Application of symmetric spaces and Lie triple systems in numerical analysis

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Abstract

Symmetric spaces are well known in differential geometry from the study of spaces of constant curvature. The tangent space of a symmetric space forms a Lie triple system. Recently these objects have received attention in the numerical analysis community. A remarkable number of different algorithms can be understood and analyzed using the concepts of symmetric spaces and this theory unifies a range of different topics in numerical analysis, such as polar type matrix decompositions, splitting methods for computation of the matrix exponential, composition of self adjoint numerical integrators and time symmetric dynamical systems.

In this paper we will give an introduction to the mathematical theory behind these constructions, and review recent results. Furthermore, we are presenting new results related to time reversal symmetries, self adjoint numerical schemes and Yoshida type composition techniques.

1 Introduction

In numerical analysis there are numerous examples of objects forming a *group*, i.e. we have a composition law and an inverse. Examples are the group of orthogonal matrices or the group of Runge-Kutta methods. *Semi groups*, where we have a composition but no inverse are also well known, e.g. the set of all matrices and explicit Runge-Kutta methods are two examples.

There are important examples of objects that are neither a group nor a semi group, where the class of objects is closed under a 'sandwich type' product, $(a, b) \mapsto aba$. For example the collection of all symmetric positive definite matrices and all self adjoint Runge-Kutta methods. Symmetric composition of numerical integrators are e.g. studied in [7]. If inverses are well defined, we may replace the sandwich product with the algebraically nicer *symmetric product* $(a, b) \mapsto ab^{-1}a$. Spaces closed under such products are called symmetric spaces and are the objects of study in this paper.

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Recall the theory of Lie groups, where fundamental tools are the Lie algebra (tangent space at the identity) and the exponential map from the Lie algebra to the Lie group. The Lie algebra is closed under commutators. In the theory of symmetric spaces there is a similar notion of tangent space. The resulting object is called a Lie triple system (LTS), and is closed under *double commutators*, $[X, [Y, Z]]$.

Associated with symmetric spaces and Lie triple systems there are important decomposition theorems. Lie algebras can be decomposed into a direct sum of a LTS and a subalgebra. The well known splitting of a matrix as a sum of a symmetric and a skew symmetric matrix is an example of such a decomposition, the skew symmetric matrices are closed under commutators, while the symmetric matrices are closed under double commutators. Similarly, there are decompositions of Lie groups into a product of a symmetric space and a Lie subgroup. The matrix polar decomposition, where a matrix is written as the product of a symmetric positive definite matrix and an orthogonal matrix is one example. We will see that there are many other important examples, such as the decomposition of a flow into the composition of two flows, one symmetric with respect to a diffeomorphism of the domain, and the other having the diffeomorphism as a *time reversal* symmetry.

The properties of these decompositions and numerical algorithms based on them are studied in a series of recent papers. In [12] the polar type decompositions are studied in detail, with special emphasis on optimal approximation results. The paper [22] is concerned with important recurrence relations for polar type decompositions, similar to the Baker-Campbell-Hausdorff formula for Lie groups.

In the recent years the interest in geometrical integration methods for differential equations has surged. These are numerical methods which exactly preserve various continuous structures of the dynamical systems. Examples of geometrical integrators are methods preserving first integrals [**?**], volume preserving integrators [**?**] integrators preserving Lyapunov functions [**?**] and integrators for systems evolving on Lie groups and symmetric spaces [4, 10]. The present theory has applications in reducing the cost of Lie group methods [23, 11, 5], and it also introduces the new question of how to integrate dynamical systems evolving on symmetric spaces.

The polar type decompositions are closely related to the more special root space decomposition employed in numerical integrators for differential equations on Lie groups in [15]. In [13] it is shown that the generalized polar decompositions can be successfully employed in cases where the theory of [15] cannot be used.

2 General theory of symmetric spaces and Lie triple systems

In this section we present some background theory for symmetric spaces and Lie triple systems. We expect the reader to be familiar with some basic concepts of differential geometry, like manifolds, vector fields, etc. For a more detailed treatment of symmetric spaces we refer the reader to [2] and [6] which also constitute the main reference of the material presented in this section.

We shall also follow (unless otherwise mentioned) the notational convention of [2]: in particular, M is a set (manifold), the letter G is reserved for groups and Lie groups, gothic letters denote Lie algebras and Lie triple systems, latin lowercase letters denote Lie-group elements and latin uppercase letters denote Lie-algebra elements. The identity element of a group will be usually denoted by e and the identity mapping by id.

2.1 Symmetric spaces

Definition 2.1 [[6]] A *symmetric space* is a manifold M with a differentiable *symmetric product* $\cdot$ obeying the following conditions:

(i) $x \cdot x = x$,

(ii) $x \cdot (x \cdot y) = y$,

(iii) $x \cdot (y \cdot z) = (x \cdot y) \cdot (x \cdot z)$,

and moreover

(iv) every x has a neighbourhood U such that $x \cdot y = y$ implies $y = x$ for all y in U.

The latter condition is relevant in the case of manifolds M with open set topology (as in the case of Lie groups) and can be disregarded for sets M with discrete topology: a discrete set M endowed with a multiplication obeying (i)–(iii) will be also called a symmetric space.

A *pointed symmetric space* is a pair (M, o) consisting of a symmetric space M and a point o called *base point.* Note that when M is a Lie group, it is usual to set $o = e$.

The left multiplication with an element $x \in M$ is denoted by S_x,

$$S_x y = x \cdot y, \quad \forall y \in M,$$

and is called *symmetry around* x. Note that $S_x x = x$ because of (i), hence x is fixed point of S_x and it is isolated because of (iv). Furthermore, (ii) and (iii) imply S_x is an involutive automorphism of M.

Symmetric spaces can be constructed in several different ways, the following are the most important:

1. Manifolds with an intrinsically defined symmetric product. As an example, consider the n-sphere as the set of unit vectors in $\mathbb{R}^{n+1}$. The product

   $$x \cdot y = S_x y = (2xx^T - I)y$$

   turns this into a symmetric space.

2. Subsets of a continuous (or discrete) group G that are closed under the composition $x \cdot y = xy^{-1}x$, where xy is the usual multiplication in G. Groups themselves, continuous, as in the case of Lie groups, or discrete, are thus particular instances of symmetric spaces. As another example, consider the set of all symmetric positive definite matrices as a subset of all nonsingular matrices, which forms a symmetric space with the product

   $$a \cdot b = ab^{-1}a.$$

3. Symmetric elements of automorphisms on a group. An automorphism on a group G is a map $\sigma : G \to G$ satisfying $\sigma(ab) = \sigma(a)\sigma(b)$. The *symmetric elements* are defined as

$$\mathcal{A} = \{\, g \in G \mid \sigma(g) = g^{-1} \,\}.$$

   It is easily verified that $\mathcal{A}$ obeys (i)–(iv) when endowed with the multiplication $x \cdot y = xy^{-1}x$, hence it is a symmetric space. As an example, symmetric matrices are symmetric elements under the matrix automorphism $\sigma(a) = a^{-T}$.

4. Homogeneous manifolds. Given a Lie group G and a subgroup H, a homogeneous manifold $M = G/H$ is the set of all left cosets of H in G. Not every homogeneous manifold possess a product turning it into a symmetric space, however, in what follows we will see that any connected symmetric space arise in a natural manner as a homogeneous manifold.

Let G be a connected Lie group and let σ be an analytic involutive automorphism, i.e. s $\sigma \neq \mathrm{id}$ and $\sigma^2 = \mathrm{id}$. Let G^σ denote $\mathrm{fix}\sigma = \{\, g \in G \mid \sigma(g) = g \,\}$, G^σ_e its connected component including the base point, in this case the identity element e and finally let K be a closed subgroup such that $G^\sigma_e \subset K \subset G^\sigma$. Set $G_\sigma = \{x \in G : \sigma(x) = x^{-1}\}$.

Theorem 2.1 ([6]) *The homogeneous space $M = G/K$ is a symmetric space with the product $xK \cdot yK = x\sigma(x)^{-1}\sigma(y)K$ and G_σ is a symmetric space with the product $x \cdot y = xy^{-1}x$. Moreover, G_σ is isomorphic to the homogeneous space G/G^σ.*

The importance of the above result resides in the fact that *every connected symmetric space* is of the type G/K and also of the type G_σ [6], and in particular they are also homogeneous spaces. As coset representatives for G/G^σ one may choose elements of G_σ, thus any $x \in G$ can be decomposed in a product

$$x = sq \text{ where } s \in G_\sigma \text{ and } q \in G^\sigma. \tag{2.1}$$

The matrix polar decomposition is a particular example, discussed in 3.1.

The automorphism σ on G induces an automorphism on the Lie algebra $\mathfrak{g}$ and a also a canonical decomposition of $\mathfrak{g}$. Let $\mathfrak{g}$ and $\mathfrak{k}$ denote the Lie algebras of G and K respectively and denote by $\mathrm{d}\sigma$ the differential of σ at e,

$$\mathrm{d}\sigma(X) = \frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0} \sigma(\exp(tX)), \quad \forall X \in \mathfrak{g}. \tag{2.2}$$

Note that $\mathrm{d}\sigma$ is an involutive automorphism of $\mathfrak{g}$ and has eigenvalues ± 1. Moreover, $X \in \mathfrak{k}$ implies $\mathrm{d}\sigma(X) = X$. Set $\mathfrak{p} = \{X \in \mathfrak{g} :\, \mathrm{d}\sigma(X) = -X\}$. Then

$$\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p} \tag{2.3}$$

[2]. It is easily verified that

$$\begin{aligned} [\mathfrak{k}, \mathfrak{k}] &\subset \mathfrak{k}, \\ [\mathfrak{k}, \mathfrak{p}] &\subset \mathfrak{p}, \\ [\mathfrak{p}, \mathfrak{p}] &\subset \mathfrak{k}, \end{aligned} \tag{2.4}$$

that is, $\mathfrak{k}$ is a subalgebra of $\mathfrak{g}$ while $\mathfrak{p}$ is an ideal in $\mathfrak{k}$. The decomposition (2.4) is called *Cartan decomposition* whenever the Cartan–Killing form $B(X,Y) = \mathrm{tr}(\mathrm{ad}_X \mathrm{ad}_Y)$ is nondegenerate, hence it can be used to introduce a positive bilinear form $B_{\mathrm{d}\sigma} = -B(X, \mathrm{d}\sigma(Y))$.

Given $X \in \mathfrak{g}$, its canonical decomposition $\mathfrak{k} \oplus \mathfrak{p}$ is

$$X = \frac{1}{2}\Big(X + \mathrm{d}\sigma(X)\Big) + \frac{1}{2}\Big(X - \mathrm{d}\sigma(X)\Big), \tag{2.5}$$

where $X + \mathrm{d}\sigma(X) \in \mathfrak{k}$ and $X - \mathrm{d}\sigma(X) \in \mathfrak{p}$.

2.2 Lie triple systems

In Lie group theory Lie algebras are important since they describe infinitesimally the structure of the tangent space at the identity. Similarly, Lie triple systems gives the structure of the tangent space of a symmetric space.

Definition 2.2 A vector space with a trilinear composition $[X,Y,Z]$ is called a *Lie triple system* (Lts) if the following identities are satisfied:

(i) $[X,X,X] = 0$,

(ii) $[X,Y,Z] + [Y,Z,X] + [Z,X,Y] = 0$,

(iii) $[X,Y,[U,V,W]] = [[X,Y,U],V,W] + [U,[X,Y,V],W] + [U,V,[X,Y,W]]$.

A typical way to construct a Lts is by means of an involutive automorphism of a Lie algebra $\mathfrak{g}$. With the same notation as above, the set $\mathfrak{p}$ is a Lts with the composition

$$[X,Y,Z] = [[X,Y],Z].$$

Vice versa, for every Lts there exists a Lie algebra $\mathfrak{G}$ and an involutive automorphism σ such that the given Lts corresponds to $\mathfrak{p}$. The algebra $\mathfrak{G}$ is called *standard embedding* of the Lts.

In general, any subset of $\mathfrak{g}$ that is closed under the operator

$$\mathrm{T}_X = \mathrm{ad}_X^2$$

is a Lie triple system. Being close under T_X guarantees being closed under the triple commutator: we have

$$[X,[Y,Z]] = \frac{1}{3}([X+Y,[X+Y,Z]]-[X-Y,[X-Y,Z]])+\frac{1}{6}([Y+Z,[Y+Z,X]]-[Y-Z,[Y-Z,X]]),$$

hence,

$$[X,[Y,Z]] = \frac{1}{3}(\mathrm{T}_{X+Y} - \mathrm{T}_{X-Y})Z + \frac{1}{6}(\mathrm{T}_{Y+Z} - \mathrm{T}_{Y-Z})X,$$

from which we deduce that $[X,[Y,Z]]$ is a linear combination of operators of the form $\mathrm{T}_V W$ [9].

3 Application of symmetric spaces in numerical analysis

The importance of symmetric spaces in numerical analysis has been overlooked in the past. We shall present common constructions in numerical analysis that strongly rely on symmetric spaces type constructions.

3.1 Polar type matrix decompositions

Let $\mathrm{GL}(N)$ be the group of $N \times N$ invertible real matrices. Consider the map

$$\sigma(x) = x^{-\mathrm{T}}, \qquad x \in \mathrm{GL}(N). \tag{3.1}$$

It is clear that σ is an involutive automorphism of $\mathrm{GL}(N)$. Then, according to Theorem 2.1, the set of symmetric elements $G_\sigma = \{x \in \mathrm{GL}(N) : \sigma(x) = x^{-1}\}$ is a symmetric space. We observe that G_σ is the set of invertible symmetric matrices. The symmetric space G_σ is disconnected and particular mention deserves its connected component containing the identity matrix I, since it reduces to the set of symmetric positive definite matrices. The subgroup G^σ consists of all orthogonal matrices. The decomposition (2.1) is the polar decomposition, any nonsingular matrix can be written as a product of a symmetric matrix and an orthogonal matrix. If we restrict the symmetric matrix to the symmetric positive definite matrices, then the decomposition is unique.

It is well known that the polar decomposition $x = sq$ can be characterized in terms of best approximation properties. The orthogonal part q is the best orthogonal approximation of x in any orthogonally invariant norm (e.g. 2-norm and Frobnius norm). In [12] such decompositions are generalized to arbitrary involutive automorphisms, and best approximation properties are established for the general case.

To derive the corresponding decomposition of the Lie algebra, we compute $\mathrm{d}\sigma$ making use of (2.2). Given $X \in \mathfrak{gl}(N)$,

$$\begin{aligned}
\mathrm{d}\sigma(X) &= \tfrac{\mathrm{d}}{\mathrm{d}t}\big|_{t=0}\sigma(\exp(tX)) = \tfrac{\mathrm{d}}{\mathrm{d}t}\big|_{t=0}(I + tX + \mathcal{O}(t^2))^{-\mathrm{T}} \\
&= \tfrac{\mathrm{d}}{\mathrm{d}t}\big|_{t=0}(I + tX^{\mathrm{T}} + \mathcal{O}(t^2))^{-1} = \tfrac{\mathrm{d}}{\mathrm{d}t}\big|_{t=0}(I - tX^{\mathrm{T}} + \mathcal{O}(t^2)) \\
&= -X^{\mathrm{T}},
\end{aligned}$$

hence we deduce that

$$\mathfrak{k} = \{X \in \mathfrak{gl}(N) :\, \mathrm{d}\sigma(X) = X\} = \mathfrak{so}(N),$$

the classical algebra of skew-symmetric matrices, while

$$\mathfrak{p} = \{X \in \mathfrak{gl}(N) :\, \mathrm{d}\sigma(X) = -X\}$$

is the classical set of symmetric matrices. Such set is not a subalgebra of $\mathfrak{gl}(N)$ but is closed under T_X, hence is a Lie triple system.

The decomposition (2.5) is nothing else than the canonical decomposition of a matrix into its skew-symmetric and symmetric part,

$$X = P + K = \frac{1}{2}(X + \mathrm{d}\sigma(X)) + \frac{1}{2}(X - \mathrm{d}\sigma(X)) = \frac{1}{2}(X - X^{\mathrm{T}}) + \frac{1}{2}(X + X^{\mathrm{T}}).$$

The group decomposition $x = sq$ can also be studied via the algebra decomposition. In [22] an explicit recurrence is given, if $\exp(X) = x$, $\exp(S) = s$ and $\exp(Q) = q$ then S and Q can be expressed in terms of commutators of P and K. The first terms in the expansions of X and Y are

$$\begin{aligned} X &= P - \tfrac{1}{2}[P,K] - \tfrac{1}{6}[K,[P,K]] \\ &\quad + \tfrac{1}{24}[P,[P,[P,K]]] - \tfrac{1}{24}[K,[K,[P,K]]] \\ &\quad + [K,[P,[P,[P,K]]]] - \tfrac{1}{120}[K,[K,[K,[P,K]]]] - \tfrac{1}{180}[[P,K],[P,[P,K]]] + \cdots, \\ Y &= K - \tfrac{1}{12}[P,[P,K]] + \tfrac{1}{120}[P,[P,[P,[P,K]]]] \\ &\qquad + \tfrac{1}{720}[K,[K,[P,[P,K]]]] - \tfrac{1}{240}[[P,K],[K,[P,K]]] + \cdots. \end{aligned} \tag{3.2}$$

The general framework of polar-type decompositions has important applications using other automorphisms. As an example, consider $G = \mathcal{O}(n+1)$, the Lie group of orthogonal $(n+1)\times(n+1)$ matrices, with the corresponding Lie algebra $\mathfrak{g} = \mathfrak{so}(n+1)$ of skew symmetric matrices. Let σ be an involutive automorphism on G given as

$$\sigma(x) = sxs$$

where s is the Householder reflection matrix $s = I - 2e_1e_1^T = \mathrm{diag}(-1,1,\dots 1)$. The corresponding algebra automorphism is given as

$$d\sigma(X) = sXs.$$

It is straightforward to verify that the subgroup G^σ of Theorem 2.1 consists of all orthogonal $(n+1)\times(n+1)$ matrices of the form

$$q = \begin{pmatrix} 1 & 0^T \\ 0 & q_n \end{pmatrix}$$

Where $q_n \in \mathcal{O}(n)$. Thus the corresponding symmetric space is $G/G^\sigma = \mathcal{O}(n+1)/\mathcal{O}(n)$. Matrices belong to the same coset if the first column coincide, thus the symmetric space can be identified with the n-sphere S^n.

The corresponding splitting of a skew symmetric matrix $V \in \mathfrak{g} = \mathfrak{so}(n+1)$ is

$$V = \begin{pmatrix} 0 & -v^T \\ v & V_n \end{pmatrix} = \begin{pmatrix} 0 & -v^T \\ v & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & V_n \end{pmatrix} = P + K \in \mathfrak{p} \bigoplus \mathfrak{k}.$$

Thus any orthogonal matrix can be expressed as the product of the exponential of a matrix in $\mathfrak{p}$ and one in $\mathfrak{k}$. The space $\mathfrak{p}$ can be identified with the tangent space to the sphere in the point $(1,0,\dots,0)^T$.

A number of papers deals with applications of these splittings in numerical analysis. In [23], such splittings are used in the computation of matrix exponentials, in [5, 13] similar ideas are used to construct numerical integrators for differential equations on Stiefel and Grassman manifolds, while [11] deals specifically with integrators on spheres.

3.2 Symmetries and reversing symmetries of differential equations

Let Diff(M) the group of diffeomorphism of a manifold M onto itself. We say that a map $\varphi \in \text{Diff}(M)$ has a symmetry $\mathcal{R} : M \to M$ if

$$\mathcal{R}\varphi\mathcal{R}^{-1} = \varphi$$

(the multiplication indicating the usual composition of maps, i.e. $\varphi_1\varphi_2 = \varphi_1 \circ \varphi_2$), while if

$$\mathcal{R}\varphi\mathcal{R}^{-1} = \varphi^{-1},$$

we say that $\mathcal{R}$ is a reversing symmetry of φ [7]. Symmetries and reversing symmetries are very important in the context of dynamical systems and their numerical integration. For instance, nongeneric bifurcations can become generic in the presence of symmetries and vice versa. Thus, when using the integration time-step as a bifurcation parameter, it is vitally important to remain within the smallest possible class of systems. As for reversing symmetries, they give rise to the existence of invariant tori and invariant cylinders [8, 17, 18, 19].

It is a classical result that the set of symmetries possess the structure of a group – they behave like automorphisms and fixed sets of automorphisms. The group structure, however, does not extend to reversing symmetries and fixed points of anti-automorphisms, and in the last few years the set of reversing symmetries has attention of numerous numerical analysts. [7] observed that the set of fixed points of an anti-automorphism $\mathcal{A}_-$ possesses the structure of a *pseudogroup*, since it is closed under the symmetric triple product

$$\varphi_1 \cdot \varphi_2 = \varphi_1\varphi_2\varphi_1 \in \text{fix}\mathcal{A}_-, \quad \forall \varphi_1, \varphi_2 \in \text{fix}\mathcal{A}_-,$$

that McLachlan et al. call "sandwich product". We have already seen in section 2.1 that the set of fixed points of an anti-automorphism is a symmetric space.

If M is a finite dimensional smooth compact manifold, it is well known that the infinite dimensional group of Diff(M) of all smooth diffeomorphisms $M \to M$ is a Lie group, with Lie algebra Vect(M) of all smooth vector fields on M, with the usual bracket and exponential map. It should be noted, however, that the exponential map is not a one-to-one map, not even close enough to the identity element, since there exist diffeomorphisms arbitrary close to the identity which are not on any one-parameter subgroup and others which are on many [16, 14]. However, the regions where the exponential map is not surjective became smaller and smaller the closer we approach the identity, and, for our purpose, we can disregard these regions and assume that our results are formally true.

There are two different settings that we can consider in this context. The first is to analyze the set of differentiable maps that possess a certain symmetry (or a discrete number of symmetries). The second is to consider the structure of the set of symmetries of a fixed diffeomorphism. The first has a continuous-type structure while the second is more often a discrete type symmetric space.

Proposition 3.1 *The set of diffeomorphisms φ that possess $\mathcal{R}$ as an (involutive) reversing symmetry is a symmetric space of the type G_σ.*

Proof. Denote

$$\sigma(\varphi) = \mathcal{R}\varphi\mathcal{R}^{-1}.$$

It is clear that σ acts as an automorphism,

$$\sigma(\varphi_1\varphi_2) = \sigma(\varphi_1)\sigma(\varphi_2),$$

moreover, if $\mathcal{R}$ is an involution then so is also σ. Note that the set of diffeomorphisms φ that possess $\mathcal{R}$ as a reversing symmetry is the space of symmetric elements G_σ defined by the automorphism σ (cf. section 2). Hence the result follows from Theorem 2.1. □

Proposition 3.2 *The set of reversing symmetries acting on an diffeomorphism φ is a symmetric space with the composition $\mathcal{R} \cdot \mathcal{S} = \mathcal{R}\mathcal{S}^{-1}\mathcal{R}$.*

Proof. If $\mathcal{R}$ is a symmetry of φ then so is also $\mathcal{R}^{-1}$, since $\mathcal{R}^{-1}\varphi^{-1}\mathcal{R} = \varphi$ and the assertion follows by taking the inverse on both sides of the equality. In particular, if $\mathcal{R}$ is a symmetry of φ it is also true that $\mathcal{R}^{-1}$ is a reversing symmetry of φ^{-1}. Next, we observe that if $\mathcal{R}$ and $\mathcal{S}$ are two reversing symmetries of φ then so is also $\mathcal{R}\mathcal{S}^{-1}\mathcal{R}$, since

$$\mathcal{R}\mathcal{S}^{-1}\mathcal{R}\varphi(\mathcal{R}\mathcal{S}^{-1}\mathcal{R})^{-1} = \mathcal{R}\mathcal{S}^{-1}\varphi^{-1}\mathcal{S}\mathcal{R}^{-1} = \mathcal{R}\varphi\mathcal{R}^{-1} = \varphi^{-1}.$$

It follows that the composition $\mathcal{R} \cdot \mathcal{S} = \mathcal{R}\mathcal{S}^{-1}\mathcal{R}$ is an internal operation on the set of reversing symmetries of a diffeomorphism φ.

With the above multiplication, the conditions i)–iii) of Definition 2.1 are easily verified. This prove the assert in the case when ϕ has a discrete set of reversing symmetries.

□

In what follows, we assume that $\mathcal{R}$ is differentiable.

Acting on $\varphi = \exp(tX)$,

$$\mathrm{d}\sigma X = \frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0} \sigma \exp(tX) = \mathcal{R}_* X \mathcal{R}^{-1},$$

where $\mathcal{R}_*$ is the pullback of $\mathcal{R}$. The pullback is natural with respect to the Jacobi bracket,

$$[\mathcal{R}_* X \mathcal{R}, \mathcal{R}_* Y \mathcal{R}] = \mathcal{R}_*[X, Y]\mathcal{R},$$

for all vector fields X, Y. Hence the map $\mathrm{d}\sigma$ is an involutory algebra automorphism. Let $\mathfrak{k}_\sigma$ and $\mathfrak{p}$ be the eigenspaces of $\mathrm{d}\sigma$ in $\mathfrak{g} = \mathrm{diff}(M)$. Then

$$\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p},$$

where

$$\mathfrak{k} = \{X : \mathcal{R}_* X = X\mathcal{R}\}$$

is the Lie algebra of vector fields that have $\mathcal{R}$ as a symmetry and

$$\mathfrak{p} = \{X : \mathcal{R}_* X = -X\mathcal{R}\}$$

is the Lie triple system, vector fields corresponding to maps that have $\mathcal{R}$ as a reversing symmetry. Thus, as is the case for matrices, every vector field X can be split into two parts,

$$X = \frac{1}{2}\Big(X + \mathrm{d}\sigma(X)\Big) + \frac{1}{2}\Big(X - \mathrm{d}\sigma(X)\Big) = \frac{1}{2}\Big(X + \mathcal{R}_* X \mathcal{R}^{-1}\Big) + \frac{1}{2}\Big(X - \mathcal{R}_* X \mathcal{R}^{-1}\Big),$$

having $\mathcal{R}$ as a symmetry and reversing symmetry respectively.

In the context of ordinary differential equation, let us consider

$$\frac{\mathrm{d}y}{\mathrm{d}t} = F(y), \qquad y \in \mathbb{R}^N. \tag{3.3}$$

Given an arbitrary involutive function $\mathcal{R}$, the vector field F can always be canonically split into two components, having $\mathcal{R}$ as a symmetry and reversing symmetry respectively. However, if one of these components equals zero, then the system (3.3) has $\mathcal{R}$ as a symmetry or a reversing symmetry.

3.3 Selfadjoint numerical schemes

Let us consider the ODE (3.3), whose exact flow will be denoted as $\varphi = \exp(tF)$. Backward error analysis for ODEs implies that a (consistent) numerical method for the integration of (3.3) can be interpreted as the sampling at $t = h$ of the flow $\varphi_h(t)$ of a vector field F_h which is close to F,

$$\varphi_h(t) = \exp(tF_h), \quad F_h = F + h^p E_p + h^{p+1} E_{p+1} + \cdots,$$

where p is the order of the method (note that setting $t = h$, the local truncation error is of order h^{p+1}). We say that F_h is the *shadow* vector field of F.

Consider next the map σ on the set of flows depending on the parameter h defined as

$$\sigma(\varphi_h(t)) = \varphi_{-h}(-t), \tag{3.4}$$

where $\varphi_{-h}(t) = \exp(tF_{-h})$, with $F_{-h} = F + (-h)^p E_p + (-h)^{p+1} E_{p+1} + \cdots$.

The map σ is involutive, since $\sigma^2 = \mathrm{id}$, and it is easily verified by means of the BCH formula that $\sigma(\varphi_{1,h}\varphi_{2,h}) = \sigma(\varphi_{1,h})\sigma(\varphi_{2,h})$, hence σ is an automorphism. Consider next

$$G_\sigma = \{\varphi_h : \sigma(\varphi_h) = \varphi_h^{-1}\}.$$

Then $\varphi_h \in G_\sigma$ if and only if $\varphi_{-h}(-t) = \varphi_h^{-1}(t)$, namely the method φ_h is *selfadjoint*. Thus, by virtue of Theorem 2.1, the set of selfadjoint numerical schemes is a symmetric space.

Next, we perform the decomposition (2.3). We deduce from (3.4) that

$$\mathrm{d}\sigma(F_h) = \frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0} \sigma(\exp(tF_h)) = -(F + (-h)^p E_p + (-h)^{p+1} E_{p+1}) + \cdots = -F_{-h},$$

hence,

$$\mathfrak{k} = \{F_h : \mathrm{d}\sigma(F_h) = F_h\} = \{F_h : -F_{-h} = F_h\},$$

is the subalgebra of vector fields that are odd in h, and

$$\mathfrak{p} = \{F_h : \mathrm{d}\sigma(F_h) = -F_h\} = \{F_h : F_{-h} = F_h\},$$

is the Lts of vector fields that possess only even powers of h. Thus, if F_h is the shadow vector field of a numerical integrator φ_h, its canonical decomposition in $\mathfrak{k} \oplus \mathfrak{p}$ is

$$\begin{aligned} F_h &= \frac{1}{2}(F_h + \mathrm{d}\sigma(F_h)) + \frac{1}{2}(F_h - \mathrm{d}\sigma(F_h)) \\ &= \frac{1}{2}(F + \sum_{k=p}^{\infty}(1-(-1)^k)h^k E_k) + \frac{1}{2}(F + \sum_{k=p}^{\infty}(1+(-1)^k)h^k E_k), \end{aligned}$$

the first term containing only odd powers of h and the second only even powers. Then, if the numerical method $\varphi_h(h)$ is selfadjoint, it contains only odd powers of h locally (in perfect agreement with classical results on selfadjoint methods [1].

3.4 Polar decomposition and its generalization to vector fields: Connections with the generalized Scovel projection and the Thue–Morse sequence for symmetries

In a recent paper, [12] have shown that it is possible to generalize the polar decomposition of matrices to Lie groups endowed with an involutive automorphism. They have shown that every Lie group element z sufficiently close to the identity can be decomposed as $z = xy$ where $x \in G_\sigma$, the space of symmetric elements of σ, and $y \in G^\sigma$, the subgroup of G of elements fixed under σ. Furthermore, setting $z = \exp(tZ)$ and $y = \exp(Y(t))$, one has that $Y(t)$ is an odd function of t and it is a best approximant to z in G^σ in G^σ right-invariant norms constructed by means of the Cartan–Killing form, provided that G is semisimple and that the decomposition $\mathfrak{g} = \mathfrak{p} \oplus \mathfrak{k}$ is a Cartan decomposition.

Assume that φ, the exact flow of the differential equation (3.3), has $\mathcal{R}$ as a reversing symmetry (i.e. $F \in \mathfrak{p}_\sigma$, where $\sigma(\varphi) = \mathcal{R}\varphi\mathcal{R}^{-1}$), while its approximation φ_h has not. We perform the polar decompostion

$$\varphi_h = \psi_h \chi_h, \tag{3.5}$$

where χ_h is the factor we wish to get rid of, since it is the one that has $\mathcal{R}$ as a symmetry. We have $\psi_h^2 = \varphi_h \sigma(\varphi_h)^{-1}$. Hence the method obtained composing φ_h with $\sigma(\varphi_h)^{-1}$ has the reversing symmetry $\mathcal{R}$ every other step. To obtain ψ_h we need to extract the square root of the flow $\varphi_h\sigma(\varphi_h)^{-1}$. Now, if $\phi(t)$ is a flow, then its square root is simply $\phi(t/2)$. However, if $\phi_h(t)$ is the flow of a consistent numerical method ($p \geq 1$), namely the numerical integrator corresponds to $\phi_h(h)$, it is not possible to evaluate the square root $\phi_h(h/2)$ by simple means as is not the same as numerical method with half the stepsize, $\phi_{h/2}(h/2)$. The latter, however, offers an approximation to the square root: note that

$$\phi_{\frac{h}{2}}\left(\frac{h}{2}\right)\phi_{\frac{h}{2}}\left(\frac{h}{2}\right) = \exp\left(hF + h(\frac{h}{2})^p E_p\right) + \cdots,$$

an expansion which, compared with $\phi_h(h)$, reveals that he error in approximating the square root with the numerical method with half the stepsize is of the order of

$$\left(\frac{2^p - 1}{2^p}\right) h^{p+1} E_p,$$

a term that is subsumed in the local truncation error.

Choosing $\tilde{\psi}_h = \varphi_{h/2}\sigma(\varphi_{h/2})^{-1} = \varphi_{h/2}\sigma(\varphi_{h/2}^{-1})$ as an approximation to ψ_h (we stress that each flow is now evaluated at $t = h/2$), we observe that $\tilde{\psi}_h$ that has the reversing symmetry $\mathcal{R}$ at each step by design, since

$$\sigma(\tilde{\psi}_h) = \sigma(\varphi_{h/2}\sigma(\varphi_{h/2}^{-1})) = \sigma(\varphi_{h/2})\varphi_{h/2}^{-1} = \tilde{\psi}_h^{-1}.$$

Note that $\tilde{\psi}_h = \varphi_{h/2}\sigma(\varphi_{h/2}^{-1})$, where $\varphi_{h/2}^{-1}(t) = \varphi_{-h/2}^{*}(-t)$ is the inverse (or adjoint) method of $\varphi_{h/2}$. If σ is given by (3.4), then $\sigma(\varphi_{h/2}^{-1}) = \varphi_{h/2}^{*}(h/2)$ and this algorithm is precisely the generalized Scovel projection [7] to generate selfadjoint numerical schemes from an arbitrary integrator.

Proposition 3.3 *The Scovel projection is equivalent to choosing the G_σ-factor in the polar decomposition of a flow φ_h under the involutive automorphism $\sigma(\varphi) = \mathcal{R}\varphi\mathcal{R}^{-1}$, whereby square roots of flows are approximated with numerical methods with half the step-size.*

Another algorithm that can be related to the generalized polar decomposition of flows is the application of the Thue–Morse sequence to improve the preservation of symmetries by means of a numerical integrator [3]. Given an involutive automorphism $\mathcal{A}$ and a numerical method φ_h in a group G of numerical integrators, [3] construct the sequence of methods

$$\varphi^{[0]} := \varphi_h, \quad \varphi^{[k+1]} := \varphi^{[k]}\mathcal{A}\varphi^{[k]}, \qquad k = 0, 1, 2, \ldots.$$

Since $\varphi^{[k]} = \mathcal{A}^0\varphi^{[k]}$, it is easily understood that the k-th method corresponds to composing $\mathcal{A}^0\varphi^{[k]}$ and $\mathcal{A}^1\varphi^{[k]}$ according to the k-th Thue–Morse sequence[1], 01101001 . . ., as displayed below in Table 1. Note that $\varphi^{[k]}$ performs 2^k steps with stepsize h with combinations of

k	$\varphi^{[k]}$	sequence
0	φ	'0'
1	$\varphi\mathcal{A}\varphi$	'01'
2	$\varphi\mathcal{A}\varphi\mathcal{A}\varphi\varphi$	'0110'
3	$\varphi\mathcal{A}\varphi\mathcal{A}\varphi\varphi\mathcal{A}\varphi\varphi\varphi\mathcal{A}\varphi$	'01101001'

Table 1: Thue–Morse iterations for the method φ

φ_h and $\mathcal{A}\varphi_h$.

[3] showed that each iteration improves of one order the preservation of the symmetry $\mathcal{S}$, where $\mathcal{S}$ is the involutive automorphism such that $\mathcal{A}\phi = \mathcal{S}\phi\mathcal{S}^{-1}$: in other words, if the method φ_h retains $\mathcal{S}$ to order p, then $\varphi^{[k]}$ retains the symmetry $\mathcal{S}$ or order $p + k$.

Let us return to the polar decomposition (3.5), and recall that χ_h is the term we wish to approximate (since it is the one preserving the symmetry $\mathcal{S}$, here $\sigma \equiv \mathcal{A}$). Recall that we have approximated the factor $\psi_h \approx \varphi_{h/2}\sigma(\varphi_{h/2})^{-1}$. Since $\chi_h = \psi_h^{-1}\varphi_h$, one has a first

[1]Expanding $\varphi_h^{[k]}$ in an iterative manner, one readily recognizes that the exponents of the automorphism $\mathcal{A}$, taken in sequential order, constitute precisely the k-th Thue–Morse sequence

approximation $\chi_h \approx \sigma(\varphi_{h/2})\varphi_{h/2}^{-1}\varphi_h \approx \sigma(\varphi_{h/2})\varphi_{h/2} := \chi_h^{[1]}$, where in the last passage we have approximated $\varphi_{h/2}^{-1}\varphi_h$ with $\varphi_{h/2}$. If instead of halving the stepsize we perform two steps with stepsize h, it is readily seen that $\chi_{2h}^{[1]}$ is a the first iteration of the Thue–Morse sequence and corresponds to the binary conjugation of the sequence defining $\varphi^{[1]}$. Similarly, we iterate the procedure performing the polar decomposition of $\chi_{2h}^{[1]}$. We approximate the subgroup factor as above to obtain a new approximation $\chi_{4h}^{[2]} = \sigma(\varphi_h)\varphi_h\varphi_h\sigma(\varphi_h)$ et cetera, which is the binary conjugation of $\varphi^{[2]}$.

Thus, at each step, the order of symmetry is increased by one unit as it follows from [3]. However, for exact preservation of the symmetry $\mathcal{S}$ one needs an infinite Thue–Morse sequence. The fact that the length of Thue–Morse sequences doubles at each iteration makes it difficult to prove any relation between the real χ_h factor in the polar decomposition of φ_h and the approximating sequence $\chi_h^{[k]}$.

3.5 A Yoshida-type technique for systems with symmetries

In a famous paper appeared in 1990, [20] showed how to construct high order time-symmetric integrators starting from lower order time-symmetric symplectic ones. Yoshida showed that, if φ is a selfadjoint numerical integrator of order $2p$, then

$$\varphi_{\alpha h}(\alpha t)\varphi_{(\beta h)}(\beta t)\varphi_{\alpha h}(\alpha t)$$

is a selfadjoint numerical method of order $2p+2$ provided that the coefficients α and β satisfy the condition

$$\begin{aligned} 2\alpha + \beta &= 1 \\ 2\alpha^{2p+1} + \beta^{2p+1} &= 0, \end{aligned}$$

whose only real solution is

$$\alpha = \frac{1}{2 - 2^{1/(2p+1)}}, \qquad \beta = -\frac{2^{1/(2p+1)}}{2 - 2^{1/(2p+1)}}. \tag{3.6}$$

In the formalism of this paper, time-symmetric methods correspond to G_σ-type elements with σ as in (3.4) and it is clearly seen that the Yoshida technique can be used in general to improve the order of approximation of G_σ-type elements.

In this section we shall show that a Yoshida-type procedure can be instead applied to improve the order of the retention of symmetries and not just reversing symmetries. To be more specific, let $\mathcal{S}$ be a symmetry of the given differential equation, namely $\mathcal{S}_*F = F\mathcal{S}$, with $\mathcal{S} \neq \mathrm{id}$, $\mathcal{S}^{-1} = \mathcal{S}$ and $\mathcal{S}_*$ denoting the pullback of $\mathcal{S}$ to $\mathfrak{g} = \mathrm{Vect}(M)$ (see § 3.2). Here, the involutive automorphism is given by

$$\sigma\varphi_h(t) = \mathcal{S}\varphi_h(t)\mathcal{S},$$

so that

$$\mathfrak{p} = \{P : \mathcal{S}_*P = -P\mathcal{S}\}, \quad \mathfrak{k} = \{K : \mathcal{S}_*K = K\mathcal{S}\}.$$

Let us assume that $\varphi_h(t)$ is the flow of a selfadjoint numerical method (the numerical method is obtained for $t = h$) of order $2p$,

$$\varphi_h(t) = \exp(tF_h),$$

where

$$F_h = F + h^{2p} E_{2p} + h^{2p+2} E_{p+2} + \cdots$$

and

$$E_j = P_j + K_j, \quad P_j \in \mathfrak{p}, K_j \in \mathfrak{k}.$$

We consider the composition

$$\varphi_h^{[1]}(t) = \varphi_{ah}(at)\sigma(\varphi_{bh}(bt))\varphi_{ah}(at). \tag{3.7}$$

which reduces to

$$\varphi_h^{[1]}(t) = \exp(atF_{ah}) \exp(bt\, \mathrm{d}\sigma(F_{bh})) \exp(atF_{ah}).$$

Application of the symmetric BCH formula, together with the fact that $\mathrm{d}\sigma$ acts by changing the signs on the $\mathfrak{p}$-components only, allows us to write the relation (3.7) as

$$\begin{aligned} \varphi_h^{[1]}(t) \;\; = \;\; & \exp((2a+b)tF + (2at(ah)^{2p} - bt(bh)^{2p})P_{2p} \\ & + (2at(ah)^{2p} + bt(bh)^{2p})K_{2p} + \mathcal{O}\big(th^{2p+2}\big) + \mathcal{O}\big(t^3h^{2p}\big) + \cdots). \end{aligned} \tag{3.8}$$

We recall that the corresponding numerical method is obtained letting $t = h$. Setting

$$2a + b = 1 \tag{3.9}$$

for consistency, and

$$2a^{2p+1} - b^{2p+1} = 0, \tag{3.10}$$

to annihilate the lowest order $\mathfrak{p}$-term, we observe that the resulting method $\varphi_h^{[1]}(t)$ is still time-symmetric (because of the symmetric BCH formula), has still order $2p$ but it satisfies the symmetry $\mathcal{S}$ to order $2p+2$. This procedure allows us to gain two extra degrees in the retention of symmetry per iteration, compared with the Thue–Morse sequence of [3] yielding one extra degree in symmetry per iteration.

Note that, differently from the case of the Yoshida technique, whereby the second step (corresponding to β in (3.6)) is required to be negative, for our sequence, (3.9)-(3.10) imply that

$$a = \frac{1}{2 + 2^{1/(2p+1)}}, \qquad b = \frac{1/2^{2p+1}}{2 + 2^{1/(2p+1)}}$$

hence all the time steps are positive. In general, the procedure can be iterated in the following manner: Assume that $\varphi_h^{[k]}(t)$ is known and it is associated with a time-symmetric method of order $2p$ which retains the symmetry $\mathcal{S}$ to order $2(p+k)$. Then,

$$\varphi_h^{[k+1]}(t) = \varphi_{a_{k+1}h}^{[k]}(a_{k+1}t)\sigma(\varphi_{b_{k+1}h}^{[k]}(b_{k+1}t))\varphi_{a_{k+1}h}^{[k]}(a_{k+1}t) \tag{3.11}$$

yields a numerical method that retains the symmetry $\mathcal{S}$ to order $2(p+k+1)$ provided that

$$a_{k+1} = \frac{1}{2+2^{1/(2(p+k)+1)}}, \qquad b_{k+1} = \frac{1/2^{(2(p+k)+1)}}{2+2^{1/(2(p+k)+1)}}.$$

One might question what is the advantage of this technique when compared to the Yoshida technique, since the latter increases of two units the order of the numerical integrator hence the retention of symmetry in a similar manner. As we have mentioned above, our procedure can be applied to stiff problems, whereas the Yoshida technique is not suitable for stiff problems since it requires the second step to be negative.

4 Numerical experiments

In this section we illustrate some of the results discussed in this paper by numerical experiments.

4.1 The Yoshida-type technique for systems with symmetries

Let $u \in \mathrm{GL}(\mathbb{R}, N)$ and consider the differential equation

$$u' = b(u)u, \quad u(0) = I, \qquad t \in [0, T], \tag{4.1}$$

where b is a $N \times N$ matrix function of u and I is the usual $N \times N$ identity matrix. We assume that b has the form

$$b(u) = l_- - l_+, \qquad l = u l_0 u^{-1},$$

where l_0 is a fixed symmetric matrix and l_-, l_+ denote the lower and upper triangular parts of the matrix l respectively. Differential equations of this kind appear time and again in conjunction with *isospectral flows,* since the eigenvalues of the matrix l do not change with time. The numerical solution of isospectral flows has been discussed at length in [21].

The differential equation (4.1) possesses the symmetry $\mathcal{S}u = u^{-\mathrm{T}}$, namely $\sigma(\varphi) = \mathcal{S}\varphi\mathcal{S}$ and the set G^σ corresponds to orthogonal matrices. In particular, if the initial condition is an orthogonal matrix (as in our case), the theoretical solution $u(t)$ stays orthogonal for all $t \in [0, T]$. This retention of symmetry of this differential equation by means of the Thue–Morse technique was discussed in [3].

Unfortunately, when solving numerically (4.1) with standard numerical schemes, like for instance Runge–Kutta or multistep methods, orthogonality of the solution is usually lost: although orthogonality reduces to a quadratic constraint, even method preserving quadratic conservation laws might fail to be orthogonal if the matrix b is not skew-symmetric in the internal stages of the method. This happens, for instance, when (4.1) is solved with the *implicit midpoint rule,* that in this case reads

$$u_{n+1} = u_n + h b(u_{n+\frac{1}{2}}) u_{n+\frac{1}{2}}, \qquad u_{n+\frac{1}{2}} = \frac{u_n + u_{n+1}}{2},$$

whenever u_{n+1} is obtained by fixed point iteration, the first iteration being approximated by a forward Euler step.

The implicit midpoint rule (IMR), however, possesses a time-reversing symmetry, hence the shadow vector field F_h expands in even powers of h only. Thus, we can apply a step of the Yoshida-type technique (3.7) to improve of two units the retention of the symmetry $\mathcal{S}$ (i.e. of orthogonality). Since the order of the method is two, we choose

$$a = \frac{1}{2+2^{1/3}}, \qquad b = \frac{2^{1/3}}{2+2^{1/3}}$$

and solve the second step in the variables $x = \mathcal{S}u = u^{-\mathrm{T}}$. The differential equation for x is given by

$$x' = b(xl_0'x^{-1})x,$$

which is obtained from (4.1) taking into account that $b(l)^{\mathrm{T}} = -b(l^{\mathrm{T}})$.

The improvement of the retention of orthogonality is displayed in Figure 4.1 for a 3×3 problem with matrix

$$l_0 = \begin{bmatrix} 1 & \frac{1}{2} & 0 \\ \frac{1}{2} & 2 & \frac{3}{2} \\ 0 & \frac{3}{2} & -3 \end{bmatrix},$$

with $T = 5$. The errors are sampled for $h = \frac{1}{20}, \frac{1}{40}, \ldots, \frac{1}{640}$ and the reference solution is computed with the Matlab routine `ode45` with absolute and relative tolerance set to `1e-12`. Clearly, the order of the resulting method is still two, while orthogonality is retained to order four. The slopes of the lines corresponding to h^2 and h^4 are reported in the figure for reference.

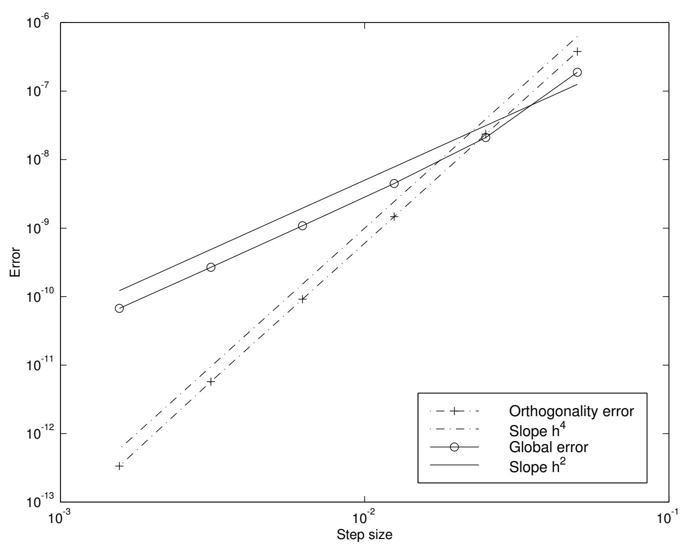

Figure 1: Orthogonality error and global error for one step of the Yoshida-type sequence applied to the IMR (logarithmic scale). The symmetry is retained to two orders of accuracy higher than the order of the scheme.

5 Conclusions

The structures of symmetric spaces and Lie triple systems are frequently encountered in numerical analysis. We have seen examples of how these concepts form a unifying approach to a number of different algorithmic problems in numerical analysis. This mathematical theory is an important tool in the study of numerical integration of differential equations and in linear algebra.

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