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by

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Data-Sparse Approximation of a Class of Operator-Valued Functions

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Abstract

In the papers [4]-[7] a method for the data-sparse approximation of the solution operators for elliptic, parabolic and hyperbolic PDEs has been developed based on the Dunford-Cauchy representation to the operator-valued functions of interest combined with the hierarchical matrix approximation of the operator resolvents. In the present paper, we discuss how these techniques can be applied to approximate a hierarchy of the operator-valued functions generated by an elliptic operator $\mathcal{L}$.

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1 Introduction

In the papers [11]-[14] and [9], a class of hierarchical matrices ($\mathcal{H}$-matrices) has been analysed which are data-sparse and allow an approximate matrix arithmetic with almost linear complexity.

In the present paper, we apply the $\mathcal{H}$-matrix technique to approximate different classes of mappings generated by integrals of functions of an elliptic operator $\mathcal{L}$. These mappings are of the form function-to-operator, operator-to-operator or sequence of operator-to-operator.

As examples of *function-to-operator mappings* we consider the solution operators to parabolic PDEs (the operator exponential), to elliptic PDEs (the normalised hyperbolic sine function) and to hyperbolic PDEs (the operator cosine function), where these operators are represented by the Dunford-Cauchy integral (cf. [4]-[7]). The latter representation together with a proper quadrature formula (Sinc quadrature or Gauss-Lobatto quadrature) and an $\mathcal{H}$-matrix representation of the resolvents leads to a data-sparse representation to the solution operators of interest. A short version of this paper was published in [7].

As an example of an *operator-to-operator mapping* we consider the solution operator to the Lyapunov equation. We use two integral representations of the solution operator, namely (i) by a double Dunford-Cauchy integral and (ii) by an improper integral with the operator exponential. The proper exponentially convergent quadrature formulae and the $\mathcal{H}$-matrix approximations to the elliptic resolvents or to the operator exponential lead to data-sparse approximations where the overall cost is of linear-logarithmic complexity.

As an example of a *sequence of operators-to-operator mapping* we discuss the solution operator to the Riccati equation by an iterative scheme involving the solution of Lyapunov-Sylvester equations in each step. Together with data-sparse approximations to these solutions, we arrive at algorithms of almost linear complexity.

Note that the data-sparse $\mathcal{H}$-matrix approximation of almost optimal complexity to the following operator-valued functions

$$\begin{aligned}
\mathcal{F}_1(\mathcal{L}) &:= e^{-t\mathcal{L}}, \\
\mathcal{F}_2(\mathcal{L}) &:= \mathcal{L}^{-\alpha},\ \alpha > 1, \\
\mathcal{F}_{3,k}(\mathcal{L}) &:= \cos(t\sqrt{\mathcal{L}})\mathcal{L}^{-k}, \qquad k \in \mathbb{N}, \\
\mathcal{F}_4(\mathcal{L}) &:= \int_0^\infty e^{t\mathcal{L}^*} G e^{t\mathcal{L}} dt,
\end{aligned} \tag{1.1}$$

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of an elliptic operator $\mathcal{L}$ was addressed in [6] (see §3 for more details). In this paper we derive a new quadrature rule for the operator $\mathcal{F}_4(\mathcal{L})$ which is more efficient than the previous one from [4, 6]. The method is now based on a double integral representation to the solution operator for equations with the general family of so-called elementary operators (cf. [26]).

In §§3.1-3.2 we are looking for a data-sparse approximation of the solution $X \in \mathcal{A}$ to the operator equation

$$SX := \sum_{j=1}^{M} U_j X V_j = Y$$

for certain operators U_j, V_j.

Finally (see §4), we construct an explicit approximation by resolvents to the operator sign-function which can be applied, for example, to represent the solution operator of the algebraic Riccati equation.

2 Goals and Overview

2.1 Hierarchy of the Operator-Valued Functions

In this section we define a hierarchy of operator-valued functions which can be represented by various mappings generated by an elliptic operator $\mathcal{L}$ in a Banach space X. In the following, we will develop various discretisations to these mappings. The hierarchy of operator-valued functions consists of function-to-operator mappings, operator-to-operator and sequence of operators-to-operator mappings which arise in applications related to partial differential equations, control theory and linear algebra.

One basic function of an elliptic operator $\mathcal{L}$ is the inverse $\mathcal{L}^{-1}$. A fast implementation of $\mathcal{L} \mapsto \mathcal{L}^{-1}$ is of interest in finite element methods for elliptic and parabolic problems. On the other hand, the data-sparse approximation of $\mathcal{L}^{-1}$ plays a central role in our further constructions. However, this topic is already addressed in [11, 12, 13, 9], where the modern $\mathcal{H}$-matrix approximation technique has been presented.

2.1.1 Functions of the First Level

Let $\Gamma_S \subset \mathbb{C}$ denote a path enveloping the spectrum of $\mathcal{L}$ and Γ_I be a path which envelopes but does not intersect Γ_S. For a given function which is analytic inside of Γ_I (the subscript I abbreviates "integration"). Below, we write Γ instead of Γ_I. We can define a bounded operator

$$F(\mathcal{L}) = \frac{1}{2\pi i} \int_\Gamma F(z)(zI - \mathcal{L})^{-1} dz$$

provided that this Dunford-Cauchy integral converges. The above integral defines a *function-to-operator mapping* $F(\cdot) \to F(\mathcal{L})$ generated by a fixed elliptic operator $\mathcal{L}$.

As a *first example* of such a mapping we consider the solution operator

$$T(t) = e^{-\mathcal{L}t} = \int_\Gamma e^{-zt}(zI - \mathcal{L})^{-1} dz$$

to the initial value problem

$$u'(t) + \mathcal{L}u(t) = 0, \quad u(0) = u_0, \tag{2.1}$$

where $\mathcal{L}$ is a strongly P-positive operator in a Banach space X and $u(t)$ is a vector-valued function $u : \mathbb{R}_+ \to X$ (see [4] for more details). Given the solution operator and the initial vector u_0, the solution of the initial value problem can be represented by $u(t) = T(t)u_0$. As a simple example of a partial differential equation which can be described by (2.1), one can consider the classical heat equation

$$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = 0$$

with corresponding boundary and initial conditions, where the operator $\mathcal{L}$ is defined by

$$D(\mathcal{L}) = \{v \in H^2(0,1) : \ v(0) = 0, v(1) = 0\},$$
$$\mathcal{L}v = -\frac{d^2 v}{dx^2} \qquad \text{for all } v \in D(\mathcal{L}).$$

Our *second example* deals with the boundary value problem

$$\frac{d^2u}{dx^2} - \mathcal{L}u = 0, \qquad u(0) = 0, \quad u(1) = u_1, \tag{2.2}$$

in a Banach space X (see [5]). The solution operator is the normalised hyperbolic operator sine family

$$E(x) \equiv E(x;\mathcal{L}) = \left(\sinh(\sqrt{\mathcal{L}})\right)^{-1} \sinh(x\sqrt{\mathcal{L}}),$$

so that $u(x) = E(x)u_1$. This function $E(x)$ is the result of the function-to-operator mapping

$$\left(\sinh(\sqrt{\cdot})\right)^{-1} \sinh(x\sqrt{\cdot}) \rightarrow E(x;\mathcal{L})$$

generated by the operator $\mathcal{L}$. The simplest PDE from the class (2.2) is the Laplace equation in a cylindric domain:

$$\begin{aligned} \frac{d^2u}{dx^2} + \frac{d^2u}{dy^2} &= 0, \qquad x \in [0,1],\ y \in [c,d], \\ u(0,y) &= 0, \qquad u(1,y) = u_1(y). \end{aligned}$$

In the *third example* we consider the following initial-value problem for the second order differential equation with an operator coefficient:

$$u''(t) + \mathcal{L}u(t) = 0, \qquad u(0) = u_0, \quad u'(0) = 0,$$

with the solution operator (the operator cosine family)

$$C(t;\mathcal{L}) = \cos(t\sqrt{\mathcal{L}}) = \int_\Gamma \cos(t\sqrt{z})(zI - \mathcal{L})^{-1} dz,$$

which represents the function-to-operator mapping $\cos\left(t\sqrt{\cdot}\right) \rightarrow C(t;\mathcal{L})$ (see [6] for more details). The simplest example of PDEs from this class is the classical wave equation

$$\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = 0$$

subject to the corresponding boundary and initial conditions.

2.1.2 Functions of the Second Level

The next hierarchy level is formed by the *operators-to-operator mappings*. Let $\{\mathcal{G}_0(t) : t \in [t_0, t_1]\}$ be an operator family in X and let the integral

$$\mathcal{F} = \int_{t_0}^{t_1} \mathcal{G}_0(t) dt$$

exist, then this integral represents an operators-to-operator mapping $\mathcal{G}_0 \mapsto \mathcal{F}$. As an example we consider the *Sylvester equation*

$$AX + XB = G, \qquad (A, B, G \text{ given})$$

with the solution X given by the integral over $\mathcal{G}_0(t) := e^{-tA}Ge^{-tB}$,

$$\mathcal{F}(G; A, B) = \int_0^\infty e^{-tA}Ge^{-tB} dt,$$

where we suppose that A, B are such that this integral exists. A particular case is the *Lyapunov equation*

$$\mathcal{L}X + X\mathcal{L}^* = G$$

with the solution

$$\mathcal{F}(G;\mathcal{L}) = \int_0^\infty e^{-t\mathcal{L}^*}Ge^{-t\mathcal{L}} dt$$

generated by an (elliptic) operator $\mathcal{L}$.

2.1.3 Functions of the Third Level

On the next hierarchy level, one can consider a sequence of operators-to-operator mappings which arises for example in the case of the (nonlinear) *Riccati equation*

$$AX + XA^\top + XFX = G, \tag{2.3}$$

where $A, F, G \in \mathbb{R}^{n\times n}$ are given and $X \in \mathbb{R}^{n\times n}$ is the unknown matrix. This equation is of fundamental importance in many applications in control theory. There are numerous methods to solve (2.3) (see, e.g., [10] and the literature therein) and one of the best is based on the matrix function $\mathrm{sign}(H)$. An alternative method is based on Newton's iteration. At each iteration step the Lyapunov equation

$$(A - FX_n)X_{n+1} + X_{n+1}(A - FX_n)^\top = -X_nFX_n + G := G_n$$

has to be solved. Assuming the convergence $X_n \to X$, we have the sequence of operators-to-operator mapping

$$X_n \to X_{n+1} \to \ldots \to X := \mathcal{F}(F, G, A)$$

of the kind

$$X = \lim_{n\to\infty} X_n, \qquad X_{n+1} := \int_0^\infty e^{-t(A-FX_n)} G_n e^{-t(A-FX_n)^\top} dt.$$

Under usual assumptions on the data, the Newton method converges quadratically.

We discuss in more details an algorithm based on the application of the *matrix* sign-*function*, which can be defined by

$$\mathrm{sign}(H) = \frac{1}{\pi i}\int_{\Gamma_I} (zI - H)^{-1} dz - I \tag{2.4}$$

with Γ_I being any simply closed curve in the complex plane whose interior contains all eigenvalues of H with positive real part. We require that H has no eigenvalues on the imaginary axis.

An equivalent definition uses the canonical Jordan decomposition $H = YJY^{-1}$ of H. Let the diagonal part of J be given by the matrix $D = \mathrm{diag}(d_1, ..., d_n)$. Set $S = \mathrm{diag}(s_1, ..., s_n)$ with $s_i = \left\{\begin{array}{ll} +1 & \text{if } \Re e(d_i) > 0 \\ -1 & \text{if } \Re e(d_i) < 0 \end{array}\right\}$. Then we define $\mathrm{sign}(H) = YSY^{-1}$.

The following algorithm gives the solution to the Riccati equation by means of the sign function:

1. For $H = \begin{pmatrix} A & M \\ R & -A^\top \end{pmatrix}$ determine $\begin{pmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{pmatrix} := \mathrm{sign}(H)$.
2. Find X as the solution of the minimisation problem (say, by the least squares method)

$$\min \left\| \begin{pmatrix} W_{12} \\ W_{22} + I \end{pmatrix} X - \begin{pmatrix} I + W_{11} \\ W_{21} \end{pmatrix} \right\|.$$

In §4 we propose some exponentially convergent quadrature formulae for the Dunford-Cauchy integral in (2.4) which is built by a sum of resolvents $(z_kI - H)^{-1}$. In this way, the data-sparse solution to the Riccati equation can be based on the $\mathcal{H}$-matrix approximation of the inversion operator.

2.2 Towards Approximations of Optimal Complexity

For the numerical treatment, the operator $\mathcal{F}$ of interest has to be approximated by $n \times n$ matrices. In our approach, we are looking for a family of data-sparse matrices (more specifically, $\mathcal{H}$-matrices) $M_i \in \mathbb{R}^{n\times n}$, such that (with a proper projection $\mathcal{P}_n : X \to \mathbb{R}^n$) the error satisfies the estimate

$$\phi(N) := \|\mathcal{P}_n\mathcal{F}\mathcal{P}_n^* - \sum_{i=1}^N M_i^{-1}\| \le \varepsilon$$

in the corresponding operator norm. The parameter $n \in \mathbb{N}$ can be viewed as $n = \dim(V_h)$, where V_h is used for the Galerkin approximation of the related elliptic PDE with a given tolerance.

We require that the class of matrices approximating the operator-valued function allows an almost linear cost estimate by $\mathcal{O}(n \log^q n)$ for the approximate matrix arithmetic and the memory. Clearly, the inversion of a *general* $n \times n$-matrix has a complexity of at least $\mathcal{O}(n^2)$. Here, however, we consider the class of matrices arising from FEM and BEM applications. Then the new concept of data-sparse approximations can be applied based on so-called hierarchical matrices ($\mathcal{H}$-matrices) [11, 12, 13, 9]. The almost linear complexity of the $\mathcal{H}$-matrix arithmetic yields a cost of $\sum M_i^{-1}$ bounded by $\mathcal{O}(Nn\log^q n)$ arithmetic operations.

Due to n-width arguments for analytic functions (see, e.g., [1] and references therein), we need $\mathcal{O}(\log 1/\varepsilon)$ parameters for their ε-approximation (say, by polynomials or Sinc-functions). In order to get a polynomial operation count with respect to $\log 1/\varepsilon$, we would like to ensure that $N = \mathcal{O}(\log^q 1/\varepsilon)$, i.e., $\phi(N)$ must be exponential in N (e.g., $\phi(N) \le c\exp(-\gamma N^\alpha)$, $\alpha, \gamma > 0$). In our applications we approximate the *analytic function* $\mathcal{F} = \mathcal{F}(\mathcal{L})$ for an elliptic operator $\mathcal{L}$ by a sum $\sum_{i=1}^N c_i(z_i I - \mathcal{L})^{-1}$ of N elliptic resolvents, such that the sum converges exponentially, i.e., $N = \mathcal{O}(\log^q 1/\varepsilon)$. Furthermore, in conventional FEM, the operator $\mathcal{L}$ itself can be approximated by a sparse $n \times n$ stiffness matrix $\mathcal{L}_h$ with $\mathcal{O}(n)$ non-zero entries, which leads to the $\mathcal{H}$-matrix inverse $(z_i I - \mathcal{L}_h)^{-1}$ with arithmetical costs of $\mathcal{O}(n\log^p n)$. Therefore, our final complexity bound for the approximation ansatz $\sum M_i^{-1}$ leads to $\mathcal{O}(n\log^q(1/\varepsilon)\log^p n)$ arithmetical operations.

In the present paper, our goals are the following ones:

- Representation of the mentioned operator-valued functions by an exponentially converging sum of elliptic resolvents.
- Construction of well parallelisable algorithms with almost linear complexity
- Discussion of some applications (PDEs, control problems).

2.3 Integral Representation to Operators of (f_S, f_R)-Type

Let $A : X \to X$ be a linear densely defined closed operator in X with the spectral set $sp(A)$. In this paper, we restrict ourselves to the class of (f_S, f_R)-type operators which will be defined below. Let Γ_S be a curve in the complex plane $z = \xi + i\eta$ defined by the equation $\xi = f_S(\eta)$ in the coordinates ξ, η. We denote by

$$\Omega_{\Gamma_S} := \{z = \xi + i\eta : \xi > f_S(\eta)\} \tag{2.5}$$

the domain inside of Γ_S. In what follows, we suppose that this curve lies in the right half-plane of the complex plane and contains $sp(A)$, i.e., $sp(A) \subset \Omega_{\Gamma_S}$.

The form of the curve enveloping the spectrum of A and the behaviour of the resolvent as a function of z contain important information about the operator A and allow to develop a calculus of functions of A (cf. [3, 4, 5, 6, 8]).

Definition 2.1 *Given an operator $A : X \to X$, let $f_S(\cdot)$ and $f_R(\cdot)$ be functions such that*

$$\|(zI - A)^{-1}\|_{X \to X} \le f_R(z) \qquad \text{for all } z \in \mathbb{C} \backslash \Omega_{\Gamma_S}.$$

Note that Γ_S is defined by means of f_S (cf. (2.5)). Then we say that the operator $A : X \to X$ is of (f_S, f_R)-type.

Note that a strongly P-positive operator (defined in [3]) is also an operator of (f_S, f_R)-type with the special choice

$$f_S(\eta) = a\eta^2 + \gamma_0, \quad f_R(z) = M/(1 + \sqrt{|z|}), \quad a > 0,\ \gamma_0 > 0,\ M > 0.$$

In order to get exponentially convergent discretisations, we are interested in operators of (f_S, f_R)-type with an exponentially increasing function f_S. Let $\mathcal{L}$ be a linear, densely defined, closed operator of (f_S, f_R)-type in a Banach space X. We choose an *integration curve* $\Gamma_I := \{z = f_I(\eta) + i\eta\}$ enveloping the so-called "spectral curve" $\xi = f_S(\eta)$ (see Figure 2.1). Let $F(z)$ be an complex-valued function that is analytic inside of the integration curve Γ_I. The next simple theorem offers conditions under which one can define a bounded operator $F(\mathcal{L})$. Its proof is given in [6].

Theorem 2.2 *Let $\xi = f_I(\eta)$ be an even function and assume that the improper integral*

$$\int_{-\infty}^{\infty} |\Phi_1(\eta)| f_R(f_I(\eta) - i\eta)d\eta \qquad \text{with } \Phi_1(\eta) = F(f_I(\eta) - i\eta)\,[f_I'(\eta) - i]$$

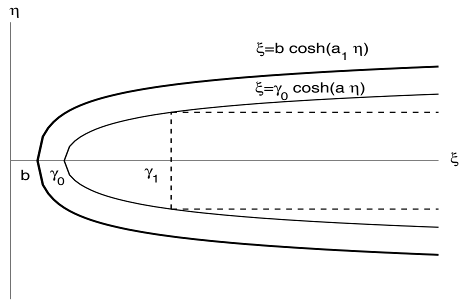

Figure 2.1: The spectral curve Γ_S and the integration curve Γ_I.

converges. Then the Dunford-Cauchy integral

$$F(\mathcal{L}) = \frac{1}{2\pi i}\int_{\Gamma_I} F(z)(zI - \mathcal{L})^{-1}dz = -\frac{1}{2\pi i}\int_{-\infty}^{\infty} \Phi_1(\eta)[(f_I(\eta) - i\eta)I - \mathcal{L}]^{-1}d\eta$$

defines a bounded operator $F(\mathcal{L})$.

We further consider examples of quadrature rules applied to the integrals in Theorem 2.2. Our particular application is concerned with the operator exponential $\mathcal{F}_1(\mathcal{L})$, and with the solution operator $\mathcal{F}_4(\mathcal{L})$ (see (1.1)) to the Lyapunov equation arising in control theory.

2.4 Representation of the Operator Exponential by Resolvents

2.4.1 Dunford-Cauchy Integral

In this section we briefly recall the results from [6]. Let $\mathcal{L}$ be a linear elliptic operator of (f_S, f_R)-type, where

$$f_S(\eta) = \gamma_0 \cosh(a\eta) \text{ with } \gamma_0 > 0, \quad f_R(z) = 1/|\Im m\, z| \text{ if } \Re e\, z > \gamma_0. \tag{2.6}$$

The function $f_S(\eta)$ defines the so-called spectral curve

$$\Gamma_S = \{z = \xi + i\eta : \xi = \gamma_0 \cosh(a\eta)\} \tag{2.7}$$

containing the spectrum $sp(\mathcal{L})$ of the operator $\mathcal{L}$.

Definition 2.3 *The class of (f_S, f_R)-type operators specified by f_S, f_R from (2.6) is denoted by $\mathbf{E}_{S,R}$.*

For the sake of simplicity, in what follows, we consider operators with real spectra bounded from below by $\gamma_0 > 0$ (cf. (2.6)). We use the infinite strip

$$D_d := \{z \in \mathbb{C} : \ -\infty < \Re e\, z < \infty, \ |\Im m\, z| < d\} \tag{2.8}$$

as well as the finite rectangles $D_d(\epsilon)$ defined for $0 < \epsilon < 1$ by

$$D_d(\epsilon) = \{z \in \mathbb{C} : \ |\Re e\, z| < 1/\epsilon, \ |\Im m\, z| < d(1-\epsilon)\}.$$

For $1 \le p \le \infty$, introduce the space $\mathbf{H}^p(D_d)$ of all operator-valued functions which are analytic in D_d, such that for each $\mathcal{F} \in \mathbf{H}^p(D_d)$ there holds $\|\mathcal{F}\|_{\mathbf{H}^p(D_d)} < \infty$ with

$$\|\mathcal{F}\|_{\mathbf{H}^p(D_d)} := \begin{cases} \lim_{\epsilon\to 0}\left(\int_{\partial D_d(\epsilon)} \|\mathcal{F}(z)\|^p |dz|\right)^{1/p} & \text{if } 1 \le p < \infty, \\ \lim_{\epsilon\to 0} \sup_{z\in D_d(\epsilon)} \|\mathcal{F}(z)\| & \text{if } p = \infty. \end{cases}$$

Next, we consider an integral representation of $e^{-t\mathcal{L}}$ with $\mathcal{L} \in \mathbf{E}_{S,R}$, where the integrand is proved to be in the class $\mathbf{H}^p(D_d)$. The proof of the lemma is given in [6].

Lemma 2.4 *Let $\mathcal{L}$ be an operator of the class $\mathbf{E}_{S,R}$. Choose the (integration) curve $\Gamma_I = \{z = \xi + i\eta : \xi = b\cosh(a_1\eta)\}$ with $a_1 < a,\ b \in (0, \gamma_0)$. Then the operator exponential $I(t;\mathcal{L}) = e^{-t\mathcal{L}}$ can be represented by the Dunford-Cauchy integral*

$$I(t;\mathcal{L}) = \frac{1}{2\pi i}\int_{\Gamma_I} e^{-zt}(zI - \mathcal{L})^{-1}dz = -\frac{1}{2\pi i}\int_{-\infty}^{\infty} F_1(\eta, t)d\eta, \tag{2.9}$$

where the integrand

$$F_1(\eta, t) = e^{-zt}(ba_1\cosh(a_1\eta) + i)(zI - \mathcal{L})^{-1} \quad \text{with } z = b\cosh(a_1\eta) + i\eta,\ \eta \in \mathbb{R}, \tag{2.10}$$

can be estimated on the real axis by

$$\|F_1(\eta, t)\| \lesssim ba_1(1 + |\eta|)^{-1}e^{a_1|\eta| - bt\cosh(a_1\eta)} \quad \text{for } \eta \in \mathbb{R}.$$

Moreover, $F_1(\cdot, t)$ can be extended analytically into the strip D_d of the width $d > 0$ and belongs to the class $\mathbf{H}^p(D_d)$ for all $p \in [1, \infty]$.

2.4.2 Sinc-Quadrature Applied to the Exponential

Following [28, 8, 6], we construct a quadrature rule for the integral in (2.9) by using the Sinc approximation. Given $f \in \mathbf{H}^p(D_d), h > 0$, and $N \in \mathbb{N}$, we use the notations

$$I(f) = \int_{\mathbb{R}} f(\xi)d\xi, \tag{2.11}$$

$$T(f, h) = h\sum_{k=-\infty}^{\infty} f(kh), \qquad T_N(f, h) = h\sum_{k=-N}^{N} f(kh), \tag{2.12}$$

$$\eta(f, h) = I(f) - T(f, h), \qquad \eta_N(f, h) = I(f) - T_N(f, h)$$

(I: integral; T: trapezoidal rule, η, η_N: quadrature errors). Further, we need the notation of one-sided limits:

$$f(\xi \pm id^-) = \lim_{\delta \to d; \delta < d} f(\xi \pm i\delta) \qquad \text{for } \xi, d \in \mathbb{R}.$$

The following approximation result for functions from $\mathbf{H}^1(D_d)$ describes the accuracy of $T_N(f, h)$. The proof of Lemma 2.5 can be found again in [6].

Lemma 2.5 *For any operator valued function $f \in \mathbf{H}^1(D_d)$ satisfying the condition*

$$\|f(\xi)\| < c(1 + |\xi|)^{-1}\exp(a|\xi| - be^{a|\xi|}), \qquad a, b, c > 0,$$

for all $\xi \in \mathbb{R}$, there holds

$$\|\eta_N(f, h)\| \le \frac{2c}{ab}\left[\frac{e^{-b}e^{-2\pi d/h}}{1 - e^{-2\pi d/h}} + \frac{2}{1 + Nh}\exp(-be^{ahN})\right] \tag{2.13}$$

with the constant d from $\mathbf{H}^1(D_d)$.

The operator exponential $I(t;\mathcal{L}) = e^{-t\mathcal{L}}$ is represented as integral according to Lemma 2.4. Applying the quadrature rule T_N to the operator valued function $f(\eta) := -\frac{1}{2\pi i}F_1(\eta, t)$, where $F_1(\eta, t)$ is given by (2.10), we obtain for the operator family $\{I(t) \equiv I(t;\mathcal{L}) : t > 0\}$ (cf. (2.11)) that

$$I(t) \approx T_N(t) \equiv T_N(f, h) = -\frac{h}{2\pi i}\sum_{k=-N}^{N} F_1(kh, t). \tag{2.14}$$

The error analysis is given by the following theorem.

Theorem 2.6 *Given the spectral curve Γ_S from (2.7) associated with $f_S(\eta) = \gamma_0 \cosh(a\eta)$, choose the integration curve $\{z = f_I(\eta) + i\eta : \eta \in \mathbb{R}\}$ with $f_I(\eta) := b\cosh(a_1\eta)$, $b \in (0,\gamma_0)$, $a_1 < a\}$ and set $h = \frac{\log N}{a_1 N}$. Then*

$$\|I(t) - T_N(t)\| \lesssim \frac{1}{t}\left(e^{-bt-2\pi dN/\log N} + \frac{e^{-btN}}{1+(\log N)/a_1}\right). \tag{2.15}$$

Proof. Substituting in (2.13) F_1 for f, a_1 for a, bt for b and specifying $h = \frac{\log N}{a_1 N}$, we conclude (2.15) from $\|\eta_N(F_1,h)\| \lesssim \frac{1}{t}\left[e^{-bt-2\pi dN/\log N} + e^{-btN}/\left(1+(\log N)/a_1\right)\right]$. ∎

The exponential convergence of our quadrature rule allows to introduce the following algorithm for the approximation of the operator exponential with a given tolerance $\varepsilon > 0$. Note that the time-variable $t \in (0,\infty)$ appears only in the coefficients $\gamma_k(t)$ of the quadrature rule (2.16), while all resolvents are independent of t.

Proposition 2.7 *a) Let $\varepsilon > 0$ be given. In order to obtain $\|I(t) - T_N(t)\| \lesssim \frac{\varepsilon}{t}$ uniformly with respect to $t > 0$, choose*

$$a_1 > a, \quad b \in (0,\gamma_0), \quad N = \mathcal{O}(|\log\varepsilon|), \quad h = \frac{\log N}{a_1 N},$$
$$z_k = f_I(kh) + ikh \ (k = -N,\dots,N) \quad \text{with } f_I(\eta) = b\cosh(a_1\eta),$$
$$\gamma_k(t) = e^{-z_k t}\frac{h}{2\pi i}\left(ba_1\cosh(a_1 kh) + i\right).$$

Then $T_N(t)$ is a linear combination of $2N+1$ resolvents with scalar weights depending on t:

$$T_N(t) = \sum_{k=-N}^{N} \gamma_k(t)(z_k I - \mathcal{L})^{-1}, \tag{2.16}$$

so that the computation of $T_N(t)$ requires $2N+1 = \mathcal{O}(|\log\varepsilon|)$ evaluations of the resolvents $(z_k I - \mathcal{L})^{-1}$, $k = -N,\dots,N$.

c) The evaluations (or approximations) of the resolvents can be performed in parallel. Note that the shifts z_k are independent of t.

d) Having evaluated the resolvents, $T_N(t)$ can be determined in parallel for different t-values $t_1, t_2, \dots$.

Proof. Use (2.15) for the error estimate. (2.14) shows $\gamma_k(t) = -\frac{h}{2\pi i}F_{11}(kh,t)$. ∎

2.4.3 Exponentially Convergent Algorithm for the Operator Exponential with $t \geq 0$

Algorithm (2.14) does not provide uniform exponential accuracy as $t \to 0$. In this section we show that a slightly modified algorithm for the weighted operator exponential $T_\sigma(t) = \mathcal{L}^{-\sigma}e^{-t\mathcal{L}}$ $(t \geq 0, \sigma > 1)$ guarantees uniform exponential convergence for all $t \geq 0$. Applied to the parabolic initial-value problem

$$\frac{du}{dt} + Au = 0, \quad u(0) = u_0,$$

we can get $u(t) = T_\sigma(t)u_{0,\sigma}$ with $u_{0,\sigma} = \mathcal{L}^\sigma u_0$ provided that $u_0 \in D(\mathcal{L}^\sigma)$, i.e., in this case we need sufficient regularity of the initial data. Choose a curve (integration curve) $\Gamma_I = \{z = \xi + i\eta : \xi = b\cosh(a_1\eta)\}$ as before with $a_1 < a$, $b \in (0,\gamma_0)$. Then the weighted operator exponential $T_\sigma(t) = \mathcal{L}^{-\sigma}e^{-t\mathcal{L}}$ can be represented by the Dunford-Cauchy integral

$$T_\sigma(t) = \frac{1}{2\pi i}\int_{\Gamma_I} z^{-\sigma}e^{-zt}(zI - \mathcal{L})^{-1}dz = -\frac{1}{2\pi i}\int_{-\infty}^{\infty} F_{1,\sigma}(\eta,t)d\eta$$

with the integrand

$$F_{1,\sigma}(\eta,t) = z^{-\sigma}e^{-zt}(ba_1\cosh(a_1\eta) + i)(zI - \mathcal{L})^{-1}, \text{ where } z = b\cosh(a_1\eta) + i\eta,\ \eta \in \mathbb{R}.$$

Contrary to Lemma 2.4, the function $F_{1,\sigma}(\eta,t)$ can be estimated on the real axis by

$$\|F_{1,\sigma}(\eta,t)\| \lesssim ba_1(1+|\eta|)^{-1}e^{(1-\sigma)a_1|\eta| - bt\cosh(a_1\eta)} \lesssim ba_1 e^{-bt}e^{(1-\sigma)a_1|\eta|} \quad \text{for } \eta \in \mathbb{R}$$

for all $t \geq 0$. Moreover, $F_{1,\sigma}(\cdot, t)$ can be analytically extended into the strip D_d of the width $d > 0$ constructed above and belongs to the class $\mathbf{H}^p(D_d)$ for all $p \in [1, \infty]$. Applying the quadrature rule (2.12)

$$T_\sigma(t) \approx T_{\sigma,N}(t) = h \sum_{k=-N}^{N} F_{1,\sigma}(kh, t)$$

to the function $f(t) = F_{1,\sigma}(\eta, t)$, we can bound the error $\eta_N(f, h)$ (see [28, 4]) by

$$\|\eta_N\| = \|T_\sigma(t) - T_{\sigma,N}(t)\| \leq ce^{-bt} \left[\frac{e^{-\pi d/h}}{2 \sinh \pi d/h} + \frac{e^{-(\sigma-1)a_1 Nh}}{(\sigma-1)a_1} \right] \|F_{1,\sigma}\|_{\mathbf{H}^1(D_d)}.$$

Equalising the exponents by setting $h = \sqrt{\pi d/[(\sigma - 1)a_1 N]}$, we get the error estimate

$$\|\eta_N\| \leq ce^{-bt} e^{-\sqrt{\pi d(\sigma-1)a_1 N}} \|F_{1,\sigma}\|_{\mathbf{H}^1(D_d)} \quad \text{for all } t \geq 0.$$

As a consequence, we get a similar result as in Proposition 2.7.

In practice one prefers integers σ, so that $\sigma = 2$ is the first choice. To conclude this section, we note that the condition $u_0 \in D(\mathcal{L}^\sigma)$ is no longer an essential restriction if $\mathcal{L}$ is a finitely dimensional operator (say, the discrete elliptic operator). We refer to Remark 4.3 for further results concerning the matrix exponential.

2.5 Operator Valued Functions in Control Theory

In this section we recall the results in [6]. Let us consider the linear dynamical system of equations

$$\frac{dX(t)}{dt} = AX(t) + X(t)B + G, \qquad X(0) = X_0,$$

where $X(t), A, B, G \in \mathbb{R}^{n \times n}$ (A, B, G given constant matrices). The solution $X(t)$ is given by

$$X(t) = e^{tA} X_0 e^{tB} + \int_0^t e^{(t-s)A} G e^{(t-s)B} ds.$$

If all eigenvalues of A, B have negative real parts, then the limit

$$X(t) \to X_\infty = \int_0^\infty e^{tA} G e^{tB} dt \qquad (t \to \infty) \tag{2.17}$$

exists and the X_∞ satisfies the *matrix Lyapunov-Sylvester equation*

$$AX_\infty + X_\infty B + G = 0. \tag{2.18}$$

We refer to [2] concerning the proof of (2.17) in the case of a matrix equation. The operator case considered below can be treated similarly.

2.5.1 Operator-to-Operator Mapping

We set $A = \mathcal{L}^*$, $B = \mathcal{L}$ in (2.18), where $\mathcal{L} : V \to V'$ is an elliptic second order differential operator, and consider the solution of the *operator Lyapunov equation*: Find a selfadjoint continuous operator $\mathcal{Z} : L^2(\Omega) \to V$ such that

$$\mathcal{L}^* \mathcal{Z} + \mathcal{Z}\mathcal{L} + G = 0. \tag{2.19}$$

The solution $\mathcal{Z}$ of the operator Lyapunov equation is given by

$$\mathcal{Z}(\mathcal{L}) := \int_0^\infty \mathcal{G}_0(t, \mathcal{L}, G) dt, \tag{2.20}$$

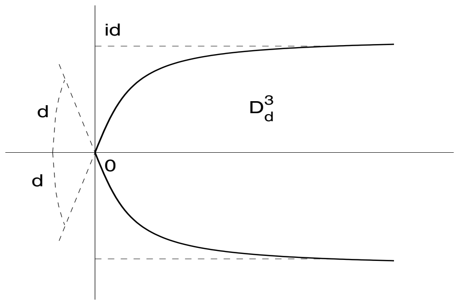

Figure 2.2: The region $\mathcal{D}_d$

where $\mathcal{G}_0(z, \mathcal{L}, G) := e^{z\mathcal{L}^*} G e^{z\mathcal{L}}$ is a continuous operator-valued function of $z \in [0, \infty)$, generated by the differential operator $\mathcal{L}$ and a selfadjoint operator $G : L^2(\Omega) \to L^2(\Omega)$ (see [2] for the matrix case).

In this section we consider a class of operator-valued functions defined by the integral representation (2.20) on $\Gamma := [0, \infty)$. The operator-valued function $\mathcal{Z}(\mathcal{L})$ defines the solution operator to the Lyapunov equation (2.19). As usual in control theory, we further assume $\Re e\, sp(-\mathcal{L}) \subset (\lambda_0, \infty)$.

To simplify the discussion, we assume that $-\mathcal{L}$ is an elliptic operator of (f_S, f_R)-type with f_S, f_R given by (2.6) such that

$$sp(-\mathcal{L}) \subset S_\mu := \{z \in \mathbb{C} : |\Im m\ z| \leq \mu, \quad \Re e\ z > \lambda_0\}, \quad \lambda_0, \mu > 0. \tag{2.21}$$

In particular, the latter condition implies that the elliptic operator $\mathcal{L}$ generates a strongly continuous semigroup $e^{t\mathcal{L}}$ such that

$$||e^{t\mathcal{L}}|| \leq C \frac{1+\mu^2}{\lambda_0 \sqrt{t}} e^{-c\lambda_0 t} \qquad \text{for all } t \in [0, \infty) \quad (|| \cdot || : \text{spectral operator norm}),$$

where $C, c > 0$ do not depend on λ_0 and t.

In the following we discuss exponentially convergent quadrature rules for the integral (2.20). The construction consists of two steps: First, we approximate the integral by a sum of operators $\mathcal{G}_0(t_k, \mathcal{L}, G)$ at quadrature points $t_k \in [0, \infty)$, and then we approximate each operator exponential involved in $\mathcal{G}_0(t_k, \mathcal{L}, G)$ as in §2.4. The resulting quadrature rule is similar to that in [10, Thm. 5] for the case of a matrix Lyapunov equation. Contrary to [10], here we consider the integral of an *operator-valued function*, moreover, we apply the more efficient approximation scheme of §2.4.

Applying the substitution $t = u^\alpha$ in the integral of (2.20) for some $\alpha \geq 0$, we obtain the equivalent representation

$$\mathcal{Z}(\mathcal{L}) = \int_0^\infty \mathcal{G}_\alpha(t, \mathcal{L}, G) dt \quad \text{with } \mathcal{G}_\alpha(t, \mathcal{L}, G) := g_\alpha(t, \mathcal{L}^*) G g_\alpha(t, \mathcal{L}) dt,$$

where

$$g_\alpha(z, \lambda) := \sqrt{1 + 2\alpha} z^\alpha \exp(z^{1+2\alpha} \lambda), \quad \alpha \geq 0, \tag{2.22}$$

so that (2.20) corresponds to the case $\alpha = 0$.

First, we recall some auxiliary approximation results for holomorphic functions based on the Sinc-approximation. Let the region[1] $\mathcal{D}_d$ (see Figure 2.2) for a given $d \in (0, \pi/2]$ be defined by

$$\mathcal{D}_d := \{z \in \mathbb{C} : |\arg(\sinh z)| < d\}. \tag{2.23}$$

We denote by $H^1(\mathcal{D}_d)$ the family of functions that are analytic in $\mathcal{D}_d$ and satisfy

$$N_1(f, \mathcal{D}_d) := \int_{\partial \mathcal{D}_d} |f(z)||dz| < \infty.$$

[1] This is the domain called $\mathcal{D}_d^3$ in [28]. Note that it is different from the strip D_d in (2.8).

Now, for $\alpha, \beta \in (0,1]$, introduce the space

$$L_{\alpha,\beta}(\mathcal{D}_d) := \left\{ f \in H^1(\mathcal{D}_d) : |f(z)| \le C \left(\frac{|z|}{1+|z|} \right)^{\alpha} e^{-\beta \, \Re e \, z} \quad \text{for all } z \in \mathcal{D}_d \right\}$$

(cf. [28]). We set

$$\phi(z) := \log\{\sinh(z)\}, \quad \text{hence}$$
$$\phi'(z) = \frac{1}{\tanh(z)}, \quad z = \phi^{-1}(w) = \log\left(e^w + \sqrt{1+e^{2w}}\right),$$

where $\phi(z)$ is the conformal map of $\mathcal{D}_d$ onto the infinite strip D_d defined by (2.8).

It is easy to check that

$$g_\alpha(\cdot, \lambda) \in L_{\alpha,\beta}, \qquad \beta \ge \min\{1, a_0\} \qquad \text{for } \lambda \in \Gamma_{\mathcal{L}},$$

where, with given $a, b_0 > 0$, $\Gamma_{\mathcal{L}} := \{z = \xi + i\eta : \xi = -b_0 - a\eta^2, \ \eta \in (-\infty, \infty)\}$ is the integration parabola to be used for technical needs.

2.5.2 Quadrature Rule I Applied to $\mathcal{Z}(\mathcal{L})$

In the sequel, the value of d involved in $\mathcal{D}_d$ (cf. (2.23)) will be chosen from the interval $0 < d < \frac{\pi}{2(1+2\alpha)}$, where we further fix the parameter $\alpha = 1/2$ involved in (2.22). Without loss of generality we can assume $\beta = \min\{1, \lambda_0/2\} \le \alpha = 1/2$ and then choose the parameter b_0 defining the integrating parabola $\Gamma_{\mathcal{L}}$, by $b_0 = \lambda_0/2$.

Lemma 2.8 *Let the spectrum of $\mathcal{L}$ lie in the strip S_μ defined by (2.21). Given $N \in \mathbb{N}$ and $\beta = \min\{1, \lambda_0/2\}$, choose $h > 0$, $t_k \in [0, \infty)$, and M by*

$$h = \sqrt[3]{\frac{\pi d}{2\lambda_0 N^2}}, \ t_k = \log\left(e^{kh} + \sqrt{1+e^{2kh}}\right), \ M = \lceil 2\beta N \rceil .$$

Then the quadrature rule

$$\mathcal{Z}_N(\mathcal{L}) := h \sum_{k=-M}^{N} \tanh(t_k) \mathcal{G}_{1/2}(t_k, \mathcal{L}, G), \tag{2.24}$$

for the integral $\mathcal{Z}(\mathcal{L}) = \int_0^\infty \mathcal{G}_0(t, \mathcal{L}, G) dt$ is exponentially convergent. The error estimate

$$\|\mathcal{Z}(\mathcal{L}) - \mathcal{Z}_N(\mathcal{L})\| \le C(1+\mu^2) e^{-(2\pi\lambda_0 d N)^{2/3}}$$

holds with C independent of N and with μ being half the width of the strip S_μ in (2.21).

Proof. See [6]. ■

If G has low rank, Lemma 2.8 already provides a low rank approximation to the solution of the Lyapunov equation. In fact, let us assume that G has a separable representation consisting of k_G terms, i.e.,

$$G := \sum_{j=1}^{k_G} a_j * f_j,$$

where $f_j : L^2(\Omega) \to \mathbb{R}$ are linear continuous functionals, while $a_j \in L^2(\Omega)$ are functions on Ω. Substitution of the above representation into $\mathcal{G}_{1/2}(t_k, \mathcal{L}, G)$ shows that also $\mathcal{G}_{1/2}(t_k, \mathcal{L}, G)$ is separable with k_G terms. Due to (2.24), $\mathcal{Z}_N(\mathcal{L})$ is separable with $k = k_G(N+M+1)$ terms (in the matrix case, this is equivalent to $\operatorname{rank} \mathcal{Z}_N(\mathcal{L}) \le k$).

We proceed with the approximation of the individual terms $\mathcal{G}_{1/2}(t_k, \mathcal{L}, G)$ in (2.24). For this purpose, we apply the basic construction from §2.4 modified by a proper translation transform explained below. We use the symbol A for both $\mathcal{L}$ and $\mathcal{L}^*$. We recall that with a given elliptic operator A and for the described choice of the parameters z_p, h, c_p, the quadrature

$$\exp_L(A) = \sum_{p=-L}^{L} c_p e^{-z_p}(z_p I - A)^{-1} \qquad \text{(see (2.16))} \tag{2.25}$$

is exponentially convergent (cf. (2.15)). To adapt the above approximation to our particular situation, we include the parameter t_k into the operator by setting $A_k := t_k\mathcal{L}$, which then leads to the bound $\lambda_{\min}(A_k) = \mathcal{O}(t_k)$. Due to the factor $\frac{1}{t}$ in (2.15), the error estimate deteriorates when $t_k \to 0$. To obtain *uniform* convergence with respect to $t_k \to 0$, we use a simple shift of the spectrum,

$$e^{A_k} = e \cdot e^{B_k} \qquad \text{for } B_k := A_k - I,$$

ensuring that $\lambda_{\min}(-B_k) = \mathcal{O}(1) > 0$. Now, we apply the quadrature (2.25) to the operator B_k, which leads to the uniform error estimate

$$\| \exp(B_k) - \exp_L(B_k)\| \le Ce^{-L/\log L} \qquad \text{for all } k = -M, ..., N,$$

where the constant C does not depend on L and k. With this procedure, we arrive at the following product quadrature.

Theorem 2.9 *Under the conditions of Lemma 2.8, the expression*

$$\mathcal{Z}_{N,L}(\mathcal{L}) := 2h \sum_{k=-M}^{N} t_k \tanh(t_k)\mathcal{S}^*_{L,k} G \mathcal{S}_{L,k} \quad \textit{with } \mathcal{S}_{L,k} := \sum_{p=-L}^{L} c_p e^{1-z_p}(z_p I - B_k)^{-1}$$

converges exponentially as $N, L \to \infty$,

$$\|\mathcal{Z}(\mathcal{L}) - \mathcal{Z}_{N,L}(\mathcal{L})\| \le C\left[(1+\mu^2)e^{-(2\pi\lambda_0 dN)^{2/3}} + e^{-L/\log L}\right].$$

Proof. Combination of the result of Lemma 2.8 with the modified quadrature (2.25) leads to the desired bound. ∎

3 New Quadrature for the Lyapunov Solution Operator

Quadrature Rule I presented in the previous section contains a *triple sum* of elliptic resolvents (one sum from $\mathcal{Z}_{N,L}$ and two sums due to $\mathcal{S}_{L,k}$ and $\mathcal{S}^*_{L,k}$). In this section we propose a new scheme which contains only a *double sum* of resolvents.

3.1 Equations with Elementary Operators

Let $\mathcal{A}$ be a complex Banach algebra with identity e and $\mathcal{B}$ be a Banach algebra of operators on $\mathcal{A}$ considered as a Banach space. Given $\{U_j\}$, $\{V_j\} \subset \mathcal{A}$ let $S \in \mathcal{B}$ be defined by

$$SX = \sum_{j=1}^{M} U_j X V_j$$

where $\{U_j\}$ and $\{V_j\}$ are commutative subsets of $\mathcal{A}$, but $\{U_j\}$ need not commute with $\{V_j\}$. The operator S (such operators are usually called *elementary operators*) was studied in [26] where it was shown that if $\Sigma(X, \mathcal{A})$ denotes the spectrum of $X \in \mathcal{A}$, then

$$\Sigma(S, \mathcal{B}) \subset \sum_{j=1}^{M} \{\lambda\,\mu : \; \lambda \in \Sigma(U_j, \mathcal{A}), \; \mu \in \Sigma(V_j, \mathcal{A})\} =: \Sigma_{UV}.$$

Furthermore, if $f(\lambda)$ is holomorphic in a domain that contains Σ_{UV}, then there exist Cauchy domains $D_i^V \supset \Sigma(V_i, \mathcal{A})$, $D_i^U \supset \Sigma(U_i, \mathcal{A})$, $1 \le i \le M$, such that for any $X \in \mathcal{A}$

$$
\begin{aligned}
f(S)X &= \frac{1}{(2\pi i)^M} \int_{\partial D_1^V} \cdots \int_{\partial D_M^V} f\left(\sum_{j=1}^M \lambda_j U_j\right) X \prod_{j=1}^M (\lambda_j I - V_j)^{-1} d\lambda_j \\
&= \frac{(-1)^M}{(2\pi)^{2M}} \int_{\partial D_1^V} \cdots \int_{\partial D_M^V} \int_{\partial D_1^U} \cdots \int_{\partial D_M^U} f\left(\sum_{j=1}^M \lambda_j \mu_j\right) \\
&\times \prod_{j=1}^M (\mu_j I - U_j)^{-1} d\mu_j X \prod_{j=1}^M (\lambda_j I - V_j)^{-1} d\lambda_j
\end{aligned}
\tag{3.1}
$$

where ∂D_i^V, ∂D_i^U denote the boundaries of D_i^V and D_i^U, respectively and I the unit operator. There is a number of papers dealing with invertibility and spectral properties of elementary operators (see, for example [19, 20]).

Let us consider the following operator equation

$$SX = G \tag{3.2}$$

and suppose that S^{-1} exists. Then, using formula (3.1) applied to the function

$$f\left(\sum_{j=1}^M \lambda_j \mu_j\right) \equiv \left(\sum_{j=1}^M \lambda_j \mu_j\right)^{-1}$$

we get

$$X = \frac{(-1)^M}{(2\pi)^{2M}} \int_{\partial D_1^V} \cdots \int_{\partial D_M^U} \left(\sum_{j=1}^M \mu_j \lambda_j\right)^{-1} \prod_{j=1}^M (\mu_j I - U_j)^{-1} d\mu_j G \prod_{j=1}^M (\lambda_j I - V_j)^{-1} d\lambda_j. \tag{3.3}$$

The following special case of equation (3.2) with bounded operators was considered in [16]:

$$\sum_{j,k=0}^n c_{jk} A^j X B^k = Y \ , \tag{3.4}$$

where $c_{jk} \in \mathbb{R}$, $B \in \mathcal{L}(B_1)$, $A \in \mathcal{L}(B_2)$, $Y \in \mathcal{L}(B_1, B_2)$ are given bounded operators, $X \in \mathcal{L}(B_1, B_2)$ is the operator we are looking for, B_1, B_2 are Banach spaces, $\mathcal{L}(B_i)$ and $\mathcal{L}(B_1, B_2)$ denote the sets of linear bounded operators acting in B_i and from B_1 into B_2, respectively. It was shown that the unique solution is given by

$$X = -\frac{1}{4\pi^2} \oint_{\Gamma_A} \oint_{\Gamma_B} \frac{(A - \lambda I)^{-1} Y (B - \mu I)^{-1}}{P(\lambda, \mu)} d\lambda d\mu \tag{3.5}$$

provided that $P(\lambda, \mu) = \sum_{j,k=0}^n c_{jk} \lambda^j \mu^k \neq 0$ for $(\lambda, \mu) \in \Sigma(A) \times \Sigma(B)$, where $\Sigma(A)$, $\Sigma(B)$ are the respective spectral sets of A and B, Γ_A and Γ_B denote paths in the resolvent sets $\rho(A), \rho(B)$ of A, B surrounding $\Sigma(A)$ and $\Sigma(B)$. The representations (3.3), (3.5) are useful in many applications (see, for example, [16, 17]) and can be justified also for unbounded operators provided the resolvents possess appropriate properties (see Lemma 3.1 below).

Particular cases of the equations (3.2), (3.4) are the Sylvester equation

$$AX + XB = G \tag{3.6}$$

and the Lyapunov equation

$$AX + XA^\top = G.$$

The Lyapunov (Sylvester) equation is involved, for example, while using Newton's method for solving Riccati matrix equations arising in optimal control problems (cf. [20, 24]). One has to solve the Riccati equation

$$AX + XA^\top + XBB^\top X = -C^\top C$$

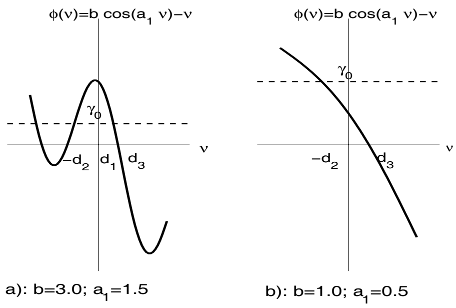

Figure 3.1: Calculation of the width of the analyticity strip.

for constructing a near-optimal reduced-order model for a dynamical system

$$\begin{aligned} \dot{x} &= Ax + Bu, \quad x(0) = x_0, \\ y &= Cx \end{aligned} \tag{3.7}$$

with state $x \in \mathbb{R}^n$, input $u \in \mathbb{R}^p$ and output $y \in \mathbb{R}^q$ and with $A \in \mathbb{R}^{n\times n}$, $B \in \mathbb{R}^{n\times p}$, $C \in \mathbb{R}^{n\times q}$. Here the optimal control u can be realised as $u(t) = -B^\top X x(t)$, $t \in (0, \infty)$.

Consider a control problem where the state is governed by partial differential equations. The spatial discretisation of the partial differential operator by a finite element or finite difference method (yielding a system matrix A) leads to a system of ordinary differential equations of the type (3.7) with large and sparse matrices and finally to a Riccati equation which can be reduced to a sequence of Lyapunov equations. There are direct and iterative methods to solve the Lyapunov equation (cf. [16, 20, 21, 23, 25, 31]). The direct ones are preferred when solving equations with matrices of moderate size. Direct methods are often based on various decompositions of the matrix (e.g., the Schur decomposition) with complexity $\mathcal{O}(n^3)$, which restricts their use to problems with relatively small n. Iterative methods (SOR, ADI and others) are applied to the Lyapunov equation when the matrix A is large. In order to ensure computational stability and to decrease the number of iteration steps various preconditioning techniques are used (cf. [22]).

The aim of this section is to find exponentially convergent approximations to the solutions of (3.2), (3.4). One can use these approximations to solve efficiently quadratic equations like the Riccati equation.

3.2 Exponentially Convergent Quadrature Rule II

Below we consider a method to solve the Sylvester equation based on a Sinc quadrature.

For the sake of simplicity, we consider operators with a real spectrum bounded from below by $\gamma_0 > 0$ and with resolvents estimated by $f_R(z) = 1/\Im m\ z$, $\Re e z > \gamma_0$ (say, for self-adjoint positive definite operators). As above, we denote the class of such operators by $\mathbf{E}_{S,R}$. Analogously, one can consider operators with spectrum in a half-strip, where the resolvent is bounded by $f_R(z) = 1/\Im m\ (z - c)$ for some constant c. We choose the parameter $b_C \in (0, \gamma_{0C})$ with $C = A$ or $C = B$, where γ_{0C} is defined as in (2.7) after substituting $\mathcal{L} = C$. Let d_{1C} be the minimal positive solution (if existing) of the equation

$$\varphi(\nu) \equiv b_C \cos(a_C \nu) - \nu = \gamma_{0C}, \quad 0 < b_C < \gamma_{0C},\ a_C > 0,\ C = A, B. \tag{3.8}$$

Moreover, let $-d_{2C}$ be the maximal negative solution ($d_{2C} > 0$) of this equation and $d_C = \min\{d_{1C}, d_{2C}\}$ (see Figure 3.1).

Using the simple transform $\hat{X} = A^{-1} X B^{-1}$, we translate the equation (3.6) into

$$A^2 \hat{X} B + A \hat{X} B^2 = G. \tag{3.9}$$

Lemma 3.1 *Let A, B be operators of the class $\mathbf{E}_{S,R}$. Choose the integration curves*

$$\begin{aligned} \Gamma_{IA} &= \{\lambda = \xi + i\eta : \xi = b_{IA} \cosh(a_{IA}\eta),\ 0 < a_{IA} < a_{SA},\ 0 < b_{IA} < b_{SA}\}, \\ \Gamma_{IB} &= \{\lambda = \xi + i\eta : \xi = b_{IB} \cosh(a_{IB}\eta),\ 0 < a_{IB}, 0 < b_{IB} < \gamma_0\}. \end{aligned}$$

Due to (3.5), the solution of the operator equation (3.9) can be represented by the Dunford-Cauchy integral

$$\hat{X} = -\frac{1}{4\pi^2}\int_{\Gamma_{IA}}\int_{\Gamma_{IB}}(\lambda^2\mu + \lambda\mu^2)^{-1}(\lambda I - A)^{-1}G(\mu I - B)^{-1}d\lambda d\mu \tag{3.10}$$

or, after parametrisation, by

$$\hat{X} = -\frac{1}{4\pi^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}F(\eta,\zeta)d\eta d\zeta, \tag{3.11}$$

where the integrand

$$F(\eta,\zeta) = \frac{(a_{IA}b_{IA}\sinh(a_{IA}\eta) + i)(a_{IB}b_{IB}\sinh(a_{IB}\zeta) + i)}{\lambda^2\mu + \lambda\mu^2}(\lambda I - A)^{-1}G(\mu I - B)^{-1}, \tag{3.12}$$

$$\lambda = b_{IA}\cosh(a_{IA}\eta) + i\eta, \quad \mu = b_{IB}\cosh(a_{IB}\zeta) + i\zeta$$

can be estimated on the real axis by

$$\|F(\eta,\zeta)\| \lesssim C(1+|\eta|)^{-1}(1+|\zeta|)^{-1}e^{-1/2a_{IA}|\eta|}e^{-1/2a_{IB}|\zeta|} \qquad (\eta,\zeta\in\mathbb{R}). \tag{3.13}$$

Moreover, it can be extended analytically into the strip D_d of width $d > 0$(see (2.8)) and belongs to the class $\mathbf{H}^p(D_d)$ for all $p \in [1,\infty]$ with respect to each variable.

Proof. Since the operators A, B are of (f_S, f_R)-type with f_S, f_R given by

$$f_{SA}(\eta) = \gamma_{0A}\cosh(a_{SA}\eta)\,,\ f_{RA}(z) = \begin{cases} 1/|\Im m\ z|, & \Re e\ z > \gamma_{0A}, \\ |z - z_0|^{-1} & \Re e\ z \le \gamma_{0A}, z_0 = (\gamma_{0A}, 0), \end{cases}$$

$$f_{SB}(\eta) = \gamma_{0B}\cosh(a_{SB}\eta)\,,\ f_{RB}(z) = \begin{cases} 1/|\Im m\ z|, & \Re e\ z > \gamma_{0B}, \\ |z - z_0|^{-1} & \Re e\ z \le \gamma_{0B}, z_0 = (\gamma_{0B}, 0), \end{cases}$$

we can choose the integration parabolae Γ_{IA}, Γ_{IB} as above. Then the solution to the operator equation (3.9) can be represented by the Dunford-Cauchy integral (3.10). After the parametrisation by (3.11) the integrand $F(\eta,\zeta)$ defined in (3.12) can be estimated for $\eta,\zeta \in \mathbb{R}$ by

$$\begin{aligned}\|F(\eta,\zeta)\| &\lesssim \|G\|(1+|\eta|)^{-1}(1+|\zeta|)^{-1}(e^{a_{IA}|\eta|} + e^{a_{IB}|\zeta|})^{-1} \\ &\lesssim \|G\|(1+|\eta|)^{-1}(1+|\zeta|)^{-1}e^{-\frac{1}{2}a_{IA}|\eta|}e^{-\frac{1}{2}a_{IB}|\zeta|}.\end{aligned}$$

The above estimate shows that both the integrals (3.10) and (3.11) converge. Next we show that the integrand can be extended analytically with respect to η into the strip D_{d_A} (resp., with respect to ζ into D_{d_B}) of width $d_A > 0$ (resp., $d_B > 0$) (see (2.8)) and belongs to the class $\mathbf{H}^p(D_{d_A})$ for all $p \in [1,\infty]$ with respect to the variable η (the same for ζ).

We obtain

$$\begin{aligned}\lambda^2\mu = {} & [b_{IB}b_{IA}^2\cosh(a_{IB}\zeta)\cosh^2(a_{IA}\eta) - \eta^2 b_{IB}\cosh(a_{IB}\zeta) - 2\zeta\eta b_{IA}\cosh(a_{IA}\eta)] \\ & + i[2\eta b_{IB}b_{IA}\cosh(a_{IA}\eta)\cosh(a_{IB}\zeta) + \zeta(b_{IA}^2\cosh^2(a_{IA}\eta) - \eta^2)].\end{aligned}$$

Taking into account that $\cosh(x \pm iy) = \cos y\cosh x \pm i\sin y\sinh x$ and replacing η by a complex variable $z_\eta = \eta + i\nu \in D_{d_A}$ and ζ by a complex variable $z_\zeta = \zeta + i\nu \in D_{d_B}$ we see that $\lambda^2\mu$ has the asymptotical behaviour $e^{a_{IB}|\zeta|}e^{2a_{IA}|\eta|}$ for $|\eta|, |\zeta|$ large enough. Considering analogously other terms in the integrand $F(\eta,\zeta)$, we conclude that it belongs to the class $\mathbf{H}^p(D_{d_A})$ for all $p \in [1,\infty]$, with respect to the variable η and to the class $\mathbf{H}^p(D_{d_B})$ for all $p \in [1,\infty]$, with respect to the variable ζ.

The analyticity of the integrand can be violated only if:
(a) $b_{IA}\cosh(a_{IA}(\eta + i\nu)) - \nu + i\eta = 0$ or the set

$$\begin{aligned}Z_A &= \{b_{IA}\cosh(a_{IA}(\eta + i\nu)) - \nu + i\eta :\ \eta \in (-\infty,\infty),\ |\nu| < d_A\} \\ &= \{b\cos(a_{IA}\nu)\cosh(a_{IA}\eta) - \nu + i(b_A\sin(a_{IA}\nu)\sinh(a_{IA}\eta) + \eta) : \\ &\qquad \eta \in (-\infty,\infty),\ |\nu| < d_A\}\end{aligned}$$

intersects the part of the real axis $\eta > \gamma_{0A}$, where the spectrum of A is situated (in this case the resolvent of A becomes unbounded); or
(b) $b_{IB}\cosh(a_{IB}(\zeta + i\nu)) - \nu + i\zeta = 0$ or the set

$$\begin{aligned} Z_B &= \{b_{IB}\cosh(a_{IB}(\zeta + i\nu)) - \nu + i\zeta :\ \zeta \in (-\infty,\infty),\ |\nu| < d_B\} \\ &= \{b_B\cos(a_{IB}\nu)\cosh(a_{IB}\zeta) - \nu + i(b_B\sin(a_{IB}\nu)\sinh(a_{IB}\zeta) + \zeta) : \\ &\qquad \zeta \in (-\infty,\infty),\ |\nu| < d_B\} \end{aligned}$$

intersects the part of the real axis $\zeta > \gamma_{0B}$, where the spectrum of B is situated (in this case the resolvent of B becomes unbounded). The intersection of Z_A with the real axis (if $\eta = 0$) is given by

$$Z_A|_{\eta=0} = \{b_A\cos(a_{IA}\nu) - \nu : |\nu| < d_A\}.$$

Now, we need the following condition to be valid:

$$\varphi(\nu) \equiv b_A\cos(a_{IA}\nu) - \nu < \gamma_{0A}.$$

Let d_{1A} and $-d_{2B}$ be defined as above as particular solutions of equation (3.8). Then the width of the strip in which $F(\eta,\zeta)$ can be extended analytically with respect to the variable η is $d = \min\{d_{1A}, d_{2B}\}$ (see also Figure 3.1). It follows from (3.13) that the integrand belongs to $\mathbf{H}^p(D_d)$ for all $p \in [0,\infty)$. The behaviour with respect to the variable ζ can be analysed analogously. It is also easy to see that $\lambda^2\mu + \lambda\mu^2 \neq 0$ in both strips D_{d_A} and D_{d_B}. ■

Remark 3.2 *Similarly to Lemma 3.1, one can easily prove the following Dunford-Cauchy representation to the solution of the Lyapunov-Sylvester equation (3.6),*

$$X = -\frac{1}{4\pi^2}\int_{\Gamma_{IA}}\int_{\Gamma_{IB}} (\lambda + \mu)^{-1}(\lambda I - A)^{-1}G(\mu I - B)^{-1}d\lambda d\mu.$$

However, the corresponding quadrature rule does not converge exponentially.

3.3 Error Analysis for the Quadrature Rule II

In this section we use the notations from §2.4.1. We will need the following lemma which can be proven similarly to Lemma 2.5 (see [6]).

Lemma 3.3 *For any operator valued function $f \in \mathbf{H}^1(D_d)$, there holds*

$$\eta(f,h) = \frac{i}{2}\int_{\mathbb{R}}\left\{\frac{f(\xi - id^-)e^{-\pi(d+i\xi)/h}}{\sin[\pi(\xi - id)/h]} - \frac{f(\xi + id^-)e^{-\pi(d-i\xi)/h}}{\sin[\pi(\xi + d)/h]}\right\}d\xi$$

providing the estimate

$$\|\eta(f,h)\| \le \frac{e^{-\pi d/h}}{2\sinh(\pi d/h)}\|f\|_{\mathbf{H}^1(D_d)}.$$

If, in addition, f satisfies on $\mathbb{R}$ the condition

$$\|f(\xi)\| \le c\exp(-\alpha|\xi|), \qquad \alpha, c > 0,$$

then taking $h = \sqrt{2\pi d/(\alpha N)}$, we obtain

$$\|\eta_N(f,h)\| \le c_1 e^{-\sqrt{2\pi d\alpha N}}$$

with a constant $c_1 > 0$ independent of N.

Given integers N_A, N_B, we set

$$h_A = 2\sqrt{\pi d_A/(a_{IA}N_A)}, \quad h_B = 2\sqrt{\pi d_B/(a_{IB}N_B)} \tag{3.14}$$

and approximate the integral (3.11) by the double quadrature sum

$$\hat{X} \approx \hat{X}_{N_A,N_B} = h_A h_B \sum_{k=-N_A}^{N_A} \sum_{j=-N_B}^{N_B} F(kh_A, jh_B). \tag{3.15}$$

Due to Lemmata 3.1 and 3.3, we have the following error estimate indicating exponential convergence of quadrature rule II.

Theorem 3.4 *There holds*

$$\|\hat{X} - \hat{X}_{N_A,N_B}\| \leq Ce^{-\sqrt{\pi d_A a_{IA} N_A + \pi d_B a_{IB} N_B}}$$

with a constant $C > 0$ independent of N_A and N_B.

The exponential convergence of our quadrature rule allows to introduce the following parallel algorithm to approximate the solution of the Sylvester (Lyapunov) equation with operators A, B from the class $\mathbf{E}_{S,R}$.

Algorithm 3.5 *a) Given $\varepsilon > 0$, choose integers $N_A = \mathcal{O}(\log^2 \varepsilon)$, $N_B = \mathcal{O}(\log^2 \varepsilon)$, set h_A and h_B as in (3.14) and determine*

$$z_{A,k} = b_{IA} \cosh (a_{IA} k h_A) \qquad (k = -N_A, \ldots, N_A),$$
$$z_{B,j} = b_{IB} \cosh (a_{IB} k h_B) \qquad (j = -N_B, \ldots, N_B).$$

b) Find the resolvents $(z_k I - A)^{-1}$, $k = -N_A, \ldots, N_A$, $(z_j I - B)^{-1}$, $j = -N_B, \ldots, N_B$.
c) Find the approximations $\hat{X}_{N_A,N_B}$ for the solution $\hat{X}$ of the Sylvester equation in the form (3.15).

Compared with the quadrature rule I (see Theorem 2.9), the new Algorithm 3.5 includes only a double sum of resolvents (it seems that it cannot be improved further).

To realise the constructive $\mathcal{H}$-matrix approximation, we build the $\mathcal{H}$-matrix representation for each individual resolvent (or its discrete version) from (3.15). The latter sum contains $(2N_A+1)(2N_B+1)$ terms, where we set $N_A = \mathcal{O}(\log^2 \varepsilon)$, $N_B = \mathcal{O}(\log^2 \varepsilon)$. The overall complexity of our quadrature rule II amounts to $\mathcal{O}(n \log^q n \log^4 \varepsilon)$, where n is the problem size corresponding to the spatial discretisation to the elliptic operators A and B.

4 Resolvent Approximation to $\mathrm{sign}(H)$

4.1 An Exponential Convergent Quadrature Rule

Let $t_j = j\pi/n, n = 0, ..., 2n-1$, be an equidistant grid. Then for a given continuous function $f(x)$, the trigonometric polynomial

$$u(t) = P_n f = \sum_{j=0}^{n} \alpha_j \cos(jt) + \sum_{j=1}^{n-1} \beta_j \sin(jt)$$

with the coefficients

$$\alpha_0 = \frac{1}{2n} \sum_{k=0}^{2n-1} f_k, \quad f_k = f(t_k), \quad \alpha_n = \frac{1}{2n} \sum_{k=0}^{2n-1} (-1)^k f_k,$$
$$\alpha_j = \frac{1}{n} \sum_{k=0}^{2n-1} f_k \cos(jt_k), \quad \beta_j = \frac{1}{n} \sum_{k=0}^{2n-1} f_k \sin(jt_k), \qquad j = 1, ..., n-1,$$

is the trigonometric interpolant satisfying $u(t_j) = f_j, j = 0, ..., 2n-1$. Another representation of this polynomial is

$$(P_n f)(t) = \sum_{k=0}^{2n-1} f(t_k) L_k(t) = \frac{1}{2n} \sin(nt) \sum_{k=0}^{2n-1} (-1)^k f(t_k) \cot \frac{t-t_k}{2}$$

with the Lagrange basis

$$L_j(t) = \frac{1}{2n}\sin n(t-t_j)\cot\frac{t-t_j}{2}, \qquad t \neq t_j, \quad j = 0, ..., 2n-1.$$

If f is analytic and 2π-periodic, then there exists a strip $D = \mathbb{R} \times (-s, s) \subset$ with $s > 0$ such that f can be extended to a holomorphic and 2π-periodic bounded function $f : D \to \mathbb{C}$ and the remainder in trigonometric interpolation can be estimated uniformly on $[0, 2\pi]$ by

$$\|P_n f - f\|_\infty \leq M\frac{\coth(s/2)}{\sinh(ns)},$$

where M denotes a bound for the holomorphic function f on D. We can summarise this result by the estimate $\|P_n f - f\|_\infty = \mathcal{O}(e^{-ns})$. Using the interpolant $P_n f$ instead of f, one gets the quadrature rule

$$\int_0^{2\pi} f(\tau)d\tau \approx \sum_{m=0}^{2n-1}\gamma_m f_m \tag{4.1}$$

with the quadrature coefficients

$$\gamma_m = \int_0^{2\pi} L_m(\tau)d\tau = \sum_{k=0}^{2n-1}\left(\frac{\pi}{n}\delta_{mk} - (-1)^{k-m}\frac{\pi}{4n^2}\right) = \pi/n.$$

Thus, in the case of analytic and 2π-periodic integrands, we arrive at a quadrature error $\mathcal{O}(e^{-ns})$.

4.2 Quadratures in the Case of Uniformly Bounded Operators

Let H be a bounded operator, $\Gamma_S = \{z = z_0 + r_S e^{i\phi} \in \mathbb{C} : \phi \in [0, 2\pi)\}$, $z_0 = x_0 \in \mathbb{R}_+, 0 \leq r_S < x_0$, be the boundary of a disc Ω_S which contains the spectral set Σ of H, and $\Gamma_I = \{z = z_0 + r_I e^{i\phi} \in \mathbb{C} : \phi \in [0, 2\pi)\}$, $0 \leq r_I < x_0$, be the integration path in (2.4). After parametrising the integral (2.4), we get

$$\begin{aligned} \operatorname{sign}(H) &= \frac{1}{\pi i}\int_{\Gamma_I}(zI - H)^{-1}dz - I = \frac{1}{\pi}\int_0^{2\pi} F(\phi)d\phi - I, \\ F(\phi) &= r_I e^{i\phi}((z_0 + r_I e^{i\phi})I - H)^{-1}, \qquad \phi \in [0, 2\pi]. \end{aligned} \tag{4.2}$$

For a complex argument $\phi_c = \phi + i\psi$, the analyticity of the integrand $F(\phi_c) = ir_c e^{i\phi}\left((z_0 + r_R e^{i\phi})I - H\right)^{-1}$, $r_R = r_I e^{-\psi}$, can be violated only if $\psi > 0$, since in this case the resolvent circle $z = z_0 + r_R e^{i\phi}$ lies inside of the spectral circle so that the resolvent can be unbounded. From the inequalities $r_I - \rho < r_R < x_0$ (this inequality guarantees that the resolvent circle lies outside the spectral one), where ρ is the distance between the integration and the spectral circles, we get $-\ln\frac{x_0}{r_I} < \psi < \ln\frac{r_I}{r_I - \rho}$. Thus, the integrand $F(\phi)$ in (4.2) is a 2π-periodic function which can be holomorphically extended into the strip $S = \{w = \phi + i\psi : \phi \in (-\infty, \infty), |\psi| < s\}$, where $s = \min\{\ln\frac{x_0}{r_I}, \ln\frac{r_I}{r_I - \rho}\}$.

Now, applying the quadrature rule (4.1) to the integral (4.2), we get the following approximation of the operator sign function:

$$\operatorname{sign}(H) \approx \operatorname{sign}_N(H) := \frac{1}{N}\sum_{k=0}^{2N-1} F\left(\frac{k\pi}{N}\right) - I, \tag{4.3}$$

where the quadrature error is $\mathcal{O}(e^{-Ns})$.

Remark 4.1 *In applications, A may be a finite element or finite difference approximation of a second order elliptic differential operator for which $r_I = \mathcal{O}(h^{-k})$, $k > 0$, where h is the spatial discretisation parameter. In this case we have $s = \ln\frac{r_I}{r_I - \rho} = \ln\frac{1}{1 - ch^k} = \mathcal{O}(h^k) \to 0$ as $h \to 0$ so that the error of the algorithm (4.3) is of the order $\mathcal{O}(e^{-ch^k N})$ with some positive constant c. This leads to a polynomial complexity relying on the estimate $N = \mathcal{O}(h^{-k'})$ with $k' > k$.*

Due to Remark 4.1, for many applications we may need a special method being robust with respect to $\operatorname{cond}(H)$.

4.3 *Sinc*-Based Approximation in the General Case

Let Ω^+ be the set of eigenvalues of H with positive real part and Ω^- be the corresponding set with negative real part. Consider the matrix-valued function $\mathcal{J} = \mathcal{J}(H)$ given by the integral representation

$$\mathcal{J} = \frac{1}{\pi i}\int_\Gamma (\zeta I - H)^{-1} d\zeta = \mathrm{sign}(H) + I, \tag{4.4}$$

where Γ is the circle in the complex plane with the diameter $[x_1, x_2] \in \mathbb{R}$, $x_1, x_2 > 0$, which encloses Ω^+. The parameter $\kappa := x_2/x_1$ will be used in the following (it can be regarded as the condition number of H). We are interested in an accurate approximation of $\mathcal{J}(H)$ by a sum of few resolvents $(z_k I - H)^{-1}$ with different parameters z_k.

Under the substitution $\zeta \mapsto t := c_0^{-1}(\zeta - \zeta_0)$ with $\zeta_0 = \frac{x_1+x_2}{2}$, $c_0 = \frac{x_2-x_1}{2}$, the integral $\mathcal{J}$ takes the form

$$\mathcal{J} = \frac{1}{\pi i}\int_{\Gamma_0} (tI - B)^{-1} dt, \quad B = c_0(H - z_0 I),$$

where $\Gamma_0 = \partial\mathcal{U}$ is the unit circle, while $\mathcal{U}$ is the unit disc centred at $t = 0$. Next, we transform the integral over Γ_0 to an integral over the reference interval $K := [-1, 1]$. To that end we use the Zhukovski mapping

$$z = \frac{1}{2}\left(t + \frac{1}{t}\right),$$

which maps $z : \Gamma_0 \to [-1, 1]$. Denote by $\Omega_z^+, \Omega_z^- \in \mathbb{C}$ the respective images of Ω^+ and Ω^- under the mapping $t \mapsto z$. We also set $\Omega_z := \Omega_z^+ \cup \Omega_z^- \subset \mathbb{C}$.

It is worth noting that the transforms $t_1 := z + \sqrt{z^2 - 1}$, $t_2 := z - \sqrt{z^2 - 1}$ map K onto the upper and lower halves of Γ_0, respectively. Therefore, since $dt = 2\frac{t^2}{t^2-1}dz$, the target integral over the two-sided slit curve K can be written as

$$\mathcal{J}(H) = \mathcal{J}_1(B) - \mathcal{J}_2(B),$$

where

$$J_k(B) := \frac{2}{\pi i}\int_K (t_k(z)I - B)^{-1} \frac{t_k^2(z)}{t_k^2(z) - 1} dz, \quad k = 1, 2.$$

One can easily check that both functions $t_k(z)$, $k = 1, 2$, have a regular behaviour as $z^2 \to 1$ with $z \in K$, namely, $t_1(z) \to 1$ as $z \to 1$ and $t_2(z) \to -1$ as $z \to -1$. On the other hand, it can be shown by a simple calculation that

$$\left|\frac{t_1^2(z)}{t_1^2(z) - 1} - \frac{t_2^2(z)}{t_2^2(z) - 1}\right| \le \frac{c}{\sqrt{1 - z^2}} \quad \text{as} \quad z^2 \to 1,\ \Im m z = 0. \tag{4.5}$$

Following [28], introduce the eye-shaped region

$$\mathcal{D} := \{z \in \mathbb{C} : \left|arg\left(\frac{z+1}{z-1}\right)\right| < d\},$$

where $d \in (0, \pi)$ is a given parameter. As in [28, Example 4.2.8], we define the functions

$$w = \Phi(z) := \log\frac{z - a}{b - z}, \qquad \Phi'(z) = \frac{b - a}{(z - a)(b - z)}, \tag{4.6}$$

and the corresponding sequence of collocation points

$$z_k = \frac{a + be^{k\delta}}{1 + e^{k\delta}}, \tag{4.7}$$

where $\delta > 0$ is the grid parameter. In our particular example, we set $a = -1$, $b = 1$. As a matter of fact, w is a conformal map of $\mathcal{D}$ onto the strip $\mathcal{D}_d$,

$$\mathcal{D}_d := \{w \in \mathbb{C} : |\Im m w| < d\}.$$

If $d \in (0, \pi)$ the class $\mathbf{L}_{\alpha,\beta}(\mathcal{D})$ is defined as the family of all matrix-valued functions F which are holomorphic in $\mathcal{D}$ and for some constant $C > 0$ satisfy the inequality

$$\|F(z)\| \leq C|z-a|^{\alpha}|b-z|^{\beta} \qquad \text{in } \mathcal{D}.$$

We rewrite our integral in the form

$$\mathcal{J}(B) = \int_K F(z)dz$$

with

$$F(z) = \frac{2}{\pi i}\left[(t_1(z)I - B)^{-1}\frac{t_1^2(z)}{t_1^2(z)-1} - (t_2(z)I - B)^{-1}\frac{t_2^2(z)}{t_2^2(z)-1}\right].$$

Theorem 4.2 *Assume that $\mathcal{D} \cap \Omega_z = \emptyset$ and let $N \in \mathbb{N}$ be given. Choose the parameter $\delta = \left(\frac{4\pi d}{N}\right)^{1/2}$ in (4.7). Then there exists a constant C_0, independent of N, such that*

$$\left\|\int_K F(z)dz - \delta\sum_{k=-N}^{N}\frac{F(z_k)}{\Phi'(z_k)}\right\| \leq C_0 e^{-(\pi d N)^{1/2}}, \tag{4.8}$$

where Φ' and z_k are given by (4.6), (4.7) with $a = -1$, $b = 1$.

Proof. The assumption $\mathcal{D} \cap \Omega_z = \emptyset$ combined with (4.5) implies that $F \in \mathbf{L}_{1/2,1/2}(\mathcal{D})$. Now the results of [28, Example 4.2.8] (see also Theorem 4.2.6 therein) modified by the usual arguments (see [5],[6] for more details) to the case of matrix-valued functions lead to the desired exponential convergence. ∎

It can be shown that the constant C_0 in (4.8) can be estimated by

$$C_0 \leq C\int_{\partial\mathcal{D}} \|F(z)\|\,|dz|,$$

where C does not depend on F. If H represents the finite element stiffness matrix for the second order elliptic operator, then we can derive $C_0 = \mathcal{O}(\kappa) = \mathcal{O}(h^{-2})$, where $h > 0$ is the corresponding mesh size. Therefore, a quadrature error of order $\varepsilon > 0$ can be achieved with $N = \mathcal{O}(|\log h|^2 + |\log\varepsilon|^2)$ (compare with the number of Newton's iteration in [10] to compute $\mathrm{sign}(H)$ alternatively).

We conclude the paper by the following remark that describes the uniform convergence of the quadrature rule for the matrix exponential $e^{-t\mathcal{L}}$ with respect to $t \geq 0$.

Remark 4.3 *Our analysis of the quadratures in Theorem 2.6 indicates that the approximation to the integral (2.9) is no longer uniform in $t \in [a, \infty)$ if $a = 0$. It is remarkable that in the limit case $t = 0$ the target integral is nothing but $1/2\mathcal{J}(\mathcal{L})$ with $\mathcal{J}$ given by (4.4). Therefore, assuming that $\mathcal{L} \in \mathbb{R}^{n\times n}$, we can apply a similar quadrature to the integral (2.9) as in (4.8) just by substituting $(\zeta I - H)^{-1}$ by the corresponding ansatz $e^{-\zeta t}(\zeta I - H)^{-1}$. Clearly, all assumptions of Theorem 4.2 are valid for the new integrand and we arrive at the same approximation result as in (4.8), now uniformly in $t \geq 0$. Again the number of terms can be estimated by $N = \mathcal{O}(|\log(\mathrm{cond}(\mathcal{L}))|^2 + |\log\varepsilon|^2)$, where one can expect $\mathrm{cond}(\mathcal{L}) = \mathcal{O}(h^{-2})$ for quasi-uniform meshes.*

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