THE LANCZOS TAU FRAMEWORK FOR TIME-DELAY SYSTEMS: PADÉ APPROXIMATION AND COLLOCATION REVISITED*

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Abstract. We reformulate the Lanczos tau method for the discretization of time-delay systems in terms of a pencil of operators, allowing for new insights into this approach. As a first main result, we show that, for the choice of a shifted Legendre basis, this method is equivalent to Padé approximation in the frequency domain. We illustrate that Lanczos tau methods straightforwardly give rise to sparse, self-nesting discretizations. Equivalence is also demonstrated with pseudospectral collocation, where the non-zero collocation points are chosen as the zeroes of orthogonal polynomials. The importance of such a choice manifests itself in the approximation of the H^2-norm, where, under mild conditions, super-geometric convergence is observed and, for a special case, super convergence is proved; both of which are significantly faster than the algebraic convergence reported in previous work.

Key words. delay-differential equations, Lanczos tau methods, spectral methods, Padé approximation, rational approximation, H^2-norm, matrix equations, orthogonal polynomials

MSC codes. 65L03, 34K06, 15A24

1. Introduction.

We consider a time-delay system described by

$$\begin{aligned} \dot{\mathbf{x}}(t) &= A_0\mathbf{x}(t) + A_1\mathbf{x}(t-\tau) + B\mathbf{u}(t), \\ \mathbf{y}(t) &= C\mathbf{x}(t), \end{aligned} \tag{1.1}$$

where $\tau \in \mathbb{R}_+$ is the constant delay, $\mathbf{x}(t) \in \mathbb{C}^n$ the state variable, $\mathbf{u}(t) \in \mathbb{C}^p$ the input, and $\mathbf{y}(t) \in \mathbb{C}^q$ the output at time t. The transfer function of this system is given by

$$G(s) = C\big(sI_n - A_0 - A_1e^{-s\tau}\big)^{-1}B. \tag{1.2}$$

Due to the presence of time-delay, the information required to define a forward solution at $t = 0$, for a given input, is not determined by $\mathbf{x}(0)$, but by the function segment $[-\tau, 0] \ni \theta \mapsto \mathbf{x}(\theta)$. More generally, the solution for all $t \geq t_0$ is uniquely defined by the solution for the time frame $[t_0 - \tau, t_0]$. Hence, the state at time t, in the natural meaning of minimal information to determine the future evolution, corresponds to the function segment $\xi_t : [-\tau, 0] \to \mathbb{C}^n$, with $\xi_t(\theta) = \mathbf{x}(t + \theta)$, which explains why a time-delay model represents an infinite-dimensional dynamical system. This infinite-dimensional nature implies that existing techniques for the analysis and design of delay-free systems cannot be readily applied. New methods thus have to be developed, most of which start by discretizing the infinite-dimensional system into a finite-dimensional approximation.

A common approach in the frequency domain is to replace the exponential function by a rational approximation, such as the Padé approximant (see e.g. Glover et al., 1991). One can also discretize at the level of the state space. There are two main variants taking this approach. As the system is linear and time-invariant, one can approximate the solution operator $\mathcal{S}_T$, which maps the function ξ_t to ξ_{t+T}. Such

*Preprint version.

Funding: This work was supported by KU Leuven project C14/22/092 and by FWO-Flanders under grant number G.092.721N.

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an approach is for instance adopted for linearized stability analysis in the bifurcation analysis package by Engelborghs et al. (2002), where $\mathcal{S}_T$ is approximated using a linear multistep method. Similarly, in the context of stability analysis of periodic delay-differential equations, Butcher et al. (2004) propose to discretize $\mathcal{S}_T$ as its action on a Chebyshev series approximation of ξ_t, where T is taken to be the period. The other option to discretize at the state space level, is to look at the infinitesimal generator $\mathcal{A}$ of the C_0-semigroup $\{\mathcal{S}_t\}_{t\geq 0}$, with action

$$\mathcal{A}\xi_t = \lim_{T\to 0^+} \tfrac{1}{T}(\mathcal{S}_T - I)\xi_t.$$

When the input and output in (1.1) are taken into account, this results in a standard state space description of a delay-free system, which captures part of the system behaviour of the original system. The main advantage of these methods is thus that one can often readily apply existing techniques for the analysis and design of finite-dimensional systems to this approximation. The earliest method in this category, to the best of our knowledge, is the Lanczos tau method of Ito and Teglas (1986), which relies on a truncated Legendre basis. This approach was extended to other bases, and shown to perform well when computing the characteristic roots, in Vyasarayani et al. (2014).

Another, particularly successful, approach in this class is pseudospectral collocation, introduced by Breda et al. (2005). It was initially presented for the eigenvalue problem, but later successfully extended to construct delay-free approximations, which can for instance be used for bifurcation analysis (Breda et al., 2016). This method collocates the action of the infinitesimal generator on a grid of nodes. In practice these are usually the Chebyshev extremal nodes, a set of nodes which are distributed more densely near the end points. This distribution evades Runge's phenomenon, which one can face in more naive collocation strategies (Boyd, 2001). Pseudospectral collocation is tightly linked to rational approximation of the exponential, which was for instance used in the initial paper to prove super-geometric convergence of the characteristic roots. Aside from theoretical interest, this link can also be exploited in practice. An example is a heuristic by Wu and Michiels (2012) to select a discretization degree such that all the characteristic roots to the right of the imaginary axis are sufficiently well approximated.

Another application of these discretizations is in the computation of system norms. An example of particular importance is the H^2-norm, which, for an exponentially stable, linear, time-invariant system with transfer function G, is given by

$$\|G\|_{H^2} = \left(\frac{1}{2\pi}\int_{-\infty}^{+\infty} \|G(i\omega)\|_F^2 \,\mathrm{d}\omega\right)^{\frac{1}{2}}, \tag{1.3}$$

where i is the imaginary unit and $\|A\|_F = \sqrt{\mathrm{tr}(AA^*)}$ the Frobenius norm. This norm is often used in robust control as a measure of disturbance rejection and, in the context of model reduction, to quantify the approximation error at the transfer function level. As it is a global characteristic, in the sense that it depends on the transfer function's behaviour along the entire imaginary axis, its computation is rather challenging. For delay-free systems an efficient method involving the algebraic Lyapunov equation is well known (Zhou et al., 1995, Lemma 4.6). The natural extension in the delay setting is the so-called delay Lyapunov equation, a boundary value problem defining a matrix-valued function. In Jarlebring et al. (2011), a spectral discretization of this equation is proposed to compute the H^2-norm, yielding super-geometric

convergence of this norm, at the cost of $\mathcal{O}(n^6N^3)$ operations, where N is the degree of the approximation. Alternatively, Vanbiervliet et al. (2011) propose to instead approximate the system using a pseudospectral discretization and then compute its H^2-norm through the standard algebraic Lyapunov equation. This improves the time complexity to $\mathcal{O}(n^3N^3)$ operations, but reduces the convergence rate to third order algebraic convergence.

In the final section of this article, we illustrate how using a Lanczos tau method for the approximation of the system allows us to recover super-geometric convergence, and sometimes even results in super convergence, giving us the best of both worlds. This unexpected improvement served as the initial motivation to revisit the Lanczos tau method in this work.

Overview. After reviewing some preliminaries in section 2, we present an operator pencil formulation of the Lanczos tau framework (section 3). We continue by discussing some properties of these methods in section 4. In particular, we show how these naturally lead to sparse, nested discretizations and how they are deeply connected to other approximations. We prove equivalence to pseudospectral collocation, when the non-zero collocation points are chosen as the zeroes of an orthogonal polynomial, and a surprising link to Padé approximation, when using shifted Legendre polynomials. Finally, we conclude by illustrating super-geometric convergence, and for some cases proving super convergence, of the H^2-norm in section 5.

Notation. Throughout this work we will rely on some classical orthogonal polynomials shifted to the interval $[-\tau, 0]$. To lighten notation we shall denote these shifted polynomials by their usual names in the literature for the interval $[-1, 1]$. In particular we will use T_k and U_k to denote the shifted Chebyshev polynomials of the first and second kind, respectively, and $P_k^{(\alpha,\beta)}$ the similarly transformed Jacobi polynomials, of which the shifted Legendre polynomials P_k are a special case. We give a review of these polynomials in subsection 2.3.

2. Preliminaries. Before presenting the Lanczos tau framework, we review some basic notions and previous work needed in our later development.

2.1. The abstract Cauchy problem. To build towards a discretization of the functional differential equation (1.1), we detail how one can reformulate it in terms of an abstract Cauchy problem on an infinite-dimensional vector space, where the unknown, corresponding to the state, is a function defined over an interval of length τ. To handle inputs, we explicitly decouple the current state from the history (resulting in the so-called 'head-tail' representation) as in Curtain and Zwart (1995). More precisely, we consider as state space

$$X := \mathbb{C}^n \times L^2([-\tau, 0]; \mathbb{C}^n). \tag{2.1}$$

Let $\mathcal{A} : D(\mathcal{A}) \to X$ be the differential operator with domain

$$D(\mathcal{A}) = \left\{(\mathbf{z}, \zeta) \in X : \zeta \in AC, \tfrac{\mathrm{d}}{\mathrm{d}\theta}\zeta \in L^2, \mathbf{z} = \zeta(0)\right\}$$

(where L^2 and AC have domain $[-\tau, 0]$ and codomain $\mathbb{C}^n$) and action

$$\mathcal{A}\begin{pmatrix}\mathbf{z}\\ \zeta\end{pmatrix} = \begin{pmatrix}(A_0\varepsilon_0 + A_1\varepsilon_{-\tau})\zeta\\ \mathcal{D}\zeta\end{pmatrix},$$

where, for later convenience, we introduce evaluation functionals $\varepsilon_\theta\zeta = \zeta(\theta)$ and differentiation operator $\mathcal{D}\zeta = \frac{\mathrm{d}}{\mathrm{d}\theta}\zeta$. Next, let operators $\mathcal{B} : \mathbb{C}^p \to X$ and $\mathcal{C} : X \to \mathbb{C}^q$ be defined by

$$\mathcal{B}\mathbf{u} = (B\mathbf{u}, \mathbf{0}) \quad \text{and} \quad \mathcal{C}z = C\mathbf{z},$$

where $\mathbf{u} \in \mathbb{C}^p$ and $z = (\mathbf{z}, \zeta) \in X$.

We can now rewrite (1.1) as the abstract Cauchy problem

$$\begin{aligned} \dot{z}(t) &= \mathcal{A}z(t) + \mathcal{B}\mathbf{u}(t), \\ \mathbf{y}(t) &= \mathcal{C}z(t), \end{aligned} \tag{2.2}$$

where $z(t) = (\mathbf{z}(t), \zeta_t) \in D(\mathcal{A})$. The relation between corresponding solutions of (1.1) and (2.2) is then given by

$$\mathbf{z}(t) = \mathbf{x}(t) \quad \text{and} \quad \zeta_t(\theta) = \mathbf{x}(t+\theta), \quad \forall \theta \in [-\tau, 0].$$

For a more detailed description of the mapping between representations, and further detail on the inclusion of input and output, we refer to Curtain and Zwart (1995).

2.2. Pseudospectral collocation. As we will discuss relations between pseudospectral collocation and Lanczos tau methods, we outline how the system (2.2), and thus also (1.1), can be discretized using the former method. A more comprehensive treatment is given in Breda et al. (2015). Given a positive integer N, we consider a mesh Ω of $N+1$ distinct points in the interval $[-\tau, 0]$, namely

$$\Omega = \{\theta_k : k = 0, \ldots, N\}, \tag{2.3}$$

where

$$-\tau \leq \theta_0 < \cdots < \theta_{N-1} < \theta_N = 0.$$

This allows us to replace the continuous space X, defined in (2.1), with the space X_N of discrete functions defined on the mesh Ω, i.e. any tuple $(\mathbf{z}, \zeta) \in X$ is approximated by a block vector $\mathbf{x}_N \in X_N$, with

$$\mathbf{x}_{N,k} = \zeta(\theta_k), \quad k = 0, \ldots, N-1, \quad \text{and} \quad \mathbf{x}_{N,N} = \mathbf{z}.$$

Let $\mathcal{P}\mathbf{x}_N$ be the unique $\mathbb{C}^n$-valued interpolating polynomial of degree at most N, satisfying

$$(\mathcal{P}\mathbf{x}_N)(\theta_k) = \mathbf{x}_{N,k}, \quad k = 0, \ldots, N.$$

This way we can approximate the operator $\mathcal{A}$ by the finite-dimensional operator $\mathcal{A}_N : X_N \to X_N$, defined by

$$\begin{cases} (\mathcal{A}_N \mathbf{x}_N)_k = (\mathcal{D}\mathcal{P}\mathbf{x}_N)(\theta_k), & k = 0, \ldots, N-1, \\ (\mathcal{A}_N \mathbf{x}_N)_N = (A_0 \varepsilon_0 + A_1 \varepsilon_{-\tau})(\mathcal{P}\mathbf{x}_N). \end{cases}$$

Note that in doing so, we implicitly enforce the boundary condition of the 'head-tail' representation, namely $(\mathcal{P}\mathbf{x}_N)(0) = \mathbf{x}_{N,N} = \mathbf{z}$, where $\mathcal{P}\mathbf{x}_N$ can be seen as the approximation of ζ.

Using the Lagrange representation of $\mathcal{P}\mathbf{x}_N$,

$$(\mathcal{P}\mathbf{x}_N)(\theta) = \sum_{k=0}^{N} \mathbf{x}_{N,k}\, \ell_k(\theta),$$

where the Lagrange polynomials ℓ_k are those real-valued polynomials of degree N satisfying $\ell_k(\theta_j) = \delta_{jk}$, with δ_{jk} the usual Kronecker delta, one can get an explicit matrix expression

$$\mathcal{A}_N = \begin{pmatrix} [\underline{\mathcal{D}}] \\ \mathbf{a} \end{pmatrix},$$

where $[\underline{\mathcal{D}}]$ consists of the first N block rows of the $(N+1)\times(N+1)$ differentiation matrix

$$[\mathcal{D}]_{jk} = I_n \ell_k'(\theta_j),$$

and $\mathbf{a}$ is a block row vector with

$$\mathbf{a}_k = A_0\ell_k(0) + A_1\ell_k(-\tau),$$

where $j = 0,\dots,N$ and $k = 0,\dots,N$.

In the same way we can approximate $\mathcal{B}$ and $\mathcal{C}$ by

$$\mathcal{B}_N = \begin{pmatrix}\mathbf{0} & \cdots & \mathbf{0} & B^T\end{pmatrix}^T \quad \text{and} \quad \mathcal{C}_N = \begin{pmatrix}\mathbf{0} & \cdots & \mathbf{0} & C\end{pmatrix}.$$

As such, we arrive at a finite-dimensional approximation of (1.1)

$$\begin{aligned}\dot{\mathbf{x}}_N(t) &= \mathcal{A}_N\mathbf{x}_N(t) + \mathcal{B}_N\mathbf{u}(t),\\ \mathbf{y}_N(t) &= \mathcal{C}_N\mathbf{x}_N(t).\end{aligned} \tag{2.4}$$

We can thus also approximate the transfer function (1.2) by

$$J_N(s) = \mathcal{C}_N\big(sI_{n(N+1)} - \mathcal{A}_N\big)^{-1}\mathcal{B}_N. \tag{2.5}$$

The following result on the structure of this approximation was proved by Gumussoy and Michiels (2010).

PROPOSITION 2.1. *The transfer function* (2.5) *satisfies*

$$J_N(s) = C(sI_n - A_0 - A_1 p_N(s,-\tau))^{-1}B,$$

where the function

$$[-\tau,0] \ni \theta \mapsto p_N(s,\theta)$$

is the unique polynomial of degree N satisfying

$$\begin{cases} p_N(s,0) = 1,\\ p_N'(s,\theta_k) = s p_N(s,\theta_k), \quad k = 0,\dots,N-1.\end{cases}$$

Furthermore, $p_N(s,\theta)$ is a rational function of s for all θ.

The effect of approximating (1.1) by (2.4) can thus be interpreted, in the frequency domain, as the effect of approximating the exponential function $s \mapsto e^{-s\tau}$ in (1.2) by the rational function $s \mapsto p_N(s,-\tau)$.

A common choice of mesh points in the literature consists of scaled and shifted Chebyshev extremal points, that is,

$$\theta_k = -\tfrac{\tau}{2}\big(\cos\big(\tfrac{\pi k}{N}\big) + 1\big), \quad k = 0,\dots,N.$$

The choice of this mesh is motivated by the resulting fast convergence of the eigenvalues of $\mathcal{A}_N$ to the corresponding characteristic roots of (1.1). More specifically, in Breda et al. (2005, Theorem 3.6) it is proved that super-geometric accuracy, i.e. approximation error $\mathcal{O}\big(N^{-N}\big)$, is obtained using these nodes.

To conclude this section, and to introduce the operator approach of section 3, note that we can rewrite $\mathbf{a}$ in terms of a block vector expression of the evaluation functionals, namely

$$\mathbf{a} = A_0[\varepsilon_0] + A_1[\varepsilon_{-\tau}],$$

where $[\varepsilon_\theta]_k = I_n\ell_k(\theta)$. Similarly, we have for $\mathcal{C}_N$

$$C\begin{pmatrix}\mathbf{0} & \cdots & \mathbf{0} & I_n\end{pmatrix} = C[\varepsilon_0].$$

2.3. Orthogonal polynomials. The Lanczos tau framework presented in the next section will rely on the notion of a degree-graded series of polynomials orthogonal with respect to an inner product $\langle \cdot, \cdot \rangle$, with induced norm $\|\phi\| = \sqrt{\langle \phi, \phi \rangle}$.[1] That is, a set of polynomials $\{\phi_k\}_{k=0}^{\infty}$ which has as defining property that ϕ_k is of degree k and $\langle \phi_j, \phi_k \rangle = 0$ if and only if $j \neq k$. Usually, the inner product chosen is of the form

$$\langle \phi_j, \phi_k \rangle = \int_{-\tau}^{0} \phi_j(\theta) \overline{\phi_k(\theta)}\, w(\theta)\, \mathrm{d}\theta\,,$$

with $w(\theta) \geq 0$, $\forall \theta \in [-\tau, 0]$, the weight function. The choice of w, together with a normalization condition, then uniquely defines the orthogonal sequence.

Throughout this work we will use the Jacobi polynomials $P_k^{(\alpha,\beta)}$ shifted to the interval $[-\tau, 0]$, which are given by the weight function

$$w(\theta) = \left(-\tfrac{2}{\tau}\theta\right)^{\alpha} \left(\tfrac{2}{\tau}\theta + 2\right)^{\beta},$$

and normalization condition $P_k^{(\alpha,\beta)}(0) = \binom{k+\alpha}{k}$. As special cases we have

$$T_k = \binom{k-\frac{1}{2}}{k}^{-1} P_k^{\left(-\frac{1}{2},-\frac{1}{2}\right)} \quad \text{and} \quad U_k = (k+1)\binom{k+\frac{1}{2}}{k}^{-1} P_k^{\left(\frac{1}{2},\frac{1}{2}\right)},$$

the shifted Chebyshev polynomials of, respectively, the first and second kind, and the shifted Legendre polynomials

$$P_k = P_k^{(0,0)}.$$

A thorough overview of the properties of these and many other orthogonal polynomials is given by Szegő (1939).

Finally, we note that, in practice, Chebyshev polynomials are generally preferred for the approximation of a function $f : [-\tau, 0] \to \mathbb{C}$ by a truncated series

$$f(\theta) \approx \sum_{k=0}^{N} \frac{\langle f, \phi_k \rangle}{\|\phi_k\|^2} \phi_k(\theta),$$

as fast convergence in N is guaranteed for sufficiently smooth functions. In particular, Mastroianni and Szabados (1995, Corollary 2) showed that functions with $m-1$ absolutely continuous derivatives, and the mth derivative of bounded variation, give mth order algebraic decay of the coefficients of this series. Additionally, Bernstein (1912, p. 94) proved that for a function which is analytically continuable to an ellipse in the complex plane, this improves to geometrical decrease $\mathcal{O}\left(\rho^N\right)$, with $0 < \rho < 1$ determined by to the size of the ellipse. In the limiting case where the function is entire, this becomes super-geometric decrease. We will use such a truncated series in the next section.

3. The Lanczos tau framework. We start by selecting an inner product $\langle \cdot, \cdot \rangle$ on the space $\mathbb{P}$ of polynomials $[-\tau, 0] \to \mathbb{C}$. Let $\{\phi_k\}_{k=0}^{\infty}$ be a degree-graded sequence of orthogonal polynomials with respect to this inner product, as in the previous section. Obviously, for any N, $\Phi_N = \{\phi_k\}_{k=0}^{N}$ is an orthogonal basis for $\mathbb{P}_N \subset \mathbb{P}$, the space of polynomials of degree at most N. Rather than replacing X by the discrete space X_N, as in subsection 2.2, in order to arrive at an approximation of (2.2), and thus (1.1), we will now replace it by the space $\mathbb{P}_N^n$, the space of polynomials of degree

[1] We assume the convention that $\langle \cdot, \cdot \rangle$ is linear in the first argument and antilinear in the second.

at most N that map to $\mathbb{C}^n$. The operation of differentiation, encapsulated in the action of the operator $\mathcal{A}$ in (2.2), reduces the degree of a polynomial with one. On the left hand side we will thus also have to map an element of $\mathbb{P}_N^n$ to an element of $\mathbb{P}_{N-1}^n$. The idea of Lanczos (1938) was to do so by truncating the series expansion, which was later applied to functional differential equations by Ito and Teglas (1986); it is their method which we will reformulate as an operator pencil. For an orthogonal sequence this truncation namely corresponds to the component-wise orthogonal projector $\mathcal{T}_{N-1}$, with action

$$\left(\mathcal{T}_{N-1}\xi\right)_j = \left(\xi\right)_j - \tfrac{\left\langle (\xi)_j, \phi_N \right\rangle}{\|\phi_N\|^2}\phi_N, \quad j = 1, \ldots, n.$$

Then letting, as in subsection 2.1, ε_θ denote the evaluation functional in θ, $\mathcal{D}$ the component-wise differentiation operator, and $\mathbf{0}$ the zero polynomial, we propose the following approximation of (1.1):

$$\begin{aligned} \begin{pmatrix} \varepsilon_0 \\ \mathcal{T}_{N-1} \end{pmatrix} \tfrac{\mathrm{d}}{\mathrm{d}t}\xi_{tN} &= \begin{pmatrix} A_0\varepsilon_0 + A_1\varepsilon_{-\tau} \\ \mathcal{D} \end{pmatrix} \xi_{tN} + \begin{pmatrix} B \\ \mathbf{0} \end{pmatrix} \mathbf{u}(t), \\ \mathbf{y}_N(t) &= C\varepsilon_0\xi_{tN}, \end{aligned} \tag{3.1}$$

where $\xi_{tN} \in \mathbb{P}_N^n$. The relation between solutions of (3.1) and solutions of (1.1) and (2.2) can then be described by

$$\mathbf{x}(t) = \mathbf{z}(t) \approx \xi_{tN}(0) \quad \text{and} \quad \zeta_t \approx \xi_{tN}.$$

Note that the evolution equation (3.1) is in an implicit form. To show that solutions of the corresponding initial value problem exist and are uniquely defined, we derive a matrix-vector representation, induced by expressing elements of $\mathbb{P}_N^n$ in the basis Φ_N. That is, $\xi_{tN} = \sum_{k=0}^{N} \mathbf{x}_{N,k}(t)\phi_k$, with $\mathbf{x}_{N,k}(t) \in \mathbb{C}^n$, $k = 0, \ldots, N$. Doing so, we get as block matrix realization of the operators

$$\left[\varepsilon_\theta\right]_k = I_n\phi_k(\theta), \quad \left[\mathcal{D}\right]_{jk} = I_n\tfrac{\left\langle \phi_k', \phi_j \right\rangle}{\|\phi_j\|^2}, \quad \text{and} \quad \left[\mathcal{T}_{N-1}\right]_{jk} = I_n\tfrac{\left\langle \phi_k, \phi_j \right\rangle}{\|\phi_j\|^2} = I_n\delta_{jk},$$

where $[\,\cdot\,]$ signifies the expression in coordinates, $j = 0, \ldots, N-1$, and $k = 0, \ldots, N$. This then gives the explicit state space realization

$$\begin{aligned} \mathcal{E}_N\dot{\mathbf{x}}_N(t) &= \mathcal{A}_N\mathbf{x}_N(t) + \mathcal{B}_N\mathbf{u}(t), \\ \mathbf{y}_N(t) &= \mathcal{C}_N\mathbf{x}_N(t), \end{aligned} \tag{3.2}$$

with

$$\begin{aligned} \mathcal{E}_N &= \begin{pmatrix} [\varepsilon_0] \\ [\mathcal{T}_{N-1}] \end{pmatrix} = \begin{pmatrix} \phi_0(0) & \cdots & \phi_{N-1}(0) & \phi_N(0) \\ & I_{N-1} & & \mathbf{0} \end{pmatrix} \otimes I_n, \\ \mathcal{A}_N &= \begin{pmatrix} A_0[\varepsilon_0] + A_1[\varepsilon_{-\tau}] \\ [\mathcal{D}] \end{pmatrix}, \quad \mathcal{B}_N = \begin{pmatrix} B \\ \mathbf{0} \end{pmatrix}, \quad \text{and} \quad \mathcal{C}_N = C[\varepsilon_0]. \end{aligned}$$

This matrix realization is also amenable to implementation. However, note that the elements of $[\mathcal{D}]$ should generally not be computed explicitly; see the book by Boyd (2001) for better approaches.

Due to a basic property of orthogonal polynomials, the zeroes of ϕ_k are located in the open interval $(-\tau, 0)$ (Szegő, 1939, Theorem 3.3.1), so it holds that $\phi_N(0) \neq 0$.

Hence, the matrix $\mathcal{E}_N$ is always invertible. The invertibility of its matrix expression also implies that

$$\begin{pmatrix} \varepsilon_0 \\ \mathcal{T}_{N-1} \end{pmatrix}^{-1}$$

is a well defined operator from $\mathbb{C}^n \times \mathbb{P}^n_{N-1}$ to $\mathbb{P}^n_N$, and forward solutions of (3.1) are thus uniquely defined.

Taking the Laplace transform of (3.1) gives

$$\begin{aligned} s \begin{pmatrix} \varepsilon_0 \\ \mathcal{T}_{N-1} \end{pmatrix} \hat{\xi}_{sN} &= \begin{pmatrix} A_0\varepsilon_0 + A_1\varepsilon_{-\tau} \\ \mathcal{D} \end{pmatrix} \hat{\xi}_{sN} + \begin{pmatrix} B \\ \mathbf{0} \end{pmatrix} \hat{\mathbf{u}}(s), \\ \hat{\mathbf{y}}_N(s) &= C\varepsilon_0 \hat{\xi}_{sN}, \end{aligned} \tag{3.3}$$

where $\hat{f}(s)$ is the transform of $f(t)$. In this way, we arrive at an expression of the transfer function of (3.1)

$$G_N(s) = C\varepsilon_0 \begin{pmatrix} s\varepsilon_0 - A_0\varepsilon_0 - A_1\varepsilon_{-\tau} \\ s\mathcal{T}_{N-1} - \mathcal{D} \end{pmatrix}^{-1} \begin{pmatrix} B \\ \mathbf{0} \end{pmatrix}. \tag{3.4}$$

To conclude this section, we provide a counterpart to Proposition 2.1.

PROPOSITION 3.1. *The transfer function* (3.4) *satisfies*

$$G_N(s) = C(sI_n - A_0 - A_1 r_N(s, -\tau))^{-1} B,$$

where the function

$$[-\tau, 0] \ni \theta \mapsto r_N(s, \theta)$$

is the unique polynomial of degree N satisfying

$$\begin{cases} r_N(s, 0) = 1, \\ \mathcal{D} r_N(s, \cdot\,) = s\mathcal{T}_{N-1} r_N(s, \cdot\,). \end{cases}$$

Furthermore, $r_N(s, \theta)$ is a rational function of s for all θ.

Proof. By expanding $r_N(s, \cdot\,)$ in a basis, it can easily be seen that it is uniquely defined. The second row of the top expression in (3.3) corresponds to a set of homogeneous equations, each of which has $r_N(s, \cdot\,)$ as a solution, by the latter's definition. As a consequence, the solutions of this set are of the form $\hat{\xi}_{sN} = r_N(s, \cdot\,)\mathbf{z}(s)$, with $\mathbf{z}(s) \in \mathbb{C}^n$. Substituting this form in the first row of the top equation leads us to

$$s\mathbf{z}(s) = A_0\mathbf{z}(s) + A_1 r_N(s, -\tau)\mathbf{z}(s) + B\hat{\mathbf{u}}(s),$$

while the output equation becomes $\hat{\mathbf{y}}_N(s) = C\mathbf{z}(s)$. The assertions follow from solving for $\mathbf{z}(s)$. ∎

From the definition of r_N we get the compact representation

$$r_N(s, \theta) = \varepsilon_\theta \begin{pmatrix} \varepsilon_0 \\ s\mathcal{T}_{N-1} - \mathcal{D} \end{pmatrix}^{-1} \begin{pmatrix} 1 \\ \mathbf{0} \end{pmatrix}. \tag{3.5}$$

Using this representation we can derive an explicit rational form, as stated in the following result.

PROPOSITION 3.2. *The rational function* (3.5) *is given by the explicit expression*

$$r_N(s,\theta) = \frac{\sum_{k=0}^{N} \phi_N^{(N-k)}(\theta)\, s^k}{\sum_{k=0}^{N} \phi_N^{(N-k)}(0)\, s^k},$$

where $\phi^{(k)}$ *is the* k*th derivative of* ϕ*.*

Proof. By expressing (3.5) in the derivative basis $\{\phi_N^{(N-k)}\}_{k=0}^{N}$, we obtain the companion matrix representation

$$r_N(s,\theta) = \begin{pmatrix} \phi_N^{(N)}(\theta) \\ \phi_N^{(N-1)}(\theta) \\ \vdots \\ \phi_N(\theta) \end{pmatrix}^T \begin{pmatrix} \phi_N^{(N)}(0) & \phi_N^{(N-1)}(0) & \cdots & \phi_N^{(1)}(0) & \phi_N(0) \\ s & -1 & & & \\ & s & -1 & & \\ & & \ddots & \ddots & \\ & & & s & -1 \end{pmatrix}^{-1} \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix},$$

from which the assertion follows directly. ∎

Note that, generally, the coefficients of this expression grow rapidly with N. For numerical reasons, solving (3.5) or using the state space realization is usually preferred in implementation.

4. Properties. We continue by showing several links to previously proposed methods, which can, partially, be unified under the Lanczos tau operator framework. Additionally, we present how Lanczos tau methods naturally lead to nested, sparse discretizations.

4.1. Relation to pseudospectral collocation. Since Lanczos tau methods for differential equations are well known to correspond to collocation in the zeroes of the truncated polynomial (Lanczos, 1938), a similar intimate connection between pseudospectral collocation and the approximation scheme of the previous section is expected; the following result holds.

THEOREM 4.1. *Assume that the non-zero mesh points of* Ω*, as defined in* (2.3)*, are chosen as the zeroes of* ϕ_N*, that is*

$$\phi_N(\theta_k) = 0, \quad k = 0, \ldots, N-1.$$

Then for any N*, the finite-dimensional approximations* (2.4) *and* (3.1) *are equivalent, i.e.* $J_N(s) = G_N(s)$*.*

Proof. Note that (2.4) can also be derived from the relations

$$\begin{cases} \varepsilon_0 \frac{\mathrm{d}}{\mathrm{d}t}\eta_{tN} = (A_0\varepsilon_0 + A_1\varepsilon_{-\tau})\eta_{tN} + B\mathbf{u}(t), \\ \varepsilon_{\theta_k} \frac{\mathrm{d}}{\mathrm{d}t}\eta_{tN} = \varepsilon_{\theta_k}\mathcal{D}\eta_{tN}, \quad k = 0, \ldots, N-1, \\ \mathbf{y}_N(t) = C\varepsilon_0\eta_{tN}, \end{cases}$$

with $\eta_{tN} \in \mathbb{P}_N^n$, by expressing η_{tN} in the Lagrange basis with respect to (2.3). Additionally, using the definition of $\mathcal{T}_{N-1}$, the bottom row of the first equation in (3.1) reads

$$\left(\tfrac{\mathrm{d}}{\mathrm{d}t}\xi_{tN}\right)_j - \left\langle \left(\tfrac{\mathrm{d}}{\mathrm{d}t}\xi_{tN}\right)_j, \phi_N \right\rangle \tfrac{\phi_N}{\|\phi_N\|^2} = (\mathcal{D}\xi_{tN})_j, \quad j = 1, \ldots, n,$$

which, under the above conditions on Ω, implies

$$\varepsilon_{\theta_k} \tfrac{\mathrm{d}}{\mathrm{d}t}\xi_{tN} = \varepsilon_{\theta_k}\mathcal{D}\xi_{tN}, \quad k = 0, \ldots, N-1.$$

Hence, the conditions imposed on the evolution of the polynomial ξ_{tN}, as a function of t, imply the conditions imposed on the evolution of the polynomial η_{tN}. But since each set of conditions uniquely defines the flow, they must be equivalent. ∎

This connection allows one to reuse the large number of results that were developed for collocation-based methods. In particular, we recover super-geometric convergence of the eigenvalues when using a Chebyshev basis of the first or second kind, as this corresponds to using the zeroes of T_N or U_N as the non-zero collocation points (Breda et al., 2015, Theorem 5.1). Such a result is not unexpected as the conditions in Propositions 2.1 and 3.1, in the limit, define the function $\theta \mapsto e^{s\theta}$. These methods are thus grounded in the approximation of the exponential by a polynomial, obtained through collocation or the truncation of a series, respectively. From the discussion in subsection 2.3, and analogous results for interpolation through Chebyshev nodes, super-geometric convergence is observed for this function as it is entire.

4.2. Sparse, nested discretizations. From a degree-graded orthogonal sequence $\{\phi_k\}_{k=0}^{\infty}$, we can trivially form a sequence of nested bases $\Phi_0 \subset \Phi_1 \subset \dots$ for $\mathbb{P}_0 \subset \mathbb{P}_1 \subset \dots$ respectively. As a consequence, it is easy to construct a matrix realization of (3.1) which is also nested, in the sense that the resulting matrices for degree N_1 are submatrices of those at degree N_2, for $N_1 < N_2$. In fact, the matrices in (3.2) have this property.

This nesting of state space representations can be exploited in Krylov algorithms for characteristic roots computation and model reduction of time delay systems of high dimension, as in the infinite Arnoldi method introduced by Jarlebring et al. (2010). This leads to far cheaper and far more flexible methods, as this nesting allows the reuse of previous computations whilst adaptively changing the discretization degree.

As an example, the self-nesting discretization initially derived for this purpose in the above article is based on collocation in zero and the zeroes of U_N. By Theorem 4.1 we can thus recast this in the framework of section 3, as this corresponds, up to a basis transform, to the choice $\Phi_N = \{U_k\}_{k=0}^{N}$.

Furthermore, note that when expressing (3.1) in a basis, it is not necessary to use Φ_N as basis for the input side of the operators (on the contrary, using Φ_N to represent the output yields neater representations of $\mathcal{T}_{N-1}$ and is thus generally preferred). One can, for instance, choose the Chebyshev polynomials of the first kind on the input side and those of the second kind as Φ_N. This leads to a highly sparse representation of $\mathcal{D}$, with $\mathcal{O}(N)$ non-zeroes instead of $\mathcal{O}(N^2)$, as exploited in the ultraspherical method introduced by Olver and Townsend (2013), yielding even more computational gains. In fact, the matrix representation of Jarlebring et al. (2010) corresponds to this choice, up to a scaling of the rows.

4.3. Relation to Padé approximation. The Padé approximant of e^s near zero and the Legendre polynomials are well known to be linked, as shown by Ahmad (1998). In the context of the approximation of time-delay systems, such a connection has also been demonstrated by Bajodek et al. (2021), which inspires a potential similar link for the Lanczos tau framework. Such a connection indeed turns out to exist, as shown by the following result.

THEOREM 4.2. *For the choice $\Phi_N = \{P_k\}_{k=0}^{N}$, the rational function*

$$s \mapsto r_N(s, -\tau),$$

as in Proposition 3.1*, is an (N, N) Padé approximant of $e^{-\tau s}$ near zero.*

Proof. From Proposition 3.1 we know that $r_N(s,-\tau)$ is a rational function of (at most) type (N,N). The defining property of a Padé approximant of this type, and thus what we must show, is that the first $2N+1$ moments match those of the exponential at zero, i.e.

$$\left[\tfrac{\mathrm{d}^n}{\mathrm{d}s^n} r_N(s,-\tau)\right]_{s=0} = \left[\tfrac{\mathrm{d}^n}{\mathrm{d}s^n} e^{-\tau s}\right]_{s=0} = (-\tau)^n \quad \forall n \leq 2N.$$

As the operators involved in (3.5) linearly map between finite-dimensional spaces, we can apply the analogue of the derivative of an inverse matrix, yielding

$$\begin{aligned}\left[\tfrac{\mathrm{d}^n}{\mathrm{d}s^n} r_N(s,-\tau)\right]_{s=0} &= \left[-\tfrac{\mathrm{d}^{n-1}}{\mathrm{d}s^{n-1}}\, \varepsilon_{-\tau} \begin{pmatrix} \varepsilon_0 \\ s\mathcal{T}_{N-1} - \mathcal{D} \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{0}^* \\ \mathcal{T}_{N-1} \end{pmatrix} \begin{pmatrix} \varepsilon_0 \\ s\mathcal{T}_{N-1} - \mathcal{D} \end{pmatrix}^{-1} \begin{pmatrix} 1 \\ \mathbf{0} \end{pmatrix}\right]_{s=0} \\ &= \left[n!\,(-1)^n\, \varepsilon_{-\tau} \left[\begin{pmatrix} \varepsilon_0 \\ s\mathcal{T}_{N-1} - \mathcal{D} \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{0}^* \\ \mathcal{T}_{N-1} \end{pmatrix}\right]^n \begin{pmatrix} \varepsilon_0 \\ s\mathcal{T}_{N-1} - \mathcal{D} \end{pmatrix}^{-1} \begin{pmatrix} 1 \\ \mathbf{0} \end{pmatrix}\right]_{s=0} \\ &= n!\, \varepsilon_{-\tau} \left[\begin{pmatrix} \varepsilon_0 \\ \mathcal{D} \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{0}^* \\ \mathcal{T}_{N-1} \end{pmatrix}\right]^n \begin{pmatrix} \varepsilon_0 \\ -\mathcal{D} \end{pmatrix}^{-1} \begin{pmatrix} 1 \\ \mathbf{0} \end{pmatrix},\end{aligned}$$

with $\mathbf{0}^* f = 0$. Let $\mathcal{M}_N = \begin{pmatrix} \varepsilon_0 \\ \mathcal{D} \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{0}^* \\ \mathcal{T}_{N-1} \end{pmatrix}$ and note that

$$(\mathcal{M}_N f)(\theta) = \int_0^\theta \left[f(\xi) - \langle f, P_N\rangle P_N(\xi)\right] \mathrm{d}\xi\,.$$

Additionally, for $f_0 = \begin{pmatrix} \varepsilon_0 \\ -\mathcal{D} \end{pmatrix}^{-1} \begin{pmatrix} 1 \\ \mathbf{0} \end{pmatrix}$ we have $f_0(\theta) = 1$, hence

$$\left[\tfrac{\mathrm{d}^n}{\mathrm{d}s^n} r_N(s,-\tau)\right]_{s=0} = n!\, \varepsilon_{-\tau} \mathcal{M}_N^n f_0.$$

It thus remains to show that for $n \leq 2N$,

$$n!\, \varepsilon_{-\tau} \mathcal{M}_N^n f_0 = (-\tau)^n.$$

The operator $\mathcal{M}_N$ maps from $\mathbb{P}_N$ to $\mathbb{P}_N$. If we embed this space in the space $\mathbb{P}$ of polynomials of arbitrary degree, we can split $\mathcal{M}_N = \mathcal{I} + \mathcal{K}_N$, where $(\mathcal{I}f)(\theta) = \int_0^\theta f(\xi)\,\mathrm{d}\xi$ and $(\mathcal{K}_N f)(\theta) = -\int_0^\theta \langle f, P_N\rangle P_N(\xi)\,\mathrm{d}\xi$. We know that $\frac{2}{\tau}(2k+1)P_k(\theta) = \frac{\mathrm{d}}{\mathrm{d}\theta}(P_{k+1}(\theta) - P_{k-1}(\theta))$ for $k \geq 1$ (consequence of Szegő, 1939, eq. 4.7.29), hence, by the fundamental theorem of calculus and the fact that $P_{k+1}(0) = P_{k-1}(0) = 1$,

$$\mathcal{K}_N f = -\frac{\langle f, P_N\rangle}{\frac{2}{\tau}(2k+1)}(P_{N+1} - P_{N-1}).$$

As P_N is orthogonal to all polynomials of degree less than N, we have

$$\mathcal{K}_N g = \mathbf{0}, \quad \forall g \in \mathbb{P}_{N-1}. \tag{4.1}$$

Note that $(\mathcal{I} + \mathcal{K}_N)^n$ is the sum of all possible sequences of $\mathcal{I}$ and $\mathcal{K}_N$ of length n. As a consequence of (4.1), we know that any subsequence of operators at most N long and containing $\mathcal{K}_N$, gives the zero function when applied to f_0. Thus $(\mathcal{I} + \mathcal{K}_N)^n f_0$ consists of $(\mathcal{I}^n f_0)(\theta) = \frac{\theta^n}{n!}$ and terms of the form $\mathcal{I}^m \mathcal{K}_N f$, with $m < n - N$. Applying the same integration rule for P_k from before, we get the following forms for $\mathcal{I}^m \mathcal{K}_N f$.

m	expression
0	$\alpha(P_{N+1} - P_{N-1})$
1	$\beta(P_{N+2} - P_N) + \gamma(P_N - P_{N-2})$
$\vdots$	$\vdots$
$N-1$	$\chi(P_{2N} - P_{2N-2}) + \cdots + \omega(P_2 - P_0)$

As $P_k(-\tau) = (-1)^k$ (Szegő, 1939, eq. 4.1.4), we get

$$\varepsilon_{-\tau}\mathcal{I}^m\mathcal{K}_N f = 0, \quad \forall m < N.$$

Since $n \leq 2N$ we have $m < 2N - N = N$, thus the last result holds, hence

$$n!\,\varepsilon_{-\tau}\mathcal{M}_N^n f_0 = n!\,\varepsilon_{-\tau}\mathcal{I}^n f_0 = (-\tau)^n, \quad \forall n \leq 2N,$$

which is precisely what had to be shown. ∎

This result and Proposition 3.1 then readily give the following.

COROLLARY 4.3. *For the choice* $\Phi_N = \{P_k\}_{k=0}^N$*, the Lanczos tau discretization* (3.1) *is a state space representation of the transfer function of the original system* (1.2) *where the exponential* $s \mapsto e^{-\tau s}$ *is replaced by a Padé approximant of type* (N, N) *around zero.*

Of course, an analogous result holds for pseudospectral collocation, via Theorem 4.1.

Finally, we can use this link and Proposition 3.2 to give an explicit expression for the resulting Padé approximant.

COROLLARY 4.4. *The* (N, N) *Padé approximant of* $s \mapsto e^{-\tau s}$ *around zero has as rational expression*

$$\frac{\sum_{k=0}^N P_N^{(N-k)}(-\tau)\, s^k}{\sum_{k=0}^N P_N^{(N-k)}(0)\, s^k}.$$

Note that this expression of the Padé approximant is identical to expression (3.4) in Ahmad (1998). This correspondence can thus be used to give an alternative proof of Theorem 4.2, be it more indirect than the approach presented here.

Whilst the results preceding this subsection straightforwardly extend to more general settings such as multiple or distributed delays, those of this subsection are unique to the single delay case. Indeed, if we replace $A_0\varepsilon_0 + A_1\varepsilon_{-\tau}$ by some other bounded linear functional in (3.1), we see by the reasoning of Proposition 3.1 that $\theta \mapsto r_N(s, \theta)$ will be evaluated in multiple points, not just $-\tau$. From Proposition 3.2, however, we know that the poles of r_N are independent of θ, hence an analogue of Corollary 4.3 cannot hold, as the (N, N) Padé approximants of e.g. $s \mapsto e^{-s}$ and $s \mapsto e^{-2s}$ do not have common poles.

5. An application: computing the H^2-norm. We conclude this article by illustrating some unexpected improvements when using a Lanczos tau method for the computation of the H^2-norm, as defined by (1.3), of (1.1).[2] For this problem two methods have been proposed in the past. One approximates the so-called delay Lyapunov equation (Jarlebring et al., 2011); the other uses a state space discretization, namely pseudospectral collocation in Chebyshev extremal nodes (Vanbiervliet et al., 2011). Whilst the latter has a lower time complexity, $\mathcal{O}(n^3N^3)$ instead of $\mathcal{O}(n^6N^3)$, it only achieves third order algebraic convergence compared to the super-geometric rate of the former.

We will see here that the choice of discretization can have a profound impact on the convergence of the second method. In particular, a Lanczos tau method satisfying the following assumption appears to recover super-geometric convergence and sometimes even displays super convergence, i.e. it gives the exact result for all N larger than some finite N_0, as we will demonstrate in Proposition 5.5.

[2]The codes used to produce the figures in this section are available at https://doi.org/10.5281/zenodo.12088674.

ASSUMPTION 5.1. *The basis function ϕ_k is symmetric when k is even and antisymmetric when k is odd, i.e. $\phi_k(-\tau-\theta) = (-1)^k\phi_k(\theta)$, $\forall\theta \in [-\tau, 0]$.*

Note that when shifted from the interval $[-\tau, 0]$ to the interval $[-\frac{\tau}{2}, \frac{\tau}{2}]$, symmetric and antisymmetric functions correspond to the classical notion of even and odd functions, respectively.

For many of the bases used in this paper, this property is a direct consequence of the defining weight function being symmetric (Szegő, 1939, eq. 2.3.3). The usual pseudospectral collocation method using Chebyshev extremal points does not satisfy any analogous property, as the non-zero collocation points are not symmetric. The less common Chebyshev zeroes extended with the node 0, however, are, per Theorem 4.1, equivalent to a Lanczos tau method that does satisfy this symmetry condition.

The idea of Vanbiervliet et al. (2011), here translated to the Lanczos tau method, is simple: approximate the H^2-norm of the system (1.1) by the H^2-norm of the approximation (3.1). As is well known (Zhou et al., 1995, Lemma 4.6) we can compute the latter, if the resulting system is exponentially stable, as

$$\|G_N\|_{H^2} = \sqrt{\operatorname{tr}\big(\mathcal{C}_N V \mathcal{C}_N^T\big)},$$

where the matrix $V \in \mathbb{C}^{nN\times nN}$ is the solution of the generalized symmetric Lyapunov equation, in the notation of (3.2),

$$\mathcal{A}_N V \mathcal{E}_N^T + \mathcal{E}_N V \mathcal{A}_N^T = -\mathcal{B}_N \mathcal{B}_N^T. \tag{5.1}$$

We can reinterpret this matrix equation in terms of operations on polynomials, which will turn out to be useful in explaining some of the results in the remainder of this section. To this end, note that we can identify the solution V by a bivariate polynomial

$$U(\theta,\theta') = \textstyle\sum_{j=0}^{N}\sum_{k=0}^{N} V_{jk}\,\phi_j(\theta)\phi_k(\theta') \in \mathbb{C}^{n\times n},$$

with V_{jk} the relevant $n\times n$ subblock of V. Formally, as our choice of coordinates with respect to the basis Φ_N imposes a bijection between $\mathbb{C}^{nN}$ and $\mathbb{P}_N^n$, we similarly have an induced bijection between the tensor spaces $\mathbb{C}^{nN\times nN} \cong \mathbb{C}^{nN}\otimes\mathbb{C}^{nN}$ and $\mathbb{P}_N^n \otimes \mathbb{P}_N^n$ via the basis $\Phi_N \otimes \Phi_N$.

Inspired by this bijection, we extend our operator notation to bivariate polynomials, to have left multiplication mean application to the first variable and transposed right multiplication to be application to the second variable, i.e. we have $\varepsilon_\theta U \varepsilon_{\theta'}^T := U(\theta,\theta')$. This notation is justified by the tensor nature of U. Indeed, denoting by $[\,\cdot\,]$ the matrix realization as in section 3, we get

$$\varepsilon_\theta U \varepsilon_{\theta'}^T = [\varepsilon_\theta] V [\varepsilon_{\theta'}]^T \in \mathbb{C}^{n\times n}.$$

We then have the following result.

PROPOSITION 5.2. *The H^2-norm of the transfer function* (3.4) *of the Lanczos tau approximation* (3.1)*, if exponentially stable, is given by*

$$\|G_N\|_{H^2} = \sqrt{\operatorname{tr}\big(C\varepsilon_0 U \varepsilon_0^T C^T\big)},$$

where the bivariate polynomial $U : [-\tau, 0]\times[-\tau, 0] \to \mathbb{C}^{n\times n}$, of degree (N, N), is the

unique solution of the system

$$\begin{cases} \mathcal{D}U\varepsilon_0^T + \mathcal{T}_{N-1}U\big(\varepsilon_0^T A_0^T + \varepsilon_{-\tau}^T A_1^T\big) = \mathbf{0}, \\ \mathcal{D}U\mathcal{T}_{N-1}^T + \mathcal{T}_{N-1}U\mathcal{D}^T = \mathbf{0}, \\ \varepsilon_\theta U \varepsilon_{\theta'}^T = \big(\varepsilon_{\theta'} U \varepsilon_\theta^T\big)^T, \\ (A_0\varepsilon_0 + A_1\varepsilon_{-\tau})U\varepsilon_0^T + \varepsilon_0 U\big(\varepsilon_0^T A_0^T + \varepsilon_{-\tau}^T A_1^T\big) = -BB^T. \end{cases} \tag{5.2}$$

Proof. Note that we can write (5.1), without loss of generality, as

$$\begin{pmatrix} A_0[\varepsilon_0]+A_1[\varepsilon_{-\tau}] \\ [\mathcal{D}] \end{pmatrix} V \begin{pmatrix} [\varepsilon_0] \\ [\mathcal{T}_{N-1}] \end{pmatrix}^T + \begin{pmatrix} [\varepsilon_0] \\ [\mathcal{T}_{N-1}] \end{pmatrix} V \begin{pmatrix} A_0[\varepsilon_0]+A_1[\varepsilon_{-\tau}] \\ [\mathcal{D}] \end{pmatrix}^T = -\begin{pmatrix} B \\ \mathbf{0} \end{pmatrix}\begin{pmatrix} B \\ \mathbf{0} \end{pmatrix}^T.$$

Similarly, we have $\|G_N\|_{H^2}^2 = \operatorname{tr}\big(C[\varepsilon_0]V[\varepsilon_0]^T C^T\big)$. The assertions can now be recovered using the earlier identification between matrices and bivariate polynomials, by splitting these expressions into their subblocks and noting that $V = V^T$ implies $\varepsilon_\theta U \varepsilon_{\theta'}^T = \big(\varepsilon_{\theta'} U \varepsilon_\theta^T\big)^T$. Finally, uniqueness and existence are direct consequences of the corresponding properties of (5.1). ∎

We can use this result to connect the approach adopted here with the method of Jarlebring et al. (2011). The latter is based on the following characterization of the H^2-norm, again assuming the system (1.1) is exponentially stable:

$$\|G\|_{H^2} = \sqrt{\operatorname{tr}(C\lambda(0)C^T)},$$

where $\lambda \in C^1([-\tau,\tau];\mathbb{C}^{n\times n})$ is the solution of the so-called delay Lyapunov equation

$$\begin{cases} \lambda'(t) + \lambda(t)A_0^T + \lambda(t+\tau)A_1^T = \mathbf{0}, \quad t \in [-\tau, 0), \\ \lambda(-t) = \lambda(t)^T, \\ A_0\lambda(0) + A_1\lambda(-\tau) + \lambda(0)A_0^T + \lambda(\tau)A_1^T = -BB^T. \end{cases} \tag{5.3}$$

At least intuitively, we now have a link between both methods via $U(\theta,\theta') \approx \lambda(\theta - \theta')$. Indeed, assuming $\mathcal{T}_{N-1}$ to go to the identity operator as $N \to \infty$, the top and bottom equations of (5.2) and (5.3) match. We recover $\lambda(-t) = \lambda(t)^T$ from $\varepsilon_\theta U \varepsilon_{\theta'}^T = \big(\varepsilon_{\theta'} U \varepsilon_\theta^T\big)^T$ by setting $\theta = t$ and $\theta' = 0$ for $t \le 0$ and $\theta = 0$ and $\theta' = -t$ for $t > 0$. Finally, the remaining equation guarantees that, in the limit, $U(\theta,\theta')$ is a function of $\theta - \theta'$. We can thus interpret the bivariate polynomial associated with the solution of (5.1) as an approximation of $(\theta,\theta') \mapsto \lambda(\theta-\theta')$ with respect to $\Phi_N \otimes \Phi_N$.

Finally, as an additional property, these equations show an interesting symmetry in the scalar case.

LEMMA 5.3. *For a Lanczos tau discretization satisfying Assumption* 5.1 *of a scalar system* (1.1)*, i.e. a system with* $n = 1$*, it holds that the solution of* (5.2)

$$U = \mathcal{R}U\mathcal{R}^T,$$

with $\mathcal{R}$ *the reversal operator, such that* $\varepsilon_\theta \mathcal{R} = \varepsilon_{-\theta-\tau}$*.*

Proof. Decomposing U in the derivative basis of ϕ_N, that is, writing

$$U = \textstyle\sum_{j=0}^N \sum_{k=0}^N W_{jk}\, \Psi_{jk},$$

with $\Psi_{jk}(\theta,\theta') = \phi_N^{(N-j)}(\theta)\, \phi_N^{(N-k)}(\theta')$, we note that $\mathcal{D}U\mathcal{T}_{N-1}^T = -\mathcal{T}_{N-1}U\mathcal{D}^T$ implies

$$\textstyle\sum_{j=1}^N \sum_{k=0}^{N-1} W_{jk}\, \Psi_{j-1,k} = -\sum_{j=0}^{N-1} \sum_{k=1}^N W_{jk}\, \Psi_{j,k-1},$$

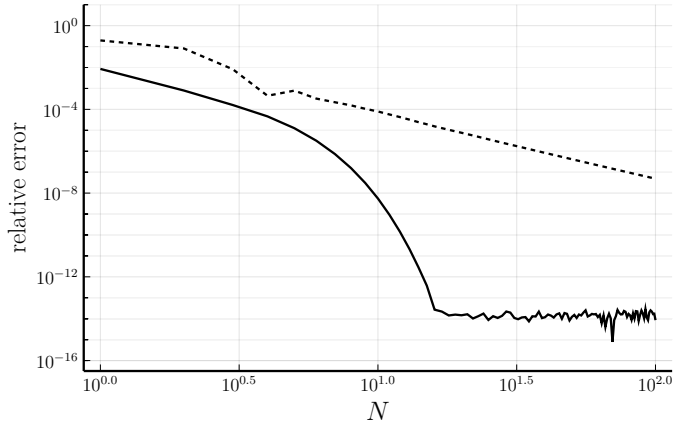

FIGURE 1. *Convergence of the H^2-norm of* (1.1) *with* $A_0 = \left(\begin{smallmatrix} -2 & 1 \\ 3 & -8 \end{smallmatrix}\right)$, $A_1 = \left(\begin{smallmatrix} -1 & -1 \\ -1 & -1 \end{smallmatrix}\right)$, $\tau = 1$, *and* $B = C = I_2$, *for different discretizations. The solid line corresponds to the Lanczos tau method with Chebyshev polynomials of the second kind, the dashed line to pseudospectral collocation in Chebyshev extremal nodes.*

and thus $W_{j+1,k} = -W_{j,k+1}$. Hence, the coefficients on an anti-diagonal of W have constant magnitude and alternating sign. As we additionally have $W_{jk} = W_{kj}$ from $\varepsilon_\theta U \varepsilon_{\theta'}^T = \left(\varepsilon_{\theta'} U \varepsilon_\theta^T\right)^T$, the anti-diagonals of even length must be zero, thus $W_{jk} = 0$ if $j+k$ is odd. Furthermore, Assumption 5.1 implies that $\phi_N^{(N-k)}$ is symmetric when k is even and antisymmetric when k is odd. Hence, for $i+j$ even, the bivariate polynomial Ψ_{jk} is the product of either two symmetric or two antisymmetric polynomials and thus $\Psi_{jk} = \mathcal{R}\Psi_{jk}\mathcal{R}^T$. The assertion then follows from the linearity of $\mathcal{R}$ and the structure of W. ∎

Note that from the point of view of the algebraic Lyapunov equation (5.1), the same structure on W follows from the companion matrix structure of the equation, when expressed in the above basis, as shown by Barnett and Storey (1967).

5.1. General A_0 and A_1. If we approximate the H^2-norm using different state space discretizations, namely pseudospectral collocation in Chebyshev extremal nodes and a Lanczos tau method satisfying Assumption 5.1, we consistently see results similar to Figure 1. We get super-geometric convergence for the Lanczos tau method instead of the third order convergence of the other discretization as described in Vanbiervliet et al. (2011).

Note that the H^2-norm depends on the behaviour of the transfer function along the entire imaginary line; however, the rational approximation of Proposition 3.1 is only accurate around zero. From this perspective, algebraic convergence is the most that one would expect from such a method (Vanbiervliet et al., 2011). The observed improvement in convergence is thus highly surprising, especially as we did not change the computational cost. Part of the explanation might stem from the link to the delay Lyapunov equation. As its solution is an analytic function defined on a finite domain, we could get super-geometric convergence for a Chebyshev basis if we in fact implicitly solve this equation using a spectral method (Tadmor, 1986). However, similar convergence would then be expected of other reasonably behaved bases, such as the Jacobi polynomials $P_k^{\left(-\frac{1}{2},-\frac{3}{4}\right)}$ which nonetheless degrade back to

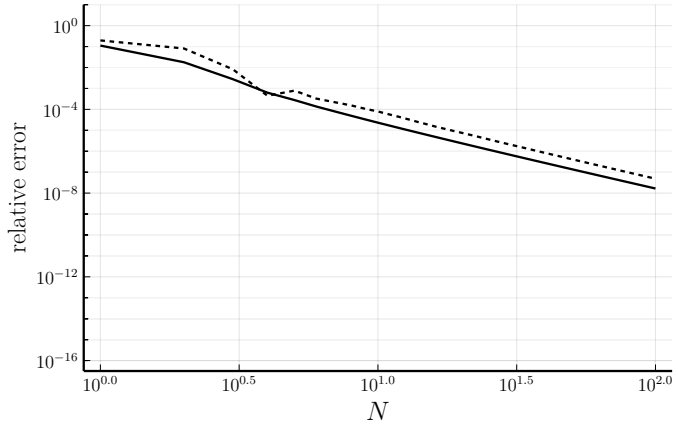

FIGURE 2. *Convergence of the H^2-norm of the system of Figure* 1*, for different discretizations. The solid line corresponds to the Lanczos tau method with Jacobi $\left(-\frac{1}{2},-\frac{3}{4}\right)$ polynomials, which do not satisfy Assumption* 5.1*, the dashed line to pseudospectral collocation in Chebyshev extremal nodes.*

third order convergence (see Figure 2). As we only note this deterioration when Assumption 5.1 is not satisfied, we presume that such a symmetry condition also plays a major part in explaining the observed super-geometric convergence. A hint is given by the following result, which shows that the rational approximation qualitatively matches the exponential better on the imaginary axis, in the sense that its magnitude equals one, precisely when this property is satisfied.

PROPOSITION 5.4. *If Φ_N is chosen such that Assumption* 5.1 *is satisfied, we have*

$$|r_N(i\omega,-\tau)| = 1, \quad \forall \omega \in \mathbb{R},$$

where r_N is as in Proposition 3.1*.*

Proof. From Proposition 3.2 we have

$$r_N(i\omega,-\tau) = \frac{\sum_{k=0}^{N} i^k \phi_N^{(N-k)}(-\tau)\,\omega^k}{\sum_{k=0}^{N} i^k \phi_N^{(N-k)}(0)\,\omega^k}.$$

Assumption 5.1 implies $\phi_N^{(N-k)}(-\tau) = (-1)^k \phi_N^{(N-k)}(0)$, hence the denominator is the complex adjoint of the numerator. ∎

5.2. A case with super convergence. We consider the system (1.1) in the scalar case, with $A_0 = A_1 = a < 0$. The zero solution of this system is then known to be exponentially stable for any $\tau \geq 0$, as proved by Hayes (1950, Theorem 1). Impressively, we see that the discretizations based on the Lanczos tau method, again under Assumption 5.1, already give the exact result at $N = 1$ (see Figure 3; the slight increase in error as N increases is due to rounding errors in the underlying matrix operations). This is once again rather surprising from the perspective of an integral over an unbounded domain, as the transfer functions barely match, even near zero (see Figure 4). We conclude by proving this effect.

For the class of systems showing this super convergence, we get as transfer function

$$G(s) = \left(s - a\left(1 + e^{-\tau s}\right)\right)^{-1}. \tag{5.4}$$

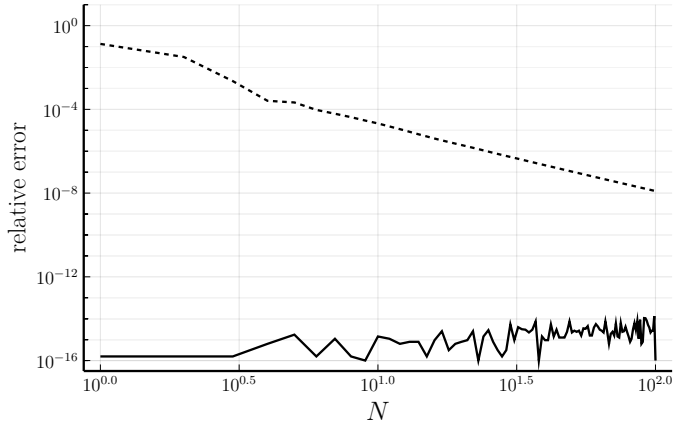

FIGURE 3. *Convergence of the H^2-norm of (1.1) with $A_0 = A_1 = -1$, $\tau = 1$, and $B = C = 1$, for different discretizations. The solid line corresponds to the Lanczos tau method with Chebyshev polynomials of the second kind, the dashed line to pseudospectral collocation in Chebyshev extremal nodes. For clarity of the figure, the relative error was lower bounded by 10^{-16}.*

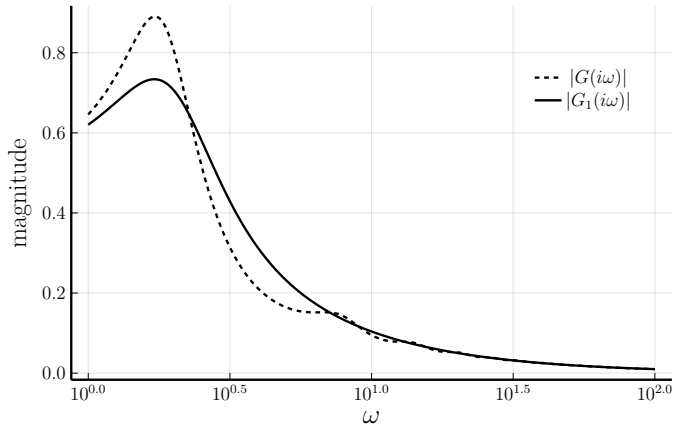

FIGURE 4. *Transfer function G of the system of Figure 3, and the approximation G_1 from a Lanczos tau method using Chebyshev polynomials of the second kind with $N = 1$.*

We can compute its H^2-norm analytically by solving the delay Lyapunov equation. As before, we have $\|G\|_{H^2} = \sqrt{\lambda(0)}$, where

$$\begin{cases} \lambda'(t) + a(\lambda(t) + \lambda(t+\tau)) = 0, \quad t \in [-\tau, 0), \\ \lambda(-t) = \lambda(t), \\ 2a(\lambda(0) + \lambda(\tau)) = -1. \end{cases}$$

It is easy to verify that $\lambda(t) = \frac{a\tau - 2a|t| - 1}{4a}$ is the solution, yielding

$$\|G\|_{H^2} = \sqrt{\frac{a\tau - 1}{4a}}.$$

We can now show the following.

PROPOSITION 5.5. *For the system with transfer function* (5.4)*, we have*

$$\|G_N\|_{H^2} = \|G\|_{H^2}$$

for $N \geq 1$, when discretized using a Lanczos tau method satisfying Assumption 5.1*.*

Proof. From Proposition 5.2 we have $\|G_N\|_{H^2} = \sqrt{\varepsilon_0 U \varepsilon_0^T}$ with U the solution of

$$\begin{cases} \mathcal{D}U\varepsilon_0^T + a\mathcal{T}_{N-1}U\left(\varepsilon_0^T + \varepsilon_{-\tau}^T\right) = \mathbf{0}, \\ \mathcal{D}U\mathcal{T}_{N-1}^T + \mathcal{T}_{N-1}U\mathcal{D}^T = \mathbf{0}, \\ \varepsilon_\theta U \varepsilon_{\theta'}^T = \left(\varepsilon_{\theta'} U \varepsilon_\theta^T\right)^T, \\ a(\varepsilon_0 + \varepsilon_{-\tau})U\varepsilon_0^T + a\varepsilon_0 U\left(\varepsilon_0^T + \varepsilon_{-\tau}^T\right) = -1. \end{cases}$$

Let μ be the univariate polynomial $U\varepsilon_0^T$. From Lemma 5.3, we then have $U\varepsilon_{-\tau}^T = \mathcal{R}U\varepsilon_0^T = \mathcal{R}\mu$. For the top equation this gives

$$\mathcal{D}\mu = -a\mathcal{T}_{N-1}(\mu + \mathcal{R}\mu). \tag{5.5}$$

The bottom equation can be rewritten as $(\varepsilon_0 + \varepsilon_0\mathcal{R})\mu + \varepsilon_0(\mu + \mathcal{R}\mu) = -\frac{1}{a}$ or

$$\varepsilon_0(\mu + \mathcal{R}\mu) = -\frac{1}{2a}. \tag{5.6}$$

By expressing these equations in a basis, it is easily seen that (5.5) and (5.6) form a system of full rank, hence this system uniquely determines a polynomial. It is straightforwardly verified that $\mu(\theta) = \lambda(-\theta) = \frac{a\tau + 2a\theta - 1}{4a}$ solves this system for a degree-graded, orthogonal basis, if $N \geq 1$, as $\mu + \mathcal{R}\mu$ is a constant function. We thus get the exact result under the given conditions. ∎

6. Conclusions. We developed a framework of operator pencil formulations of the Lanczos tau method (3.1) for the discretization of linear systems with state delay. The interpretation in terms of actions on polynomials aids theoretical derivations. We showed equivalence to rational approximation in the frequency domain and provided an explicit expression of the resulting rational function in Propositions 3.1 and 3.2, respectively.

Links were also made to pseudospectral collocation in Theorem 4.1. We illustrated how Lanczos tau methods naturally lead to nested and sparse matrix realizations, which can be exploited in Krylov methods, allowing improved performance (subsection 4.2). Particularly surprising was equivalence to Padé approximation for the choice of a shifted Legendre basis (Theorem 4.2); our proof of which strongly relied on the interpretation in terms of operations on polynomials.

Finally, we illustrated the potential benefits of the Lanczos tau framework in section 5, where, under a mild symmetry condition (Assumption 5.1), significantly increased convergence rates, compared to earlier work, were observed and partially proved for the H^2-norm. From links to the delay Lyapunov equation (Proposition 5.2), through bivariate polynomials, and from qualitative properties of the rational approximation (Proposition 5.4), we could provide intuitions for observed super-geometric convergence. Proving this effect, however, remains an open problem. A proof of a case of super convergence concluded our work (Proposition 5.5). Note that this super-geometric convergence and, in particular, super convergence are at first glance somewhat unexpected, as the H^2-norm is inherently a global characteristic; it depends on the behaviour of the transfer function along the entire imaginary axis.

Although we did not pursue multiple nor distributed delays in this paper, the development of section 3, in particular Propositions 3.1 and 3.2, the equivalence Theorem 4.1, and the benefits discussed in subsection 4.2, can easily be extended to these cases. In fact, any bounded linear functional can be substituted for $A_0\varepsilon_0 + A_1\varepsilon_{-\tau}$ in (3.1). As already noted at the end of subsection 4.3, a link to Padé approximation cannot be obtained from such an extension. Section 5 also depends on having only a single delay; how to extend the noted benefits to more general settings is thus an interesting open question.

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