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Abstract

We present a new approach to the numerical solution of Sturm–Liouville eigenvalue problems based on Magnus expansions. Our algorithms are closely related to Pruess' methods [Pre73], but provide for high order approximations at nearly the same cost as the second-order Pruess method. By using Newton iteration to solve for the eigenvalues, we are able to present an efficient algorithm for computing a range of eigenvalues and eigenfunctions. Numerical experiments display promising results, and asymptotic corrections are made to improve further the accuracy of the schemes.

Introduction

In this paper we are concerned with the numerical approximation of parameter estimation problems of the form

$$y' = A(x, \lambda)y, \tag{1}$$

where $A \in \mathbb{R}^{n\times n}$, $y \in \mathbb{R}^n$. The parameter $\lambda \in \mathbb{K}$ (where $\mathbb{K} = \mathbb{R}$ or $\mathbb{C}$) is unknown, and is to be found subject to some kind of boundary conditions. Of particular interest are conditions of the form

$$B_a y(a, \lambda) + B_b y(b, \lambda) = 0,$$

where $B_a, B_b \in \mathbb{R}^{n\times n}$ are possibly dependent on the parameter λ. Among the problems fitting this category are Sturm–Liouville and Schrödinger eigenvalue problems. Other interesting problems are AKNS eigenvalue problems obtained when generalising the inverse scattering transform for non-linear partial differential equations. A fourth example is provided by multi-point boundary-value problems. These are obtained e.g. when modeling wave propagation in range-independent multi-region fluid-solid media. Mathematically these problems are formulated as follows: Given a set of matrices $G_j \in \mathbb{R}^{m_j\times n}$ together with corresponding points $x_j \in \mathbb{R}$, $j = 1, \ldots, k$, the problem is to determine a parameter value λ such that

$$G_j y(x_j) = 0, \quad j = 1, 2, \ldots, k$$

where $\sum_{j=1}^{k} m_j = n$.

Usually an iterative routine is used to refine the approximations, and depending on the method applied and the number of parameter values we seek, the computational cost when solving such problems can be significant. By taking advantage of special methods we can construct numerical algorithms having special advantages over standard "off the shelf" methods. These methods provide an approximation more consistent with the true solution, in terms of the configuration space in which the solution evolves. An added benefit of these methods is the efficiency we can achieve by taking account of the special structure of the problems. For numerical computations large parameter values often pose problems and may lead to loss of accuracy, or even to non-convergence, an issue that we address in the sequel.

The linear matrix case

Let $A(t) \in \mathbb{R}^{n\times n}$ be a time-dependent matrix. We define the fundamental matrix of (1), as the matrix Φ satisfying the linear differential equation

$$\frac{d\Phi_a(x)}{dx} = A(x)\Phi_a(x), \quad \Phi_a(a) = \mathbb{1}. \tag{2}$$

By assuming boundedness of A in the interval of interest, the existence of a unique matrix Φ is guaranteed in a neighbourhood of $t = a$. However, the formula valid for the scalar case, $\Phi_a(x) = \exp(\int_a^x A(s)\,ds)$, is not valid in general unless A commutes, $A(t)A(s) = A(s)A(t)$, $\forall t, s$. Formal expansions for Φ of various forms have been given by several authors, e.g. by F.J. Dyson, R.V. Gamkrelidze, K.-T. Chen and M. Fliess some of which are equally applicable to nonlinear problems. We will here restrict our attention to the series expansion introduced by W. Magnus [Mag54], while Feynman some years earlier related the terms in the the "Magnus" expansion to quantum interactions.

Interested in representing the solutions of linear time-dependent equations of quantum physics, Magnus devised a new approach for representing the solution by assuming that it could be written in the form $\Phi_a(x) = \exp(\sigma(x))$, and showed that σ satisfies the equation

$$\sigma' = d\exp^{-1}(\sigma)A(t) = \sum_{n\geq 0} b_n \mathrm{ad}(\sigma)^{\mathrm{n}}\mathrm{A(t)}, \quad \sigma(0) = 0 \tag{3}$$

where $n!b_n$ are Bernoulli numbers. These expansions are central in the theory of Lie groups, and can be considered as a continuous analogue of the well known Baker–Cambell–Hausdorff formula.

The powers of the endomorphism $\mathrm{ad(p)q} = [\mathrm{p},\mathrm{q}]$ are defined as $\mathrm{ad(p)^0q} = \mathrm{q}$ and $\mathrm{ad(p)^kq} = \mathrm{ad(p)ad(p)^{k-1}q}$, where in our case the *Lie bracket* is the matrix commutator $[p,q] = pq - qp$. The first terms of the *Magnus expansion* can be obtained by Picard iteration on (3),

$$\begin{aligned} \sigma_a(t) \quad = \quad & \int_a^t A(\kappa)d\kappa - \frac{1}{2}\int_a^t \left[\int_a^\kappa A(\xi)d\xi, A(\kappa)\right] d\kappa + \\ & \frac{1}{4}\int_a^t \left[\int_a^\kappa \left[\int_a^\xi A(\nu)d\nu, A(\xi)\right] d\xi, A(\kappa)\right] d\kappa + \end{aligned} \tag{4}$$

$$\frac{1}{12}\int_a^t \left[\int_a^\kappa A(\nu)d\nu, \left[\int_a^\kappa A(\xi)d\xi, A(\kappa)\right]\right] d\kappa + \ldots,$$

We note in passing that a linear space of matrices $\mathfrak{g} \subset \mathbb{R}^{n\times n}$ closed under the matrix commutator is called a *matrix Lie algebra.* Important examples are $\mathfrak{sl}(2,\mathbb{R})$,$\mathfrak{sl}(2,\mathbb{C})$ and $\mathfrak{sl}(4,\mathbb{R})$ the sets of 2×2 real and complex and 4×4 real matrices with zero trace respectively and they are all relevant to our parameter estimation examples. Other important examples of matrix Lie algebras include $\mathfrak{su}(n,\mathbb{R})$, the set of skew symmetric matrices, and $\mathfrak{sp}(n)$, the set of symplectic vector fields. We will denote a generic Lie algebra by the symbol $\mathfrak{g}$.

By construction the Magnus expansion provides a matrix function σ in the same Lie algebra as A, a fact that holds even if we truncate the expansion(4). Therefore exponentiating σ provides an element in the corresponding Lie group G. This fact is used in the construction of numerical integrator s on homogenous spaces, where the basic transforms of solution points are given by Lie group actions[MKZ97, MK97]. Most of these methods can be constructed by applying a classical method to (3). It then follows from the linearity of the Lie algebra $\mathfrak{g}$ and the numerical methods that the approximate σ remain in $\mathfrak{g}$.

Several numerical experiments with discretisation on Lie groups show promising results with regard to accuracy and stability. Reasons for the somewhat good behaviour might lie in the fact that the configuration spaces of the discretisation and the exact systems are the same. Another feature of discrete Magnus expansions is that if they are based on symmetric collocation points then they will share the *reversibility* property $\tilde{\Phi}_a^c\tilde{\Phi}_c^a = \mathbb{1}$ of the true solution [AIFR98], a property that can be viewed as a weak version of the group property $\Phi_a^c\Phi_c^b = \Phi_a^b$, which has proven impossible to retain in general approximations.

In [IN97] the authors associate the terms of the Magnus series with rooted trees, thus systemising the analysis, see also [FC90] for a recursion formula for the terms in the Magnus expansion together with some analysis of convergence properties. It is also worth mentioning that in the physics and chemistry literature the expansion has been quite extensively used as a perturbation expansion for linear systems see e.g. [OR91, Sal87] for refferences.

Convergence of Lie group methods

In practical computations using numerical methods, the question of stability is central. Magnus expansions, or for that matter numerical methods based on Lie group actions can be viewed as methods obtained by assuming that the solution can be written in the form $y = \Lambda(\exp(\sigma), y(a))$, where Λ denotes a Lie group action. This assumption introduces singularities, since exp is not injective, and (3) is valid only in some neighborhood of $x = a$. Knowing the radius of convergence tells us how the step-size h of the numerical method should be restricted in order have a well-defined approximation.

The question of convergence has been addressed by many authors, e.g. [FC90, SBR98, Sal87], with the common result that the series has a finite radius of convergence. The results vary from statements concerning specific problems [Sal87] to more a general framework [FC90, SBR98]. W. Magnus himself obtained a less useful result stating that the expansion does not exist if the difference between two eigenvalues of

σ is a multiple of $2\pi i$. We present a simple proof, achieving the same results as those of [SBR98], and deriving an explicit expression for the constant therein.

Lemma 1 *(*A Bihari-type inequality.*) Let $h, v \in C(0,T)$ be positive and assume that $g \in C(0,T)$ is a non-decreasing positive function. Suppose that*

$$h(t) \le \int_0^t v(s) g(h(s)) ds, \quad 0 \le t.$$

Then

$$h(t) \le G^{-1}\left(\int_0^t v(s)ds\right), \quad t \le T$$

holds, where $G(s) = \int_0^s d\tau/g(\tau)$.

Proof Let $f = \int_0^t v(s)g(h(s))ds$, then $f' = v(t)g(h(t)) - v(0)g(h(0)) \le v(t)g(h(t))$. Since g is a nondecreasing function we have $f' \le v(t)g(f(t))$, or $f'/g(f) \le v(t)$, because g is positive. By integrating the inequality we arrive at $\int_0^{f(t)} \{g(s)\}^{-1} ds \le \int_0^t v(s)ds$, or $G(f(t)) \le \int_0^t v(s)ds$. From this we deduce that $h \le f \le G^{-1}(\int_0^t v(s)ds)$ for $t < T$, where $T = \sup\{t \ge 0 : \int_0^t v(s)ds \in \text{domain}\, \mathrm{G}^{-1}\}$. $\square$

Let us assume that we endow our Lie algebra $\mathfrak{g}$ with the structure of a Banach space with a norm $\|\cdot\|$. By the continuity of the commutator there exists a constant $0 \le \mu \le 2$ such that $\|[p,q]\| \le \mu \|p\| \|q\|$.

Theorem 2 *(*Convergence for Lie-type methods*) Let $A : \mathbb{R} \times G \to \mathfrak{g}$, where $G \subseteq \mathbb{R}^{n\times n}$ is a matrix Lie group and $\mathfrak{g} \subseteq \mathbb{R}^{n \times n}$ is the underlying Lie algebra. Assume that there exists a nonnegative function $m(x)$ such that $\|A(x, Y(x))\| \le m(x)$. Then the solution Y of*

$$Y' = A(x,Y)Y, \quad x \ge 0, \quad Y(0) = Y_0 \in G,$$

has a convergent representation $Y(x) = \exp(\sigma)Y_0$, $0 \le x < T$, and $T = \sup\{x \ge 0 : \int_0^x m(s)ds < \xi/\mu\}$, where $\xi = \int_0^{2\pi} \{2 + \frac{x}{2}[1 - \cot(x/2)]\}^{-1} dx = 2.1737...$.

Proof From (3) we have

$$\begin{aligned}
\|\sigma\| &= \left\| \int_0^\tau d\exp^{-1}(\sigma(s))A(s,Y)ds \right\| \\
&\le \int_0^\tau \|d\exp^{-1}(\sigma(s))A(s,Y)\|ds \quad \text{triangle inequality} \\
&\le \int_0^\tau \sum_{n\ge 0} |b_n| (\mu\|\sigma\|)^n \|A\| ds \quad \text{triangle inequality and } \|[p,q]\| \le \mu\|p\|\,\|q\| \\
&= \int_0^\tau g(\mu\|\sigma(s)\|) m(s) ds
\end{aligned}$$

where $g(x) = \sum_{n\ge 0} |b_n| x^n = 2 + x(1 - \cot(x/2))/2$. Now, since g is a nondecreasing positive function on the interval $[0, 2\pi)$, we can apply Lemma 1. With $G(s) = \int_0^s d\tau/g(\mu\tau)$ we find that G is nondecreasing and bounded in the interval

$[0, 2\pi/\mu)$, and hence the boundedness of $\|\sigma\|$ follows, with a corresponding T. In fact, $\mu\|\sigma\| = \delta < 2\pi$ when $\int_0^t \|A\| ds < \frac{1}{\mu}\int_0^{2\pi} ds/g(s) \approx 2.1737...$ By a standard inequality [Abr64] on Bernoulli numbers we have

$$\begin{aligned}\left\|b_{2n}\int_0^t \mathrm{ad}(\sigma(s))^{2n}A(s)ds\right\| &\leq \frac{4}{(2\pi)^{2n}}\left\|\int_0^t \mathrm{ad}(\sigma(s))^{2n}A(s)ds\right\| \\ &\leq \frac{4}{(2\pi)^{2n}}\int_0^t (\mu\|\sigma\|)^{2n}\|A\|ds \\ &\leq 4\left(\frac{\delta}{2\pi}\right)^{2n} \times \frac{1}{\mu}2.1737... \to 0 \quad as \quad n \to \infty,\end{aligned}$$

and we thus have a unique solution σ. □

A more careful study of the inequality $\|[\sigma(t), A(t)]\| \leq \mu(t)\|\sigma(t)\|\|A(t)\|$ shows that $\mu(0) = 0$ since σ is dependent on A. Further numerical studies of this inequality indicate that $\|\mathrm{ad}(\sigma)^n A\| \leq \mu^n\|\sigma\|^n\|A\|$, where μ is some function which can be made independent of A. By finding tight bounds on μ the bound on the radius can be improved. Particular cases when this is possible is when $A(t)$ is in a nil potent Lie algebra , and the Magnus expansion (4) is finite. Another, maybe more surprising, fact is that if A is skew symmetric we can take $\mu = \sqrt{2}$. Recalling Magnus' result on convergence we now have $\mu\int_0^t \|A(s)\|\, ds \leq 2.1737... \Rightarrow \rho(\sigma) \leq \pi$, where $\rho(\rho)$ denotes the spectral radius of ρ. On the other hand it would be interesting in knowing how sharp this result is, i.e. when we have the equivalence

$$\mu\int_0^t \|A(s)\|\, ds \leq 2.1737... \quad \Leftrightarrow \quad \rho(\sigma) \leq \pi.$$

In the case when the eigenvalues of A are large, numerical approximations are often hampered by small step-size, h. Theorem 2 indicates that truncations of Magnus series might have poor convergence properties when the eigenvalues of A are large, hence leading to a restriction on step-size. This is typical to explicit numerical methods, but in our case the problem persists even if we use implicit methods to solve the equation $\sigma' = d\exp^{-1}(\sigma)A(t,y)$. Some improvements can be made, in particular we can improve the accuracy of the truncations near the singularities. We will return to this theme later in this paper.

Numerical methods based on Magnus expansions

Having first been presented in the context of numerical solution of differential equations on manifolds in [IN97], the methods were readily extended to higher order numerical methods. By further analysis and automating the construction, we can now construct discrete Magnus expansions up to arbitrary order.

To construct our finite approximations based on the Magnus expansion, we allow point evaluations of A, giving us the possibility to construct an interpolating approximation for the interval $(x_n, x_n + h)$,

$$\tilde{A}_n(x) = \sum_{k=1}^{m} \mathcal{L}_k(x)A(x_n + c_k h), \tag{5}$$

where $\mathcal{L}_k$ is a cardinal polynomial of Lagrange interpolation based on the points c_k,

$$\mathcal{L}_i(x) = \prod_{k=1,k\neq i}^{m} \frac{x-c_k}{c_i-c_k} = \begin{cases} 1, & x=c_i, \quad j=i, \\ 0, & x=c_j, \quad j\neq i. \end{cases}$$

Lemma 3 *Let Φ be the fundamental matrix of (2) and $\tilde{\Phi}$ the fundamental matrix of $\tilde{Y}' = \tilde{A}\tilde{Y}$. Then $\|\Phi - \tilde{\Phi}\| = \mathcal{O}(h^p)$, where p is the largest integer such that*

$$\int_0^1 x^q M(x)\,dx = 0, \quad q = 0,\ldots,p-m,$$

and $M(x) = \prod_{k=1}^m (x-c_k)$.

The proof follows directly from Alekseev-Gröbner's lemma, and is given in e.g. [Zan97].

Choosing c_k as the zeros of Legendre polynomials shifted to the interval of interest it is well known that $\int_0^1 x^q M(x)\,dx = 0$ for $q=0,\ldots,m$, hence allowing us to construct $2m$th order methods based on m interpolation points. Such methods are useful if we are able to evaluate A at the Gauss–Legendre points. For other interpolation points the order will be lower, in particular for a uniform distribution of points the order will be just $p = m+1$.

The fully discrete approximation is obtained by truncating the Magnus expansion (4) after replacing A by $\tilde{A}$ and evaluating the integrals exactly. In the case A has an analytic expansion it is clear that the commutator $[A(x_n+hc_i), A(x_n+hc_j)]$ will be $\mathcal{O}(h)$, a fact we should take into account when truncating the expansions. The simplest way to do so is by rewriting the interpolating polynomial in a Taylor basis, $\tilde{A}_n(x) = \sum_{k=1}^m x^{k-1} h\tilde{f}_k$, related to the point-samples $A(x_n+c_kh) = A_k$ through a Vandermonde system

$$\begin{bmatrix} A_1 \\ A_2 \\ \vdots \\ A_m \end{bmatrix} = \begin{bmatrix} 1 & c_1 & c_1^2 & \cdots & c_1^{m-1} \\ 1 & c_2 & c_2^2 & \cdots & c_2^{m-1} \\ \vdots & & \vdots & & \vdots \\ 1 & c_m & c_m^2 & \cdots & c_m^{m-1} \end{bmatrix} \begin{bmatrix} \tilde{f}_1 \\ \tilde{f}_2 \\ \vdots \\ \tilde{f}_m \end{bmatrix}. \tag{6}$$

We have taken the liberty to normalise the terms $\tilde{f}_n$by a factor h^n to obtain cleaner expressions.

In the Taylor basis the order of the elements of a Lie algebra is simple to compute, the rule being that the order of an element is the sum of the subscripts, e.g. $\mathcal{O}[[f_4,f_2],f_1] = \mathcal{O}(h^{4+2+1})$. In our expansions further dependencies occur because of identities on commutators, e.g.

$$\begin{aligned} [A,B]+[B,A] &= 0 \\ [A,[B,C]]+[C,[A,B]]+[B,[C,A]] &= 0 \\ [A,[B,[C,D]]]+[D,[A,[B,C]]]+[C,[D,[A,B]]]+[B,[C,[D,A]]] &= [[A,C],[B,D]]. \end{aligned}$$

To account for such relations, we convert the terms to the *Hall basis* defined by the two rules[1]

$$\begin{aligned} [A,B] &\rightarrow -[B,A] \quad \text{if} \quad B < A \\ [A,[B,C]] &\rightarrow [B,[A,C]] - [C,[A,B]] \quad \text{if} \quad B < A. \end{aligned} \tag{7}$$

For Lie algebras were we know the structure constants the Hall basis is redundant since we can expand the *finite* basis of the algebra.

This is important in implementing a procedure for computing the discrete Magnus expansion. This procedure has been implemented in the symbolic computation package `Maple V`, giving us the ability to compute these discrete expansions to a high order in h. The solutions are automatically represented in a Hall basis by `Maple V`, but to further simplify the evaluation of $\tilde{\sigma}$, the Lie polynomials can be rendered in Horner's form.

Proposition 4 *Assume that* $A(t) = \sum_{n=0}^{m} t^n \tilde{f}_n$ *, then* $\sigma(t) = \sum_{k\geq 1} t^k \mathcal{X}_k$ *is given by the recursion*

$$(j+1)\mathcal{X}_{j+1} = \sum_{\sum_{k=0}^{m} n_k = j} b_m[\mathcal{X}_{n_m}, [\mathcal{X}_{n_{m-1}}, \cdots, [\mathcal{X}_{n_1}, \tilde{f}_{n_0}] \cdots]],$$

where $\mathcal{X}_1 = \tilde{f}_0$.

The proof follows by inserting $\sigma = \sum_{n\geq 1} t^n \mathcal{X}_n$ and $A = \sum_{n=0}^{m} t^n \tilde{f}_n$ into (3) and collecting equal powers of t.

To complete this section we present the coefficients for methods up to order 10. From these it is simple to extract the methods of lower order, from which we present a method of order 8 as an example. The coefficients are computed using the recursion in Proposition 4. For verification the same coefficients were computed using the `MATLAB 5` package `DiffMan` [Dif], which employs a different algorithm. In [MKO98] some of these coefficients are presented together with results concerning the number of terms in discrete Magnus expansions. To fully take advantage of symmetric collocation points the Taylor expansion is computed about the midpoint $x_n + h/2$ of the interval, leading to a further reduction in the number of terms in the expansions.

Function evaluations, f_i, are denoted by $[i]$, and commutators $[f_i, f_j]$ by $[i,j]$ etc. The terms are collected in sets of the same order in h to make it clear how to use the terms to construct numerical methods of a given order. In the following table the 'Order' is the order of the term, hence to construct a method of order k it is sufficient to include terms of order less than k.

[1] We assume that the elements of the Lie algebra are ordered through an equivalence relation "$<$", satisfying $(A < B) \& (B < C) \Rightarrow A < C$.

Order	Term	Weight	Order	Term	Weight
1	[1]	1		[2,[2,[2,[1,2]]]]	$-\frac{1}{241920}$
3	[1,2]	$-\frac{1}{12}$		[[2,[1,2]],[1,[1,2]]]	$-\frac{1}{241920}$
	[3]	$+\frac{1}{24}$		[2,[2,[1,[1,[1,2]]]]]	$+\frac{1}{241920}$
5	[1,[1,[1,2]]]	$+\frac{1}{720}$		[2,[1,[1,[1,[1,[1,2]]]]]]	$-\frac{1}{403200}$
	[2,[1,2]]	$-\frac{1}{240}$		[[1,[1,2]],[1,[1,[1,2]]]]	$+\frac{1}{1209600}$
	[2,3]	$+\frac{1}{480}$		[[1,2],[1,[1,[1,[1,2]]]]]	$+\frac{1}{1209600}$
	[1,[1,3]]	$+\frac{1}{720}$		[1,[1,[1,[1,[1,4]]]]]	$-\frac{1}{1814400}$
	[1,4]	$-\frac{1}{480}$		[1,[1,[1,[1,[1,[1,[1,2]]]]]]]	$+\frac{1}{1209600}$
	[5]	$+\frac{1}{1920}$		[1,[1,[1,[1,[1,[1,3]]]]]]	$+\frac{1}{1209600}$
7	[1,[1,[1,[1,[1,2]]]]]	$-\frac{1}{30240}$		[4,[2,[1,2]]]	$-\frac{1}{120960}$
	[[1,2],[1,[1,2]]]	$-\frac{1}{30240}$		[2,[2,[2,3]]]	$+\frac{1}{483840}$
	[2,[2,[1,2]]]	$-\frac{1}{6720}$		[[2,3],[1,3]]	$+\frac{1}{193536}$
	[2,[1,[1,[1,2]]]]	$+\frac{1}{10080}$		[3,[2,[1,3]]]	$-\frac{1}{483840}$
	[1,[1,[1,[1,3]]]]	$-\frac{1}{30240}$		[2,[2,[1,4]]]	$-\frac{1}{483840}$
	[3,[1,[1,2]]]	$+\frac{23}{120960}$		[3,[3,[1,2]]]	$+\frac{1}{138240}$
	[[1,3],[1,2]]	$+\frac{31}{120960}$		[4,[1,[1,3]]]	$+\frac{1}{967680}$
	[2,[1,[1,3]]]	$+\frac{1}{40320}$		[[1,2],[2,4]]	$+\frac{1}{290304}$
	[3,[1,3]]	$+\frac{1}{24192}$		[[1,3],[1,4]]	$+\frac{1}{193536}$
	[2,[2,3]]	$+\frac{1}{13440}$		[2,[1,[1,[1,4]]]]	$+\frac{1}{725760}$
	[1,[1,[1,4]]]	$+\frac{1}{40320}$		[[1,2],[1,[1,4]]]	$-\frac{1}{725760}$
	[2,[1,4]]	$-\frac{1}{13440}$		[[1,3],[2,[1,2]]]	$+\frac{1}{60480}$
	[4,[1,2]]	$-\frac{1}{8064}$		[[2,3],[1,[1,2]]]	$+\frac{1}{120960}$
	[3,4]	$-\frac{1}{16128}$		[[1,3],[1,[1,3]]]	$-\frac{1}{241920}$
	[1,[1,5]]	$+\frac{1}{40320}$		[[1,[1,3]],[1,[1,2]]]	$-\frac{19}{1209600}$
	[2,5]	$+\frac{1}{53760}$		[[1,2],[1,[1,[1,3]]]]	$+\frac{11}{1209600}$
9	[4,5]	$+\frac{1}{1658880}$		[3,[1,[1,[1,[1,2]]]]]	$-\frac{1}{134400}$
	[3,[1,5]]	$+\frac{1}{829440}$		[1,[1,[1,[1,5]]]]	$-\frac{1}{1814400}$
	[4,[2,3]]	$+\frac{1}{241920}$		[3,[1,[1,4]]]	$+\frac{11}{2903040}$
	[5,[1,[1,2]]]	$+\frac{1}{387072}$		[[1,2],[1,5]]	$-\frac{23}{5806080}$
	[2,[2,5]]	$+\frac{1}{1935360}$		[4,[1,[1,[1,2]]]]	$+\frac{1}{362880}$
	[3,[2,4]]	$-\frac{1}{580608}$		[3,[2,[1,[1,2]]]]	$+\frac{1}{80640}$
	[4,[1,4]]	$-\frac{1}{414720}$		[3,[1,[1,[1,3]]]]	$-\frac{1}{241920}$
	[2,[1,[1,5]]]	$+\frac{1}{1935360}$		[[1,2],[2,[1,3]]]	$-\frac{1}{120960}$
				[[1,2],[3,[1,2]]]	$-\frac{1}{120960}$
				[2,[1,[1,[1,[1,3]]]]]	$-\frac{1}{1209600}$
				[[1,3],[1,[1,[1,2]]]]	$-\frac{1}{57600}$

Example

Assume that we use four Gaussian collocation points, whereby obtaining an 8th order method by virtue of Lemma 3. Since the terms in the table are odd powers of h, we only need to retain terms up to order 7, giving the discrete expansion

$$\tilde{\sigma}^4 = f_1 - \frac{1}{12}[f_1, f_2] + \frac{1}{24} f_3 + \frac{1}{480}[f_2, f_3] + \frac{1}{720}[f_1, [f_1, f_3]]$$

$$
\begin{aligned}
&- \frac{1}{240}[f_2,[f_1,f_2]] + \frac{1}{720}[f_1,[f_1,[f_1,f_2]]] - \frac{1}{480}[f_1,f_4] \\
&- \frac{1}{16128}[f_3,f_4] - \frac{1}{13440}[f_2,[f_1,f_4]] + \frac{1}{13440}[f_2,[f_2,f_3]] \\
&+ \frac{1}{24192}[f_3,[f_1,f_3]] - \frac{1}{8064}[f_4,[f_1,f_2]] + \frac{1}{40320}[f_1,[f_1,[f_1,f_4]]] \\
&+ \frac{1}{40320}[f_2,[f_1,[f_1,f_3]]] - \frac{1}{6720}[f_2,[f_2,[f_1,f_2]]] \\
&+ \frac{23}{120960}[f_3,[f_1,[f_1,f_2]]] - \frac{16}{62431}[[f_1,f_2],[f_1,f_3]] \\
&- \frac{1}{30240}[f_1,[f_1,[f_1,[f_1,f_3]]]] + \frac{1}{10080}[f_2,[f_1,[f_1,[f_1,f_2]]]] \\
&- \frac{1}{30240}[[f_1,f_2],[f_1,[f_1,f_2]]] - \frac{1}{30240}[f_1,[f_1,[f_1,[f_1,[f_1,f_2]]]]],
\end{aligned} \tag{8}
$$

where the f_ks are related to A_k through the Vandermonde matrix (6).

Eigenvalue problems

Mathematically, Schrödinger problems arise from the standard separation of variable method applied to a linear partial differential equation, and in connection with the inverse scattering transform for solving nonlinear partial differential equations (PDEs). They also arise in quantum physics, quantum chemistry, transport theory, geophysical applications, and vibration and heat flow problems in mechanical engineering. Many eigenvalue problems have explicit solutions, and are therefore important in analytic investigation of different physical models. However most eigenvalue problems are not solvable, and computationally efficient approximation techniques are of great applicability. Although we focus on the basic Schrödinger equation in a finite domain,

$$
-y'' + q(x)y = \lambda y, \quad x \in (a,b), \tag{9}
$$

with a smooth potential, $q \in C^m(a,b)$, and appropriate boundary conditions, our schemes can be easily adapted to other types of eigenvalue problems, e.g. Sturm–Liouville problems, $-(py')' + qy = \lambda wy$. In this connection we wish to mention the periodic AKNS 2×2 eigenvalue problem

$$
Y' = \begin{bmatrix} -i\lambda & q(x) \\ r(x) & i\lambda \end{bmatrix} Y.
$$

It appears when studying the asymptotics of integrable PDEs, for example the nonlinear Schrödinger equation.

For this particular problem uniform approximation to the eigenvalues is important in order to carry out an approximate inverse scattering transform, or when approximating the asymptotics. Similarly, the soon to be described methods are well suited for monitoring the breakup of integrability of discrete PDEs. We will return to this application at a later point in time. A third class of problems that seem interesting are fourth-order Sturm–Liouville problems, $(py'')'' - (sy')' + qy = \lambda wy$ [GM95].

It is well known that for regular Schrödinger problems the eigenvalues are real, distinct and bounded from below. It is therefore customary to order the eigenvalues in the form $\lambda_{-N} < \ldots < \lambda_{-1} < 0 \leq \lambda_0 < \lambda_1 < \ldots$, where negative indices indicate negative eigenvalues.

Finding the eigenvalues and associated eigenfunctions can be a computationally challenging task, especially when a large set of eigenvalues is sought, which is important when studying e.g. the onset of chaos in numerical discretisation [MJAS96], carrying through a inverse scattering transform using the discrete Ablowitz–Ladik scheme [MJA76], for example in geophysical applications [PdH79], or just when particularly large eigenvalues are sought. At this point it is also worth mentioning that for particulary large eigenvalues asymptotic expressions like WKB are attractive alternatives to classical numerical methods.

Methods found in the literature mainly belong to two distinct classes, *shooting methods* and *matrix-based methods*. Matrix methods have the advantage of providing a set of eigenvalues, but their main disadvantage is the difficulty in providing high order approximations with uniform error bounds. In this respect shooting methods have an advantage. They are based on transforming the boundary value problem (9) into a first-order initial value problem

$$
\begin{aligned}
Y'(x) = \begin{bmatrix} 0 & 1 \\ q(x) - \lambda & 0 \end{bmatrix} Y(x) &= A(x,\lambda)Y(x) \\
B_a Y(a) + B_b Y(b) &= 0,
\end{aligned} \tag{10}
$$

where $B_a, B_b \in \mathbb{R}^{2\times 2}$ and $Y(x)^T = [y(x), y'(x)]$. The boundary conditions are stated less general here than in (9) for presentation purposes.

The eigenvalues are determined, using some iterative technique, as the solution of

$$
\Delta(\lambda) = \det\left[B_a + B_b \Phi_a^b(\lambda)\right] = 0.
$$

Numerical experience has shown that choosing some *matching point*, $a < x_M < b$, and solving the problem $\Delta(\lambda) = \det\left[B_a \Phi_a(x_M) + B_b \Phi_b(x_M)\right]$ normally gives smaller errors, however for simplicity we will only consider the matching point $x_M = b$.

We are in this paper interested in methods that yield uniform approximation to the eigenvalues. To obtain a good algorithm it is paramount to have an efficient solution algorithm for the initial value problem together with an efficient method for solving the nonlinear equation $\Delta(\lambda) = 0$. *Pruess–Fulton* methods are methods based on "approximation of the differential equation"[Can72, Pre73, PdH79], and the methods have successfully been used to solve a range of Sturm–Liouville problems. In essence the approach is to replace the potential q with a perturbed potential that renders the equation solvable. In particular *constant reference potential* approximations are popular.

A major drawback of the Pruess methods is the difficulty in obtaining higher order methods. Although this was addressed in [PJ96], the methods presented only achieved higher order for homogenous boundary conditions. It is therefore usual to implement them using Richardson extrapolation.

Shooting methods based on standard initial-value libraries, such as `Sleigen2`, often suffer from step-size restriction when solving for large eigenvalues, or when the potentials are particularly large, and are not suited for computing a large set of eigenvalues.

Applying Magnus expansions to eigenvalue problems

A typical feature of shooting methods is the need to solve the differential equation (9) repeatedly using different trial values of λ, either refining the accuracy of one eigensolution, or searching for new eigensolutions. Several extrapolation-based methods [HS93] utilise this fact and save function evaluations in a vector for later use, either to extrapolate or to solve the differential equation for different λs.

Evaluation of the function σ

Naive consideration of the complexity of discrete Magnus expansions may seem to indicate that they are not good candidates for an efficient numerical method.

However the aforementioned conservative properties and the observation that $\tilde{\sigma}$ is a polynomial in λ give ample reasons to pursue this topic further. We now have

$$\tilde{\sigma}(\lambda) = \sum_{k=0}^{M} \gamma_k \lambda^k.$$

A simple calculations shows that for an $2m$th order method, based on Gaussian collocation points, the order of $\tilde{\sigma}$ as a polynomial in λ is $M = m - 2$ when $m \geq 3$ and $M = 1$ otherwise.

In practice this means that once we have found the matrices γ_k the cost of evaluating the Magnus expansion for $\tilde{\sigma}$ is reduced to evaluating a polynomial with matrix coefficients.

As a specific application of the technique we study problems in Liouville normal form (Schrödingers' equation). In this case the matrix coefficients of the polynomial $\sigma(\lambda)$ will be dependent only on the potential, and to simplify the notation we introduce $z_i = h \sum_{j=1}^{m+1} v_{ij}^m q(n_0 + hc_i^m)$, where $q(x_n + hc_i^m)$ is the potential evaluated at the collocation point and v_{ij}^m is the associated Vandermonde matrix (6). We can now easily write down the formulas for the methods using Magnus series and an appropriate quadrature rule. These formulas are obtained by inserting z_i into e.g. (8).

Fourth order methods

We choose the two Gaussian collocation points $c_1^1 = \frac{1}{2} - \frac{\sqrt{3}}{6}$, $c_2^1 = \frac{1}{2} + \frac{\sqrt{3}}{6}$, whereby the method is given by

$$v^1 = \begin{bmatrix} 1/2 & 1/2 \\ \sqrt{3} & -\sqrt{3} \end{bmatrix}.$$

The components of the σ matrix for the fourth-order method, applied to a problem in a Liouville normal form, are given by

$$\sigma_{11}^1(\boldsymbol{\lambda}) = -\frac{hz_2}{12}, \ \sigma_{12}^1(\boldsymbol{\lambda}) = h,$$
$$\sigma_{21}^1(\boldsymbol{\lambda}) = z_1 - h\boldsymbol{\lambda}, \ \sigma_{22}^1(\boldsymbol{\lambda}) = \sigma_{11}^1(\boldsymbol{\lambda}),$$

where λ is the eigenvalue parameter.

Another fourth-order method, more suited for extrapolation, or when the values of the potential is available on a uniform grid, is obtained from the Simpson quadrature rule. The Vandermonde matrix is then

$$v_s^1 = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 2 & -4 & 2 \end{bmatrix}.$$

The sixth-order method

The sixth order method was first constructed in [AIFR98]. The same paper also presented a proof that the truncated Magnus expansion based on symmetric collocation has global error expansion in even powers of h, hence our methods can be combined efficiently with the Richardson extrapolation algorithm. Using the three Gauss–Legendre nodes $c_1^2 = \frac{5-\sqrt{15}}{10}$, $c_2^2 = \frac{1}{2}$, $c_3^2 = \frac{5+\sqrt{15}}{10}$ with the weight matrix

$$v^2 = \begin{bmatrix} 0 & 1 & 0 \\ -\sqrt{\frac{5}{3}} & 0 & \sqrt{\frac{5}{3}} \\ \frac{20}{3} & -\frac{40}{3} & \frac{20}{3} \end{bmatrix},$$

our sixth order method becomes

$$\begin{aligned}
\sigma_{11}^2(\boldsymbol{\lambda}) &= \left(-\frac{hz_2}{12} + \frac{h^2 z_1 z_2}{180}\right) - \frac{h^3 z_2}{180}\boldsymbol{\lambda} \\
\sigma_{12}^2(\boldsymbol{\lambda}) &= \left(h - \frac{h^2 z_3}{360}\right) \\
\sigma_{21}^2(\boldsymbol{\lambda}) &= \left(z_1 + \frac{z_3}{24} - \frac{hz_2^2}{120} + \frac{hz_1 z_3}{360}\right) - \left(h + \frac{h^2 z_3}{360}\right)\boldsymbol{\lambda} \\
\sigma_{22}^2(\boldsymbol{\lambda}) &= -\sigma_{11}^2(\boldsymbol{\lambda})
\end{aligned}$$

The eighth-order method

By using the four Gauss–Legendre nodes

$$\begin{aligned}
c_1^3 &= -\sqrt{\frac{15+2\sqrt{30}}{35}}, & c_2^3 &= -\sqrt{\frac{15-2\sqrt{30}}{35}}, \\
c_3^3 &= +\sqrt{\frac{15+2\sqrt{30}}{35}}, & c_4^3 &= +\sqrt{\frac{15-2\sqrt{30}}{35}},
\end{aligned}$$

the eighth-order Magnus method is given by

$$\sigma^3_{11}(\boldsymbol{\lambda}) = \left(-\frac{hz_2}{12} + \frac{h^2 z_1 z_2}{180} - \frac{hz_4}{480} - \frac{h^3 z_1^2 z_2}{1890} + \frac{h^2 z_1 z_4}{10080} + \frac{13h^2 z_2 z_3}{30240}\right)$$
$$- \left(\frac{h^3 z_2}{180} + \frac{h^3 z_4}{10080} - \frac{h^4 z_1 z_2}{945}\right)\boldsymbol{\lambda} - \frac{h^5 z_2}{1890}\boldsymbol{\lambda}^2$$
$$\sigma^3_{12}(\boldsymbol{\lambda}) = \left(h - \frac{h^2 z_3}{360} + \frac{h^3 z_1 z_3}{3780} + \frac{h^3 z_2^2}{7560}\right) - \frac{h^4 z_3}{3780}\boldsymbol{\lambda}$$
$$\sigma^3_{21}(\boldsymbol{\lambda}) = \left(z_1 + \frac{z_3}{24} - \frac{hz_2^2}{120} + \frac{hz_1 z_3}{360} - \frac{h^2 z_1^2 z_3}{3780} - \frac{hz_2 z_4}{2520} + \frac{hz_3^2}{12096} + \frac{h^2 z_1 z_2^2}{1080}\right)$$
$$- \left(h + \frac{h^2 z_3}{360} - \frac{h^3 z_1 z_3}{1890} + \frac{h^3 z_2^2}{1080}\right)\boldsymbol{\lambda} - \frac{h^4 z_3}{3780}\boldsymbol{\lambda}^2$$
$$\sigma^3_{22}(\boldsymbol{\lambda}) = -\sigma^3_{11}(\boldsymbol{\lambda})$$

where the weight matrix v^3 is

$$\begin{bmatrix} \frac{4-\sqrt{30}}{16} & \frac{4+\sqrt{30}}{16} & \frac{4+\sqrt{30}}{16} & \frac{4-\sqrt{30}}{16} \\ \frac{35}{8}\frac{\sqrt{30}-4}{\sqrt{525+70\sqrt{30}}} & -\frac{35}{8}\frac{\sqrt{30}+4}{\sqrt{525-70\sqrt{30}}} & \frac{35}{8}\frac{\sqrt{30}+4}{\sqrt{525-70\sqrt{30}}} & -\frac{35}{8}\frac{\sqrt{30}-4}{\sqrt{525+70\sqrt{30}}} \\ \frac{7\sqrt{30}}{12} & -\frac{7\sqrt{30}}{12} & -\frac{7\sqrt{30}}{12} & \frac{7\sqrt{30}}{12} \\ -\frac{245\sqrt{6}}{\sqrt{3780+504\sqrt{30}}} & \frac{245\sqrt{6}}{\sqrt{3780-504\sqrt{30}}} & -\frac{245\sqrt{6}}{\sqrt{3780-504\sqrt{30}}} & \frac{245\sqrt{6}}{\sqrt{3780+504\sqrt{30}}} \end{bmatrix}.$$

Shooting for eigenvalues

We now return to the important $\Delta(\lambda)$ function defined as

$$\Delta(\lambda) = \det\left[B_a + B_b \Phi^b_a(\lambda)\right] = 0$$

where $\Phi^t_a(\lambda) \in \mathrm{SL}(2,\mathbb{R})$ is the fundamental matrix, and whose zeros are the eigenvalues. $SL(2,\mathbb{R})$ is the group of real matrices with unit determinant, and by construction our methods preserve this property. Using the Magnus expansion we can now construct approximations to $\Phi^{t_N}_{t_1}$ in the form $\tilde{\Phi}^{t_N}_{t_1} = \tilde{\Phi}^{t_{n+1}}_{t_n}\tilde{\Phi}^{t_n}_{t_n-1}\cdots\tilde{\Phi}^{t_2}_{t_1}$, which in turn is needed to compute Δ. Newton's iteration scheme for the zeros of $\Delta(\lambda)$,

$$\frac{d\Delta(\lambda_n)}{d\lambda}(\lambda_{n+1} - \lambda_n) = -\Delta(\lambda_n), \quad n = 0, 1, \ldots$$

requires the evaluation of the derivative of Δ with respect λ. From the analytic theory of regular Sturm–Liouville problems it is known that the zeros of Δ are simple, hence Newton iterations converge quadratically for starting values, near enough to a zero. The derivative of Δ can be obtained from the derivative of the fundamental matrix by means of the formula

$$\frac{d\Delta}{d\lambda} = \det\left[\frac{d\varphi_1}{d\lambda};\varphi_2\right] + \det\left[\varphi_1;\frac{d\varphi_2}{d\lambda}\right],$$

where φ_i denotes the i-th column of the matrix $B_a + B_b\Phi_a^b(\lambda)$. The formula

$$\frac{\partial}{\partial\lambda}e^{\sigma(\lambda)} = \int_0^1 e^{(1-x)\sigma}\frac{\partial\sigma}{\partial\lambda}e^{x\sigma}\,dx$$

provides a way of finding the derivative [Wil67], but is less useful for numerical computations. The *variational equation*

$$\begin{bmatrix}\Phi\\ \Phi_\lambda\end{bmatrix}' = \begin{bmatrix}A(t) & 0\\ \partial A/\partial\lambda & A(t)\end{bmatrix}\begin{bmatrix}\Phi\\ \Phi_\lambda\end{bmatrix}, \Phi(0,\lambda) = \mathbb{1}, \quad \Phi_\lambda(0,\lambda) = 0 \tag{11}$$

provides a better way and, solving (11), we obtain the required derivative. This technique is easily extended to problems with many parameters λ_i.

Lemma 5 *Let $\hat\sigma$ be the Magnus expansion for the variational problem (11), and σ be the Magnus expansion for (2). Then* $\hat\sigma = \begin{bmatrix}\sigma & 0\\ \frac{\partial\sigma}{\partial\lambda} & \sigma\end{bmatrix}$.

Proof To simplify the notation let $D = \begin{bmatrix}1 & 0\\ \frac{\partial}{\partial\lambda} & 1\end{bmatrix}$, furthermore $\mathcal{D} = D\otimes$, where $\otimes$ is the Kronecker product, i.e. $\hat\sigma = \mathcal{D}\sigma$. A simple calculation shows that for λ-dependent matrices, p and q , $\mathcal{D}$ satisfies $\mathcal{D}pq = \mathcal{D}p\mathcal{D}q$, i.e. $\mathcal{D}$ is a homomorphism of the standard algebra of matrices. This implies that $\mathcal{D}$ is a matrix Lie algebra homomorphism, i.e. $\mathcal{D}[p,q] = [\mathcal{D}p, \mathcal{D}q]$. The statement of the lemma follows by using the homomorphism and its linearity. $\square$

The matrix exponential

For an $\mathfrak{sl}(2)$ matrix σ we have the well-known formula $\exp(\sigma) = \cosh(\phi) + \sigma\,\sinh(\phi)/\phi$, where $\phi = \sqrt{<\sigma,\sigma>}$, $<p,q>= \mathrm{trace}(\mathrm{p}^{\mathrm{T}}\mathrm{q})$.

In passing we would like to mention that for $\mathfrak{so}(3)$, the Lie algebra of skew-Hermitian matrices, similar formulae exist under the name of the *Euler–Rodriguez formula.* Moreover if we allow analytic approximations to the exponential, it can be shown that diagonal Padé approximations do provide mappings from quadratic Lie algebras to the corresponding group. Examples of quadratic Lie algebras are $\mathfrak{sp}(2n,\mathbb{R})$, $\mathfrak{su}(n)$ and $\mathfrak{so}(n,\mathbb{R})$, the algebra of symplectic vector-fields, skew-symmetric complex matrices, and skew-symmetric matrices respectively, all important in applications. For generic Lie-algebras Iserles and Celledoni [CI98] present a novel approach based on low-rank operator splitting.

To compute the matrix exponential of $\hat{\tilde\sigma} = \mathcal{D}\tilde\sigma$, we again resort to the homomorphism of $\mathcal{D}$ and obtain $\exp(\mathcal{D}\sigma) = \mathcal{D}\exp(\sigma)$, more explicitly

$$\exp(\mathcal{D}\sigma) = \begin{bmatrix}\cosh(\phi)\mathbb{1} + \frac{\sinh(\phi)}{\phi}\sigma & 0\\ \frac{\sinh(\phi)}{\phi}(\hat\phi\mathbb{1} + \frac{\partial\sigma}{\partial\lambda}) + \hat\phi\frac{\sinh(\phi)-\phi\cosh(\phi)}{\phi^3}\sigma & \cosh(\phi)\mathbb{1} + \frac{\sinh(\phi)}{\phi}\sigma\end{bmatrix}, \tag{12}$$

where $\phi = \sqrt{<\sigma,\sigma>}$, $\hat\phi =<\sigma,\sigma'>/2$.

Since the formula contains the same evaluations of cosh and sinh as for the 2×2 case, the additional cost in evaluating the exponential of $\mathcal{D}\sigma$ is small. Similar formulas can be found for other parameter-dependent problems, for example fourth-order Sturm–Liouville problems and other systems giving rise to a 4×4 σ-matrix. For larger systems other techniques must be applied for approximating the exponential, see e.g. [CI98, MVL78], however by doing so new difficulties arise, e.g. in computing the derivative of $\Phi_a(x)$ with respect to λ.

Algorithm : Simple Sturm–Liouville solver

BEGIN
  INPUT N
  Divide the domain into partitions D_n , $n = 1...N$, *according to given tolerance* ϵ.
FOR *n=1:N*
  Evaluate the potential q(x) at the collocation point in D_n
  Compute z_i *and the coefficients of the polynomials* σ_{ij}
ENDDO
  INPUT λ, Y_0, Y_N
SET E_0*=0*
1: FOR *n=1:N*
  Evaluate σ_{ij} *for the given* λ
  Find $\hat{\sigma}$ *according to Lemma 5*
  Compute $[P,Q]_n = \exp(\hat{\sigma})[P,Q]_{n-1}$ *as in (12)*
  $Y_n = P_n Y_{n-1}$
  $E_n = Q_n Y_n + P_n E_n$
ENDDO
  Compute the Newton correction to λ *using* E_n *and* Y_n
  IF *result not within tolerance* THEN GOTO 1:
  OUTPUT λ *and* Y_n
END

Y_n is the vector(or matrix) containing an approximation to the solution, $Y_n \approx \begin{bmatrix} y(a+h*n) \\ y'(a+h*n) \end{bmatrix}$. E_n is the vector containing the first variation $\partial y / \partial \lambda$ of the solution on the same points as we approximate the solution, $E_n \approx \begin{bmatrix} \partial y(a+h*n)/\partial\lambda \\ \partial y'(a+h*n)/\partial\lambda \end{bmatrix}$. Y_n and E_n the fundamental matrix solution for Y_n and E_n is then approximated using $[P,Q]_n$, the notation emphasizing the block structure of the large fundamental matrix (11).

Asymptotic behaviour

By construction the methods presented in this paper have a global order of approximation $\mathcal{O}(h^p)$. However, for large eigenvalues it is interesting to see how the errors depend on the magnitude of the eigenvalue. Most standard discretisations display deteriorating behaviour for large eigenvalues, and much effort has been put into improving this situation. The methods of Pruess [Pre73] and those of Ixaru et. al. see

[LGIVB98] for a review have addressed themselves to this problem, but only those of Ixaru seem to be practical for Schrödinger eigenvalue problems. Pruess methods are practical only for second-order approximations, or approximations using Richardson extrapolation.

The main reason we can expect poor approximations for large eigenvalues is Theorem 2. The finite radius of convergence implies that there is a relation between the maximum allowable step-size, $h_{\max}$, and the magnitude of the eigenvalues we are seeking. By simply evaluating the discrete Magnus expansion we find that $h_{\max} = \mathcal{O}(1/\sqrt{\lambda_{\max}})$.

Proposition 6 *Let σ be the exact Magnus expansion and $\tilde{\sigma}$ be the truncated Magnus expansion obtained by using m Gauss–Legendre nodes. Then we have the estimate $\|\sigma - \tilde{\sigma}\| = \mathcal{O}\big(h^{2m+1}\lambda^{m-1}\big)$.*

The result follows by induction on $\mathrm{ad}^n(f_1)f_2$, and by noting that only terms with odd n are present in the centred Magnus expansion. Typical terms causing problems for large λ are the truncations of

$$\begin{aligned}
E^{[2]} &= \tfrac{1}{2}f_2 - \tfrac{1}{12}\mathrm{ad}(f_1)f_2 + \tfrac{1}{720}\mathrm{ad}^3(f_1)f_2 - \tfrac{1}{30240}\mathrm{ad}^5(f_1)f_2 + \cdots \\
E^{[3]} &= \tfrac{1}{3}f_3 - \tfrac{1}{12}\mathrm{ad}(f_1)f_3 + \tfrac{1}{360}\mathrm{ad}^2(f_1)f_3 + \tfrac{1}{720}\mathrm{ad}^3(f_1)f_3 \\
&\;\;\vdots \\
E^{[2,2]} &= -\tfrac{1}{240}[f_2,[f_1,f_2]] + \tfrac{1}{10080}[f_2,[f_1,[f_1,[f_1,f_2]]]] - \\
E^{[2,3]} &= \tfrac{1}{480}[f_2,f_3] + \tfrac{1}{40320}[f_2,[f_1,[f_1,f_3]]] + \tfrac{23}{120960}[f_3,[f_1,[f_1,f_2]]] + \cdots \\
&\;\;\vdots
\end{aligned}$$

We note in the case that when f_i are samples form a Lie algebra it is possible to represent these sums using the basis. In order to make the formulas more comprehensive we formulate the sums as functions of f_i.

With these definitions we can now write

$$\sigma = f_1 + \sum_{i\geq 2} E^{[i]} + \sum_{i\geq j\geq 2} E^{[i,j]} + \cdots \tag{13}$$

Each term in e.g. $E^{[2]}$ are $\mathcal{O}(h^3)$ whenever $h^2\lambda \approx 1$, hence a truncation of $E^{[2]}$ will asymptotically ($h^2\lambda$ large) give a second-order approximation to the eigensolution. In order to avoid this difficulty it is better to truncate the expansion based on (13) rather than e.g. (8), since this eliminates the dependency on λ in the truncation in a systematic manner. However, to do so we need to sum up expressions for e.g. $E^{[2]}$,$E^{[3]}$ and $E^{[2,3]}$ in the case of the sixth-order method.

Lemma 7 *The terms in the discrete Magnus expansion can all be written in the form*

$$\mathcal{C}^{[k_1,k_2,\ldots,k_m]}_{n_1,n_2,\ldots,c_w} = [\mathrm{ad}^{n_1}(f_1)f_{k_1},[\mathrm{ad}^{n_2}(f_1)f_{k_2},\ldots,[\mathrm{ad}^{n_{w-1}}(f_1)f_{k_{w-1}},\mathrm{ad}^{n_w}(f_1)f_{k_w}]\ldots]],$$

in particular we have the Leibniz' rule

$$\mathrm{ad}^n(f_1)[f_{k_1}, f_{k_2}] = \sum_{m=0}^{n-1} \binom{n}{n-m} [\mathrm{ad}^m(f_1) f_{k_1}, \mathrm{ad}^{n-m}(f_1) f_{k_2}], \quad f_1, f_{k_1}, f_{k_2} \in \mathfrak{g}.$$

The proof follows by induction from the fact that $\mathrm{ad}(f_1)$ is a derivation on the Lie algebra, with a corresponding Leibniz' rule, $\mathrm{ad}(A)[B,C] = [\mathrm{ad}(A)B, C] + [B, \mathrm{ad}(A)C]$. By expressing the terms in the Magnus expansions according to Lemma 7 we avoid many complications induced by the Hall basis relations (7), but at the same time we loose the independence among the different terms. The main reason for this is the difficulties associated with keeping track of the Hall basis relations with the generating functions we are about to develop. We now define the coefficients $c_{n_1,n_2,\cdots}^{[k_1,k_2,\cdots]}$ by

$$E^{[k_1,k_2,\cdots]} = \sum_{n_1,n_2,\cdots \geq 0} c_{n_1,n_2,\cdots}^{[k_1,k_2,\cdots]} \mathcal{C}_{n_1,n_2,\cdots}^{[k_1,k_2,\cdots]},$$

and with each such discrete Magnus expansion we associate a generating function

$$\mathcal{E}^{[k_1,k_2,\ldots]}(x_1, x_2, \ldots) = \sum_{n_1,n_2,\ldots \geq 0} c_{n_1,n_2,\cdots}^{[k_1,k_2,\ldots]} x_1^{n_1+k_1} x_2^{n_2+k_2} \cdots$$

The first nontrivial terms are those of the form $E^{[k]} = \sum_{n \geq 0} c_n^{[k]} \mathrm{ad}(f_1)^n f_k$ with the generating function $\mathcal{E}^{[k]}(x) = \sum_{n\geq 0} c_n^{[k]} x^{n+k}$. By finding explicit expressions for $\mathcal{E}^{[\cdot]}$ we can evaluate the corresponding Lie series $E^{[\cdot]}$ exactly.

Lemma 8 *Assume* $A(t) = \sum_{n\geq 0} \tilde{f}_n t^n$, *then* $\tilde{\mathcal{E}}^{[k]}(x) = x(k-1)! \left\{ 1 - \frac{\sum_{n=1}^{k-1} \frac{x^n}{n!}}{e^x - 1} \right\}$, *with* $\tilde{E}^{[k]} = \frac{\tilde{\mathcal{E}}^{[k]}(\mathrm{ad}(\tilde{f}_1))}{\mathrm{ad}(\tilde{f}_1)^k} \tilde{f}_k$.

Proof The structure of $\tilde{E}^{[k]}$ is most easily found by recalling the Picard iteration used to construct the expansions

$$\sigma_{m+1} = \sum_{n\geq 0} b_n \int_0^t \mathrm{ad}(\sigma_m)^n A(\tau) d\tau, \quad \sigma_0 = \int_0^t A(\tau) d\tau. \tag{14}$$

Since we are really interested in terms of the form $\mathrm{ad}(\tilde{f}_1)^n \tilde{f}_k$, it suffices, after taking into account the skew-symmetry $[\tilde{f}_1, \tilde{f}_k] = -[\tilde{f}_k, \tilde{f}_1]$ the iteration

$$\begin{aligned} \rho_{m+1} \quad &= \quad \sum_{n_1 \geq 0} b_{n_1} \mathrm{ad}^{n_1}(\tilde{f}_1) \int_0^t \tau_1^{n_1} (\tau_1^{k-1} \tilde{f}_k) \, d\tau_1 \\ &- \quad \sum_{n_1 \geq 1} b_{n_1} \mathrm{ad}^{n_1}(\tilde{f}_1) \int_0^t \tau_1^{n_1} \rho_m \, d\tau_1, \quad m = 0, 1, \ldots, \end{aligned}$$

whose fixed-point, $\rho_\infty = \tilde{E}^{[k]} = \frac{\tilde{\mathcal{E}}^{[k]}(\mathrm{ad}(\tilde{f}_1))}{\mathrm{ad}(\tilde{f}_1)^k} \tilde{f}_k$, formally satisfies the equation

$$\tilde{\mathcal{E}}^{[k]}(\mathrm{ad}\tilde{f}_1 t)\tilde{f}_k \quad = \quad \sum_{n_1 \geq 0} b_{n_1} \mathrm{ad}^{n_1}(\tilde{f}_1) \tilde{f}_k \int_0^t \tau_1^{n_1+k-1} \, d\tau_1$$

$$-\sum_{n_1\geq 1} b_{n_1}\mathrm{ad}^{n_1}(\tilde{f}_1)\int_0^t \tau_1^{n_1}\tilde{\mathcal{E}}^{[k]}(\mathrm{ad}(\tilde{f}_1)\tau_1)\tilde{f}_k\,d\tau_1, \quad m=0,1,\ldots.$$

At this point the Lie algebra elements $\tilde{f}_1$ and $\tilde{f}_k$ are redundant in defining $c_n^{[k]}$ and we find by omitting them the differential equation

$$\frac{d\tilde{\mathcal{E}}^{[k]}(t)}{dt} = \frac{t^k}{e^t-1} - (\frac{t}{e^t-1}-1)t^{-1}\tilde{\mathcal{E}}^{[k]}(t),$$

whose solution is given by

$$\tilde{\mathcal{E}}^{[k]}(t) = t(k-1)!\left(1-\frac{\sum_{n=1}^{k-1}\frac{t^n}{n!}}{e^t-1}\right) \tag{15}$$

□

To find the generating function for the centred expansion we use the relation

$$\mathcal{E}^{[k]}(t) = \frac{1}{(k-1)!}\sum_{j=2}^{k}\binom{k-1}{j-1}(-\frac{1}{2})^{k-j}\tilde{\mathcal{E}}^{[j]}(t).$$

In particular we find using Lemma 8 the following expressions

$$\mathcal{E}^{[2]}(x) = (1-\frac{1}{2}x-\frac{x}{\exp(x)-1})/x = -\sum_{n\geq 1} b_{n+1}x^n$$

$$\mathcal{E}^{[3]}(x) = (1-\frac{1}{2}x+\frac{1}{12}x^2-\frac{x}{\exp(x)-1})/x^2 = -\sum_{n\geq 2} b_{n+2}x^n$$

$$\mathcal{E}^{[4]}(x) = -\sum_{n\geq 1}(b_{n+3}+\frac{b_{n+1}}{24})x^n.$$

An application to the Schrödinger equation

The main motivation in the previous section was to avoid the deterioration in accuracy for large eigenvalues in Schrödinger's eigenvalue problems. In this case the term causing the problems is f_1, the only term dependent on λ. After introducing $z_i = h\sum_{j=1}^{m+1} v_{ij}^m q(n_0+hc_i^m)$, where $q(x_n+hc_i^m)$ is the potential evaluated at the Gaussian collocation points, we find the following for various powers of $\mathrm{ad}(f_1)$ applied to f_2, f_3 and f_4

$$\mathrm{ad}(f_1)^{2n+1}f_2 = (4h(z_1-\lambda h))^n z_2 h J^{[2]} \tag{16}$$

$$\mathrm{ad}(f_1)^{2n}f_3 = (4h(z_1-\lambda h))^n z_3 h J^{[3]} \tag{17}$$

$$\mathrm{ad}(f_1)^{2n+1}f_4 = (4h(z_1-\lambda h))^n z_4 h J^{[4]}, \tag{18}$$

where

$$J^{[k]} = \begin{cases} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, & k \quad \text{even} \\ \begin{bmatrix} 0 & -2h \\ 2(z_1-\lambda h) & 0 \end{bmatrix}, & k \quad \text{odd} \end{cases}$$

If we let $E^{[k]} = g^{[k]}(4h(z_1 - \lambda h))J^{[k]}$, we have, by Lemma 8 and $\sum_{k\geq 0} b_k z^k = z/(e^z - 1)$, the following expressions for $g^{[k]}$

$$
\begin{aligned}
g^{[2]}(z) &= \begin{cases} \frac{1}{z}\left(\frac{\sqrt{z}\sinh(\sqrt{z})}{2-2\cosh(\sqrt{z})} + 1\right), & z > 0, \\ \frac{-1}{z}\left(\frac{\sqrt{-z}\sin(\sqrt{-z})}{2-2\cos(\sqrt{-z})} - 1\right), & z < 0, \end{cases} \\
g^{[3]}(z) &= \left(\frac{1}{12} + g^{[2]}(z)\right)/z, \\
g^{[4]}(z) &= \frac{1}{24} g^{[2]}(z) + g^{[3]}(z),
\end{aligned}
$$

and are then able compute the sums exactly as

$$
\begin{aligned}
E^{[2]} &= g^{[2]}(4h(z_1 - h\lambda))hz_2 \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \\
E^{[3]} &= g^{[3]}(4h(z_1 - h\lambda))hz_3 \begin{bmatrix} 0 & -2h \\ 2(z_1 - h\lambda) & 0 \end{bmatrix}, \\
E^{[4]} &= g^{[4]}(4h(z_1 - h\lambda))hz_4 \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.
\end{aligned}
$$

By using these expressions instead of their polynomial approximations, we obtain the sixth-order modified Magnus-type method by setting

$$
\begin{aligned}
&\sigma_{11}^2(\boldsymbol{\lambda}) = hz_2 g^{[2]}(4h(z_1 - h\boldsymbol{\lambda})) \\
&\sigma_{12}^2(\boldsymbol{\lambda}) = h - 2h^2 z_3 g^{[3]}(4h(z_1 - h\boldsymbol{\lambda})) \\
&\sigma_{21}^2(\boldsymbol{\lambda}) = \left(z_1 + \frac{1}{24}z_3 - \frac{1}{120}z_2^2 h\right) - h\boldsymbol{\lambda} + 2(z_1 - h\boldsymbol{\lambda})g^{[3]}(4h(z_1 - h\boldsymbol{\lambda})) \\
&\sigma_{22}^2(\boldsymbol{\lambda}) = -\sigma_{11}^2(\boldsymbol{\lambda}).
\end{aligned}
$$

Compared to the original method, the latter requires significantly more computations to evaluate $g^{[k]}$, however combining the non-modified and modified method we can switch between them according to a criterion based on the error committed when truncating $g^{[k]}$. The method will produce approximation with an error $\mathcal{O}(h^4(h^2\lambda))$, i.e. like a fourth-order method.

The corresponding modified eighth-order method for large λ is given by

$$
\begin{aligned}
\sigma_{11}(\boldsymbol{\lambda}) &= \left(-\frac{z_4 h}{480} + \frac{h^2 z_1 z_4}{10080} + \frac{13h^2 z_2 z_3}{30240}\right) - \frac{h^3 z_4}{10080}\boldsymbol{\lambda} \\
&+ z_2 h g^{[2]}(4h(z_1 - \boldsymbol{\lambda}h)) \\
\sigma_{12}(\boldsymbol{\lambda}) &= h + \frac{h^3 z_2^2}{7560} - 2h^2 z_3 g^{[3]}(4h(z_1 - \boldsymbol{\lambda}h))) \\
\sigma_{21}(\boldsymbol{\lambda}) &= \left(z_1 + \frac{z_3}{24} - \frac{hz_2^2}{120} - \frac{z_2 z_4 h}{2520} + \frac{z_3^2 h}{12096} + \frac{z_1 z_2^2 h^2}{1080}\right) \\
&- \left(h + \frac{z_2^2 h^3}{1080}\right)\boldsymbol{\lambda} + 2(z_1 - h\boldsymbol{\lambda})g^{[3]}(4h(z_1 - \boldsymbol{\lambda}h)z_3 h \\
\sigma_{22}(\boldsymbol{\lambda}) &= -\sigma_{11}(\boldsymbol{\lambda}).
\end{aligned}
$$

This method also behaves like a fourth-order method for large eigenvalues, and the applicability is mainly restricted to accurate approximation of small to medium sized eigenvalues.

Higher-order corrections

To eliminate further dependency on λ in the error term, we need to take into account terms of the form

$$\begin{aligned} E^{[2,2]} &= -\frac{1}{240}[f_2,[f_1,f_2]] - \frac{1}{10080}[f_1,[f_1,[f_2,[f_1,f_2]]]] - \cdots \\ E^{[3,2]} &= +\frac{13}{604800}[f_1,[f_3,[f_1,f_2]]] + \cdots \end{aligned}$$

In other words, we focus on terms of the form

$$E^{[k_1,k_2]} = \sum_{n_1,n_2\geq 0} c^{[k_1,k_2]}_{n_1,n_2}[\mathrm{ad}^{n_1}(f_1)f_{k_1}, \mathrm{ad}^{n_2}(f_1)f_{k_2}],$$

these include all terms with two f's different from f_1 according to Lemma 7

Lemma 9 *The generating function, $\mathcal{E}^{[k_1,k_2]}(x_1,x_2)$, for the discrete Magnus expansion consisting of two elements, f_{k_1}, f_{k_2}, each different from f_1, satisfies the relation*

$$\begin{aligned} \mathcal{E}^{[k_1,k_2]}(x_1\tau,x_2\tau) &= \frac{1}{x_1}\int_0^t \left(\frac{x_1+x_2}{e^{t(x_1+x_2)}-1} - \frac{x_2}{e^{\tau x_2}-1}\right)\tau^{k_2-1}\mathcal{E}^{[k_1]}(x_1\tau)\,d\tau \\ &- \frac{1}{x_2}\int_0^t \left(\frac{x_1+x_2}{e^{t(x_1+x_2)}-1} - \frac{x_1}{e^{\tau x_1}-1}\right)\tau^{k_1-1}\mathcal{E}^{[k_2]}(x_2\tau)\,d\tau \\ &+ \frac{1}{x_1}\int_0^t \left(\frac{x_2}{e^{\tau x_2}-1} - \frac{x_1+x_2}{e^{\tau(x_1+x_2)}-1}\right)\tau^{-1}\mathcal{E}^{[k_1]}(x_1\tau)\mathcal{E}^{[k_2]}(x_2\tau)\,d\tau \\ &+ \frac{1}{x_2}\int_0^t \left(\frac{x_1}{e^{\tau x_1}-1} - \frac{x_1+x_2}{e^{\tau(x_1+x_2)}-1}\right)\tau^{-1}\mathcal{E}^{[k_1]}(x_1\tau)\mathcal{E}^{[k_2]}(x_2\tau)\,d\tau \\ &+ \int_0^t \left(\frac{\tau(x_1+x_2)}{e^{\tau(x_1+x_2)}-1} - 1\right)\tau^{-1}\mathcal{E}^{[k_1,k_2]}(x_1\tau,x_2\tau)\,d\tau, \end{aligned}$$

where $\mathcal{E}^{[k_1]}$ and $\mathcal{E}^{[k_2]}$ are the generating functions given in Lemma 8.

Proof Employing again Picard iteration, the significant part is

$$\begin{aligned} E^{[k_1,k_2]} &= \sum_{n\geq 1} b_n \int_0^t \sum_{m=0}^{n-1}\sum_{l=0}^{m}\binom{m}{l}[\mathrm{ad}^l(f_1)E^{[k_1]}, \mathrm{ad}^{n-l-1}(f_1)f_{k_2}]\tau^{n+k_2-2}\,d\tau \\ &- \sum_{n\geq 1} b_n \int_0^t \sum_{m=0}^{n-1}\sum_{l=0}^{m}\binom{m}{l}[\mathrm{ad}^{n-l-1}(f_1)f_{k_1}, \mathrm{ad}^l(f_1)E^{[k_2]}]\tau^{n+k_1-2}\,d\tau \\ &- \sum_{n\geq 2} b_n \int_0^t \sum_{m=0}^{n-1}\sum_{l=0}^{m}\binom{m}{l}[\mathrm{ad}^l(f_1)E^{[k_1]}, \mathrm{ad}^{n-l-1}(f_1)E^{[k_2]}]\tau^{n-2}\,d\tau \end{aligned}$$

$$
\begin{aligned}
&+ \sum_{n\geq 2} b_n \int_0^t \sum_{m=0}^{n-1} \sum_{l=0}^{m} \binom{m}{l} [\mathrm{ad}^{n-l-1}(f_1)E^{[k_1]}, \mathrm{ad}^l(f_1)E^{[k_2]}]\tau^{n-2}\, d\tau \\
&- \sum_{n\geq 1} b_n \int_0^t \mathrm{ad}^n(f_1)E^{[k_1,k_2]}\tau^{n-1}\, d\tau
\end{aligned}
$$

By introducing the generating function $\mathcal{E}^{[k_1,k_2]}(x_1\tau, x_2\tau)$ this relation can be written in the form

$$
\begin{aligned}
\mathcal{E}^{[k_1,k_2]}(x_1\tau, x_2\tau) &= \frac{1}{x_1}\int_0^t \left(\frac{x_1+x_2}{e^{t(x_1+x_2)}-1} - \frac{x_2}{e^{\tau x_2}-1}\right)\tau^{k_2-1}\mathcal{E}^{[k_1]}(x_1\tau)\, d\tau \\
&- \frac{1}{x_2}\int_0^t \left(\frac{x_1+x_2}{e^{t(x_1+x_2)}-1} - \frac{x_1}{e^{\tau x_1}-1}\right)\tau^{k_1-1}\mathcal{E}^{[k_2]}(x_2\tau)\, d\tau \\
&+ \frac{1}{x_1}\int_0^t \left(\frac{x_2}{e^{\tau x_2}-1} - \frac{x_1+x_2}{e^{\tau(x_1+x_2)}-1}\right)\tau^{-1}\mathcal{E}^{[k_1]}(x_1\tau)\mathcal{E}^{[k_2]}(x_2\tau)\, d\tau \\
&+ \frac{1}{x_2}\int_0^t \left(\frac{x_1}{e^{\tau x_1}-1} - \frac{x_1+x_2}{e^{\tau(x_1+x_2)}-1}\right)\tau^{-1}\mathcal{E}^{[k_1]}(x_1\tau)\mathcal{E}^{[k_2]}(x_2\tau)\, d\tau \\
&+ \int_0^t \left(\frac{\tau(x_1+x_2)}{e^{\tau(x_1+x_2)}-1} - 1\right)\tau^{-1}\mathcal{E}^{[k_1,k_2]}(x_1\tau, x_2\tau)\, d\tau.
\end{aligned}
$$

□

A general solution to the integral relation in Lemma 9 has proven difficult to find. If we instead focus on particular sub-expansions like e.g.

$$
\sum_{n\geq 0} c_{n,m}[\mathrm{ad}^n(f_1)f_{k_1}, \mathrm{ad}^m(f_1)f_{k_2}],
$$

the generating function becomes $\frac{1}{m!}(\frac{d}{dx_2})^m\mathcal{E}^{[k_1,k_2]}(x_1,x_2)|_{x_2=0}$. As an example we wish to find the generating function $\mathcal{E}'$ for the series $E' = \sum_{n\geq 0} c_{n,m}[\mathrm{ad}^n(f_1)f_{k_1}, f_{k_2}]$. From our definition of the generating functions we know that $\mathcal{E}^{[k_2]}(0) = 0$, hence we find, using Lemma 9 that

$$
\begin{aligned}
\mathcal{E}'(tx_1) &= \frac{1}{x_1}\int_0^t \left(\frac{\tau x_1}{e^{tx_1}-1} - 1\right)\tau^{k_2-1}\mathcal{E}^{[k_1]}(x_1\tau)\, d\tau \\
&+ \int_0^t \left(\frac{\tau x_1}{e^{\tau x_1}-1} - 1\right)\tau^{-1}\mathcal{E}'(x_1\tau)\, d\tau.
\end{aligned}
$$

Without proceeding any further we believe that the expressions for the solution will be of a complicated nature, and numerical methods based on them will mainly be of theoretical interest.

Numerical examples

In the following section we display a number of numerical experiments. The order of convergence in the eigenvalues is shown to be in accordance with theory. Some evidence of the asymptotic behaviour of the error is also presented. We study the *relative error* defined as $\epsilon_{\rm rel}$=(exact solution − approximation)/exact solution. The exact solution is computed with the eighth-order method to machine precession.

The Mathieu equation

We look at the potential $q(x) = 2k\cos(2kx)$ on $[0,\pi]$, with boundary values $y(0) = y(\pi) = 0$. By solving for the first, fifth and fifteenth eigenvalues when $k = 5, 15$ and 25 we give experimental evidence of order of convergence in the eigenvalues. Using the non-modified sixth-order method with N =16, 64 and 256 steps, we derive the results in Table 1.

λ ($k=5$):	-5.79008	25.5108	225.055
N=16	3.73e-07	8.56e-06	9.87e-04
64	8.96e-11	2.06e-09	2.23e-09
256	3.96e-14	4.99e-13	5.39e-13
λ ($k=15$):	-22.5130	27.9679	225.503
N=16	1.47e-06	7.78e-05	1.90e-03
64	3.35e-10	1.86e-08	2.00e-08
256	9.15e-14	4.53e-12	4.84e-12
λ ($k=25$):	-40.2568	28.0628	226.401
N=16	2.59e-06	2.73e-04	1.97e-04
64	5.69e-10	6.51e-08	5.53e-08
256	1.46e-13	1.58e-11	1.33e-11

Table 1: Relative errors in eigenvalues for sixth-order non-modified method applied to the Mathieu problem

We observe from Table 1 and Table 2 that the methods display the expected order of convergence. However the improved accuracy observed in Pruess methods for large eigenvalues is not seen. To the contrary, we note a moderate deterioration for increasing eigenvalues.

A second test example

This example is supposed to highlight the effect of the modification of the standard truncated Magnus expansion. We compute five eigenvalues for the potential $q(x) = 1/(1/10+x)^2$ for $x \in (0,\pi)$. $y(0) = 0$, $y(\pi) = 0$

The italics in the table indicate when the modified method has smaller error than the non-modified method. As we can see in the tables the modified methods have higher accuracy for large eigenvalues, but the errors for small eigenvalues are not significantly changed. As a matter of fact, the modified method does not perform as well as the unmodified method for small eigenvalues.

λ $(k=5)$:	-5.79008	25.5108	225.055
N=16	2.64e-08	1.14e-06	8.69e-04
64	4.40e-13	1.67e-11	1.63e-10
256	1.72e-14	-4.32e-15	1.77e-15
λ $(k=15)$:	-22.5130	27.9679	225.503
N=16	2.26e-07	1.36e-05	1.65e-03
64	3.67e-12	1.95e-10	1.47e-09
256	1.03e-14	-1.14e-14	2.04e-14
λ $(k=25)$:	-40.2568	28.0628	226.401
N=16	5.68e-07	6.25e-05	-3.80e-07
64	9.31e-12	8.70e-10	4.08e-09
256	8.29e-15	-1.536e-14	5.77e-14

Table 2: Relative errors in eigenvalues for eighth-order non-modified method applied to the Mathieu problem

λ :	1.51986	17.5599	171.613	1298.99	12324.1
Points			modified		
N=16	1.7417e-04	5.1222e-04	*-9.0780e-04*	*3.4118e-05*	*5.2909e-06*
N=32	3.4484e-06	1.1525e-05	1.0648e-05	*-4.2456e-05*	*6.6391e-07*
N=64	6.3972e-08	1.8793e-07	2.7081e-07	*-4.7203e-08*	*-1.1332e-07*
N=128	8.2206e-10	2.9039e-09	4.4224e-09	*2.3592e-09*	*-2.8663e-08*
Points			standard		
N=16	1.1591e-04	4.6925e-04	-1.8217e-03	-1.6271e-04	-5.5648e-03
N=32	1.6890e-06	8.4167e-06	4.8049e-07	8.4672e-05	1.4955e-04
N=64	1.8681e-08	1.0958e-07	2.3973e-07	-6.4948e-06	1.6595e-05
N=128	2.2723e-10	1.4904e-09	4.2832e-09	-6.5819e-08	-2.4166e-06

Table 3: Relative errors in eigenvalues for sixth-order methods for second test example where italics indicate when modified method gives lower error.

λ :	1.51986	17.5599	171.613	1298.99	12324.1
Points			modified		
N=16	-1.5897e-05	-2.0439e-05	*-7.5603e-04*	*5.1251e-04*	*-1.0278e-04*
N=32	-2.0061e-07	-4.8103e-07	*-2.0412e-06*	*1.3067e-06*	*3.4283e-05*
N=64	*5.6632e-11*	-4.2660e-09	*-9.5619e-09*	*-3.6015e-07*	*7.5661e-07*
N=128	-2.7433e-11	-2.2750e-11	*-5.2578e-11*	*-1.1475e-09*	*-4.9335e-08*
Points			standard		
N=16	-1.1196e-05	-1.9650e-05	-1.2804e-03	-1.6276e-02	-1.4862e-03
N=32	-1.3237e-07	-4.0109e-07	-2.9561e-06	8.8018e-05	-5.7363e-03
N=64	-9.6014e-10	-3.4458e-09	-1.1111e-08	-2.1716e-06	5.0893e-05
N=128	-4.8356e-12	-1.8213e-11	-5.8908e-11	-6.0729e-09	-1.8087e-06

Table 4: Relative errors in eigenvalues for eighth-order methods for second test example where italics indicate when modified method gives lower error.

The Airy problem

We consider the eigenvalue problem

$$-y'' + xy = \lambda y, \quad x \in [0, 1],$$

with the boundary condition $y(0) = y(1) = 0$. This problem is special in that $f_k = 0$ for $k > 2$, hence the exact solution can be represented by the discrete Magnus series as

$$\sigma = f_1 + E^{[2]} + E^{[2,2]} + E^{[2,2,2]} + \cdots.$$

By solving the problem for a the 50 first positive eigenvalues (i.e. in the range $(3.16, \approx 20433)$) we can see, by plotting, how the error depends on the size of the eigenvalue for the modified and non-modified methods (the eighth-order and sixth-order methods will in this case give the same result as the fourth-order method since $f_3 = f_4 = 0$). We ran the experiment with $N = 16$ and $N = 32$ steps to monitor how the difference in $h = 1/N$ influences the errors.

We see from the plots that the modified method has an error three orders of magnitude less than the non-modified method. It is also interesting to see that the modified method has an error wich is strictly positive, a feature which might turn out significant in deriving good bounds on the error. We also see from the graphs how the singularity shifts to the right as $\mathcal{O}(1/h^2)$ when decreasing the step size h. A last, yet unexplained, feature of the results is the conservation of accuracy past the singularity at $4h(z_1 - h\lambda) = 2\pi$, which corresponds to using the Magnus expansion outside the region of convergence.

Conclusions and further development

We have demonstrated in this paper that Magnus expansions are a highly-promising technique to approximate eigenvalues of Schrödinger problems, giving an efficient approximation to a range of eigenvalues and eigen functions. Numerical and analytical

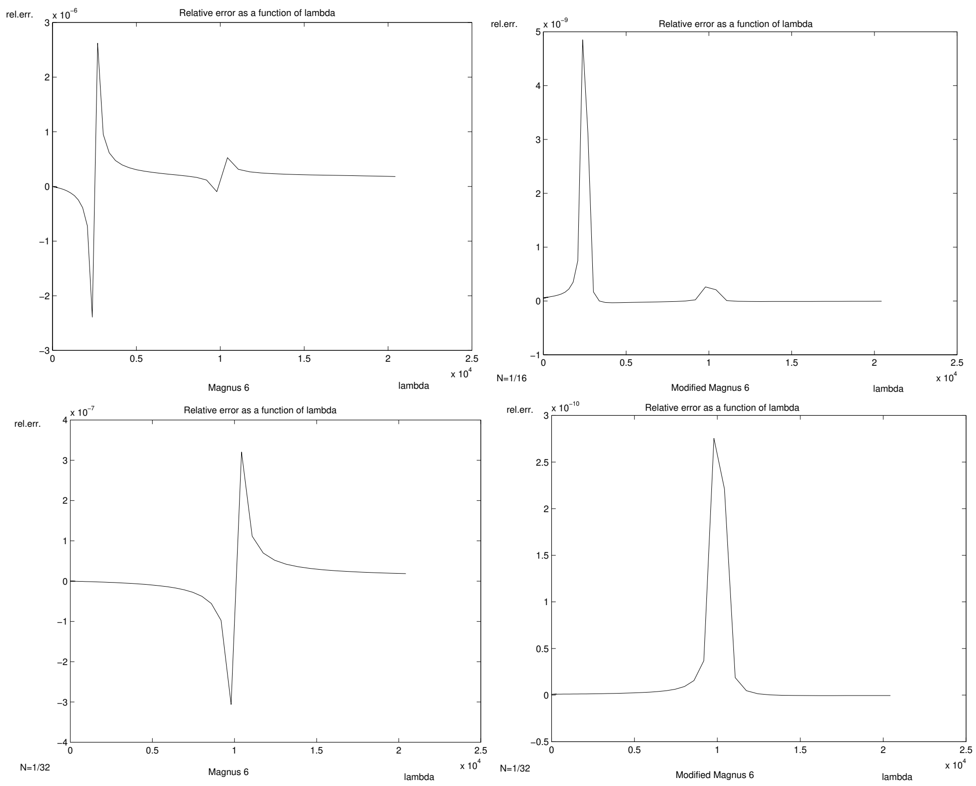

Figure 1: We number the graphs clockwise 1,2,3 and 4. Graph 1 shows the relative error in the eigenvalues with $N = 16$ for the non-modified method, graph 2 the same for the modified method. Graph 3 shows the relative error for $N = 32$ with the non-modified method and graph 4 shows the errors for the modified method.

results have shown that the accuracy degrades with increasing eigenvalues, a problem which has been addressed. Modifying the discrete Magnus expansions by correction functions, the precision of the methods has been improved, making them accurate for larger ranges of eigenvalues. The methods we have considered here are methods which represent the fundamental matrix by so called coordinates of the first kind.

While the Magnus expansion represents one alternative to approximating the solution of differential equations, several other approaches are possible in our framework of Lie groups and algebras. The complexity of the asymptotic corrections to the Magnus expansions clearly neccesitates alternative approaches, and of particular interest are expansions where the singularities of Magnus expansions are avoided altogether.

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