1\leqslant j\leqslant p} |A_{ij}| = \sup_{\|x\|_\infty\leqslant 1} \|A\cdot x\|_\infty.$$

Since $\Lambda^k \to 0$, there is a k such that $\mu = \|\Lambda^k\|_\infty < 1$. Then $\mathbf{T}^k$ is a μ-contraction for the d_∞ metric, so that Banach theorem applies and gives $x^\star$ as the unique fixed-point of $\mathbf{T}^k$. Hence $\mathbf{T}$ can have at most one fixed point. From the following inequality:

$$\begin{aligned} d_\infty(x^\star, \mathbf{T}\cdot x^\star) &= d_\infty(\mathbf{T}^k\cdot x^\star, \mathbf{T}^{k+1}\cdot x^\star) \\ &\leqslant \|\Lambda^k\|_\infty d_\infty(x^\star, \mathbf{T}\cdot x^\star) < d_\infty(x^\star, \mathbf{T}\cdot x^\star), \end{aligned}$$

we get that $x^\star = \mathbf{T}\cdot x^\star$ is the unique fixed point of $\mathbf{T}$.

(ii) Let $x^\circ \in X$. Since $d(x^\circ, x^\star) \leqslant d(x^\circ, \mathbf{T}\cdot x^\circ) + d(\mathbf{T}\cdot x^\circ, x^\star) \leqslant d(x^\circ, \mathbf{T}\cdot x^\circ) + \Lambda\cdot d(x^\circ, x^\star)$, we get:

$$(\mathbf{1}-\Lambda)\cdot d(x^\circ, x^\star) \leqslant d(x^\circ, \mathbf{T}\cdot x^\circ). \tag{20}$$

Since $\Lambda^k \to 0$ as $k\to\infty$, it is easy to prove that $\mathbf{1}-\Lambda$ is nonsingular, with nonnegative inverse $(\mathbf{1}-\Lambda)^{-1} = \sum_{k\geqslant 0}\Lambda^k \geqslant \mathbf{0}$. Therefore, multiplying both members of Inequality (20) by $(\mathbf{1}-\Lambda)^{-1}$ is licit, so as to obtain the upper bound (3) for $n=0$. The general bound for $n\geqslant 0$ follows from the fact that $\mathbf{T}$ is Λ-Lipschitz.

□

In order to prove the technical Lemma 1, we need the following fact:

Lemma 2. *Let $A \in \mathcal{M}_p^{\to 0}(\mathbb{R}_+)$ a convergent to zero nonnegative matrix and $B \in \mathcal{M}_p(\mathbb{R})$ a matrix whose entries are dominated by those of A:*

$$|B_{ij}| \leqslant A_{ij}, \qquad \textit{for all } i,j \in [\![1,p]\!].$$

Then B is convergent to zero.

Proof. Since A has nonnegative entries which bound those of B, it can be easily shown by the triangle inequality that for any exponent $k\geqslant 0$, $|B_{ij}^k| \leqslant A_{ij}^k$ for all $i,j\in[\![1,p]\!]$. This directly implies the conclusion of Lemma 2. □

Proof of Lemma 1. First, $\mathbf{1}-D_i\cdot\Lambda$ is nonsingular because $D_i\cdot\Lambda$ is convergent to zero by use of Lemma 2, since its entries are clearly dominated by those of $\Lambda \in \mathcal{M}_p^{\to 0}(\mathbb{R}_+)$. Hence so is $\Lambda - D_i$.

Then we prove that $\mathbf{1}-\Lambda$ and $\mathbf{1}-D_i\cdot\Lambda$ both have positive determinant. The segment $\mathbf{1}-\tau\Lambda$ ($\tau \in [0,1]$) connects $\mathbf{1}$ to $\mathbf{1}-\Lambda$, and all these matrices are nonsingular, because $\tau\Lambda$ converges to zero according to Lemma 2. Since $\det(\mathbf{1}) = 1 > 0$, we get by connectedness that $\det(\mathbf{1}-\Lambda) > 0$. A similar argument proves that $\det(\mathbf{1}-D_i\Lambda) > 0$, and hence $\det(D_i - \Lambda) < 0$.

Remember that for a nonsinglular matrix M, we have $M^{-1} = (\det M)^{-1} Cof(M)^T$, where $Cof(M)$ is the cofactor matrix of M, whose entries are the minors of M. Noticing that $Cof(D_i-\Lambda)_{ji} = Cof(\mathbf{1}-\Lambda)_{ji}$ for $j \in [\![1,p]\!]$ and using the fact that $\det(D_i-\Lambda) < 0$, $\det(\mathbf{1}-\Lambda) > 0$ and all entries in $(\mathbf{1}-\Lambda)^{-1}$ are nonnegative, we conclude that all entries on the i-th row of $(D_i-\Lambda)^{-1}$ are non-positive. □

A.2 Discussion About the Tightness of Error Enclosures of Section 2

In the one-dimensional case with a contracting operator of Lipschitz constant $\lambda \in (0,1)$, the ratio of the upper bound and the lower bound given by Banach fixed-point theorem is equal to $(1+\lambda)/(1-\lambda) > 1$. This quantity does not depend on the approximation x°, and uniformly tends to 1 as $\lambda \to 0$, justifying the principle: the more contracting the operator is, the tighter the obtained enclosure is.

This section aims at extending this study to the vectorial case, for the bounds obtained from Theorems 2 and 3. Let's first exhibit an expression for the ratio of this enclosure.

Lemma 3. *Let $\mathbf{T}$ be contracting of Lipschitz matrix $\Lambda \in \mathcal{M}_p^{\to 0}(\mathbb{R}_+)$ and $\eta = d(x^\circ, \mathbf{T}\cdot x^\circ)$. Fix an index $i \in [\![1,p]\!]$ and let $\varepsilon_i^+ = e_i^T\cdot(\mathbf{1}-\Lambda)^{-1}\cdot\eta$ and $\varepsilon_i^- = e_i^T\cdot(\mathbf{1}-D_i\cdot\Lambda)^{-1}\cdot\eta$ denote, respectively, the upper and lower bounds for the i-th component of $d(x^\circ, x^\star)$, as given by Theorems 2 and 3.*

Then, if $\varepsilon_i^- > 0$, the ratio of the enclosure is equal to:

$$\frac{\varepsilon_i^+}{\varepsilon_i^-} = \frac{d'}{d}\frac{c_i\eta_i + \sum_{j\neq i} c_j\eta_j}{c_i\eta_i - \sum_{j\neq i} c_j\eta_j}, \tag{21}$$

where $d = \det(\mathbf{1}-\Lambda)$, $d' = \det(\mathbf{1}-D_i\cdot\Lambda)$ and $c = (c_1,\dots,c_p) = e_i^T\cdot(\mathbf{1}-\Lambda)^{-1}$ is the i-th row of $(\mathbf{1}-\Lambda)^{-1}$.

Proof. We have:

$$\varepsilon_i^+ = c_i\eta_i + \sum_{j\neq i} c_j\eta_j, \qquad \text{and} \qquad \varepsilon_i^- = c_i'\eta_i + \sum_{j\neq i} c_j'\eta_j,$$

where $c = (c_1, \dots, c_p) = e_i^T \cdot (1-\Lambda)^{-1}$ and $c' = (c'_1, \dots, c'_p) = e_i^T \cdot (1-D_i \cdot \Lambda)^{-1}$. Reusing the discussion led in the proof of Lemma 1, we have:

$$dc_i = d'c'_i, \qquad \text{and} \qquad dc_j = -d'c'_j \quad \text{for all } j \neq i.$$

This directly provides Equation (21). □

In particular, Lemma 3 shows that the ratio now depends not only on Λ, but also on $\eta = d(x^\circ, \mathbf{T} \cdot x^\circ)$.

Let's first fix η with $\eta_i > 0$, and make Λ tend to zero. Then $\mathbf{1} - \Lambda$ and $\mathbf{1} - D_i \cdot \Lambda$ are closed to the identity matrix (hence $d, d' \approx 1$), and so are their inverses, meaning that $c_i \approx 1$ and $c_j \ll c_i$ for $j \neq i$. We thus recover the principle: the smaller Λ is, the tighter the enclosure is.

Let's now fix Λ, as small as desired. As long as $c_j > 0$ for some $j \neq i$, there exists a vector of errors η that makes the ratio arbitrarily large (take η_j large enough), or even makes ε_i^- become negative, in which case the overapproximation factor of the upper bound ε_i^+ provided by Theorem 2 is not controlled.

Let's now fix a maximal value $\kappa > 1$ for the ratio $\varepsilon_i^+/\varepsilon_i^-$. This yields the following condition over η:

$$\eta_i \geqslant \frac{\kappa d + d'}{\kappa d - d'} \frac{1}{c_i} \sum_{j \neq i} c_j \eta_j, \qquad (22)$$

which roughly states that η_i should not be too small compared to the other components of η. By stating similar constraints for all $i \in [\![1, p]\!]$, we get that η must live in a cone $\mathcal{C}_\kappa$, that we call *tightness cone*, in order to ensure an overapproximation ratio smaller than κ. Under a certain value for κ, $\mathcal{C}_\kappa$ is empty, meaning that $\mathbf{T}$ is not contracting enough to achieve this ratio, whatever η is. The cone $\mathcal{C}_\kappa$ grows to a *limit cone* $\mathcal{C}_\infty$ as $\kappa \to +\infty$, defined by replacing $(\kappa d + d')/(\kappa d - d')$ by 1 in the constraints (22). A point η outside $\mathcal{C}_\infty$ means that the componentwise error distribution is so unbalanced that some lower bound ε_i^- is negative (hence rounded to zero). Figure 4 illustrates the cones $\mathcal{C}_\kappa$ for different values of κ and the limit cone $\mathcal{C}_\infty$ arising in our toy example. In particular, we observe that η belongs to $\in \mathcal{C}_{1.2}$ but not to $\mathcal{C}_{1.17}$, which is consistent with the numerical values (6) for $\varepsilon_1^-, \varepsilon_1^+, \varepsilon_2^-, \varepsilon_2^+$ obtained in Section 2.2.

A.3 Proof of Theorem 4

Proof. The value of N_{val} must be sufficiently large to ensure that the truncation error $\|(\mathbf{1} + \mathbf{K}^{[N_{\text{val}}]})^{-1} \cdot (\mathbf{K} - \mathbf{K}^{[N_{\text{val}}]})\|_{\text{Ч}^1}$ is a convergent to zero matrix.

- We have as a direct consequence of the one-dimensional case [7, Lemma 3.5]:

$$\|\mathbf{K} - \mathbf{K}^{[N_{\text{val}}]}\|_{\text{Ч}^1} = O\left(\frac{B}{N_{\text{val}}}\right).$$

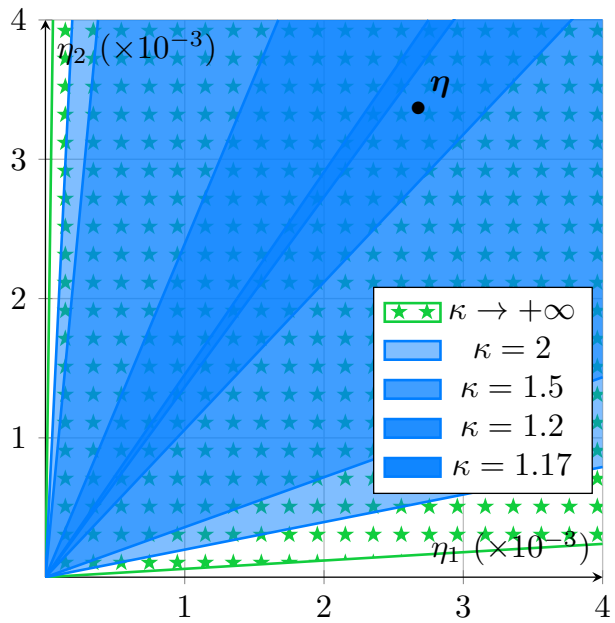

Figure 4: Tightness cones for the toy example

- For $i \geqslant 0$, the bound $\|\mathbf{K}^i\| \leqslant (6di+1)\frac{(2C)^i}{i!}$ is generalized from the one-dimensional case contained in the proof of [7, Lemma 3.3], where $C = (C_{ij})_{1\leqslant i,j\leqslant p}$ with $C_{ij} = \sup_{-1\leqslant s,t\leqslant 1} |k_{ij}(t,s)|$ is bounded by B. Since $\mathbf{K}^{[N_{\text{val}}]}$ converges to $\mathbf{K}$, we may approximate:

$$\|(\mathbf{1}+\mathbf{K}^{[N_{\text{val}}]})^{-1}\|_{\text{Ч}^1} \approx \|(\mathbf{1}+\mathbf{K})^{-1}\|_{\text{Ч}^1} = O\left(dB\exp(2B)\right).$$

We therefore have:

$$\|(\mathbf{1}+\mathbf{K}^{[N_{\text{val}}]})^{-1}\cdot(\mathbf{K}-\mathbf{K}^{[N_{\text{val}}]})\|_{\text{Ч}^1} = O\left(dB^2\exp(2B)\right),$$

which gives the estimate (16) for N_{val} to obtain a matrix with spectral radius less than 1. □