

Numerical Exploitation of Symmetry in Integral Equations^{3,4}

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Abstract: Linear integral operators describing physical problems on symmetric domains often are equivariant, which means that they commute with certain symmetries, i.e., with a group of orthogonal transformations leaving the domain invariant. Under suitable discretizations the resulting system matrices are also equivariant. A method for exploiting this equivariance in the numerical solution of linear equations and eigenvalue problems via *symmetry reduction* is described. A very significant reduction in the computational expense in both the assembling of the system matrix and in solving linear systems can be obtained in this way. This reduction is particularly important because the system matrices are typically full. The basic ideas underlying our method and its analysis involve group representation theory. We concentrate here on the use of symmetry adapted bases and their automated generation. In this paper symmetry reduction is studied in connection with quadrature formulae and the Nyström method. A software package has been posted on the internet.

Keywords: equivariant integral equations, symmetry groups, boundary element method, Nyström method, linear equation solvers, finite Fourier transform

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1. INTRODUCTION

Many problems in science and mathematics exhibit symmetry phenomena which may be exploited to analyze them, and also to effect a significant cost reduction in their numerical treatment. Usually the symmetry stems from the domain or body on which the problem is considered. The numerical treatment of problems such as partial differential equations and integral equations generally involves discretizations which ought (as far as possible) to incorporate or respect such symmetries. The present paper discusses some of the techniques in the context of integral equations. In contrast to the survey [3], which builds upon [1, 2, 4, 11, 12, 13, 25, 27], the present paper studies the exploitation of symmetry from the point of view of symmetry adapted bases and discretization via the Nyström method. Although the symmetry adapted bases approach is conceptually simpler and easier to implement (e.g., in MATLAB), the presentation in [3] is more convenient for derivations and proofs, and it also leads in a more natural way to efficient algorithms.

The basic concept is a generalization of the Fourier transform for arbitrary finite groups. We study here the general case which incorporates non-abelian groups (i.e., having irreducible representations of dimension > 1) and the possibility that some nodes or elements of the discretization remain fixed under some of the symmetries. This latter case is of considerable practical importance since it naturally occurs in the most frequently used finite element or boundary element discretizations, and since it considerably complicates the algorithmic approach.

Although the algebraic tool employed here is the classical representation theory of groups, which has been a venerated tool in physics, the systematic exploitation of these tools in numerical analysis has only recently begun, e.g., Stiefel and Fässler [9, 24]. They introduced symmetry adapted bases to analyze equivariant linear maps. These bases have been exploited in many numerically oriented papers on bifurcation theory under group actions, in the spirit of [15, 16, 28], see, e.g., [8, 10, 19, 20, 21, 29]. Our approach can be viewed as a method to *automatically* generate these symmetry adapted bases. The fact that the generation of symmetry adapted bases can be automated is of considerable importance for standard discretizations of operator equations and has been presented in the literature only on a case by case basis.

We will see that a straightforward application of the concept of symmetry adapted bases leads to implementations that are not optimal from the point of view of efficiency. We will note this and make appropriate modifications at these points. It is possible to avoid the use

of symmetry adapted bases altogether at the cost of a more complex notation. This is the point of view taken in [3] and also in our software [14].

2. GROUP THEORETICAL BACKGROUND

Let us briefly outline the group theoretical background and motivation of the symmetry reduction method. Underlying the method is a decomposition of equivariant linear operators via projectors defined by means of group representations. Deeper familiarity with these group concepts is not essential for understanding the subsequent sections of the paper.

If Γ is a finite group, H a finite dimensional complex vector space, $T : \Gamma \rightarrow L(H)$ a linear representation (i.e., an action) of Γ on H , and $A : H \rightarrow H$ a linear operator which commutes with T (i.e., is equivariant), then it is well known that H splits into a canonical direct sum

$$H = \bigoplus_{\mathbf{r}, \rho} H_{\mathbf{r}, \rho}$$

via the projectors $P_{\mathbf{r}, \rho} : H \rightarrow H_{\mathbf{r}, \rho}$ which are defined by

$$(1) \quad P_{\mathbf{r}, \rho} = \frac{\dim \mathbf{r}}{|\Gamma|} \sum_{g \in \Gamma} \mathbf{r}_{\rho, \rho}(g^{-1}) T(g)$$

where \mathbf{r} runs through a complete list \mathcal{R} of irreducible representations of Γ and $\rho = 1 : \dim \mathbf{r}$. It is well known that the equivariance of A leads to a splitting

$$(2) \quad A = \bigoplus_{\mathbf{r}, \rho} A_{\mathbf{r}, \rho}$$

where $A_{\mathbf{r}, \rho} : H_{\mathbf{r}, \rho} \rightarrow H_{\mathbf{r}, \rho}$. This can be exploited to solve linear equations or eigenvalue problems involving A . Hence the linear equations or eigenvalue problems are solved over each of the subspaces $H_{\mathbf{r}, \rho}$. We call this approach the *symmetry reduction method*.

In earlier literature, this splitting is performed by introducing a symmetry adapted basis, i.e., a collection of bases for each subspace $H_{\mathbf{r}, \rho}$, see [9, 24]. For some applications such bases can be seen easily enough. However, for large scale discretizations of operator equations where typically some of the nodes or elements are fixed under some symmetries, it is desirable to implement this approach more systematically. Thus we are led to generating the symmetry adapted bases automatically. This is the approach we describe here. The applications we have in mind are discretizations of integral equations which display some

symmetry structure. We will see that the sum in (1) and variations thereof will remain (not surprisingly) a basic theme of the method.

Guy and Mangeot [17] applied the projection operators (1) to decompose functions and integral operators into coupled subproblems. In particular, the equivariant kernels which we discuss in Section 4 lead to decoupled subproblems. In this case, the solution is expressed in terms of the resolvents of the subproblems. The smaller spectral radii of the resolvents of the subproblems can yield faster convergence of the corresponding Neumann series. Our paper does not investigate these questions but concentrates on solving discretized integral equations.

3. BASIC FACTS ABOUT GROUPS

Let us briefly review some basic facts about groups that will be needed in the sequel. For the rest of the paper Γ will be some finite group. For the applications we have in mind, Γ will be a group of orthogonal transformations in \mathbb{R}^N where N is typically 2 or 3.

Let \mathcal{U}_d denote the group of unitary matrices of size d . A (unitary) *representation* of Γ is a group homomorphism $\mathbf{r} : \Gamma \rightarrow \mathcal{U}_d$, such that the unit element $I \in \Gamma$ is mapped onto the identity matrix. The number $d_{\mathbf{r}} := d$ is called the *dimension* of \mathbf{r} .

The representation is called *irreducible* if it has no proper invariant subspaces: This means that there is no matrix P of size d with $P^2 = P \notin \{0, I\}$ (i.e., a non-trivial projection) such that $P\mathbf{r}(g)(I-P) = 0$ for all $g \in \Gamma$.

Two representations are called *equivalent* if they differ only by a similarity transformation. A maximal number of non-equivalent irreducible representations is called a *complete list* \mathcal{R} of representations for Γ .

For many of the groups which are important in applications (in particular groups of geometric symmetries) such a complete list is known and can be found in standard books such as [23]. The lists have been implemented in [14] for a number of groups.

The following result can be found in standard textbooks which discuss group representation theory:

Theorem 1 (Orthogonality Relation). *Let \mathcal{R} be a complete list of representations for a finite group Γ . For a fixed $\mathbf{r} \in \mathcal{R}$ and fixed indices $i, j = 1 : d_{\mathbf{r}}$ the map $g \mapsto \mathbf{r}_{i,j}(g)$ defines a column in $\mathbb{C}^{|\Gamma|}$ where $|\Gamma|$ denotes the order of the group. Then*

$$g \mapsto \sqrt{\frac{d_{\mathbf{r}}}{|\Gamma|}} \mathbf{r}_{i,j}(g) \quad \text{for } \mathbf{r} \in \mathcal{R} \text{ and } i, j = 1 : d_{\mathbf{r}}$$

is an orthonormal basis of $\mathbb{C}^{|\Gamma|}$.

A well-known consequence of this is

$$(3) \quad \sum_{r \in \mathcal{R}} d_r^2 = |\Gamma|.$$

If Γ is a group of orthogonal transformations in \mathbb{R}^N , then Γ acts in a natural way on the functions $x : \mathbb{R}^N \rightarrow \mathbb{R}$ by setting $(gx)(t) = x(g^{-1}t)$ for all $g \in \Gamma$ and $t \in \mathbb{R}^N$.

4. EQUIVARIANT KERNELS

For the sake of simplicity, let us restrict our attention to integral equations of the second kind. Since the identity operator turns out to be equivariant with respect to any group action, our discussion can be easily carried over to integral equations of the first kind.

Hence, consider an integral equation

$$(4) \quad x(s) + \int_D K(s, t)x(t)d\mu(t) = b(s)$$

where $d\mu$ is a standard measure on the domain $D \subset \mathbb{R}^N$, i.e., a so-called volume element for D if D has interior, or a so-called surface element for D if D is an $N - 1$ dimensional manifold.

The reader should note that we make no assumptions on the kernel, and do not discuss the nature of the Sobolev space on which the corresponding integral operators are defined. We do this to avoid a technical discussion which would be unimportant for the present aims. The proofs given below can be easily modified to accomodate for these technical matters. On the other hand, we do not want to leave the reader with the impression that we only consider *nice* kernels.

The theory of integral equations has been considerably advanced in recent decades, and it is beyond the aims and possibilities of this paper to revisit the proofs of the most general results under the aspect of a given symmetry invariance. This is (in our opinion) also not necessary since our proofs are very formal (as can be seen in the examples below) and can be easily added into the right technical context. As a simple example: If the reader thinks that an “almost everywhere” should be added in a statement, then he is most probably right.

Furthermore, in the next sections we investigate some aspects of discretization methods of integral equations. We emphasize that the choice of a specific discretization method has to be appropriate for a given integral equation. Our point is that if certain formal rules are followed when discretizing, and if the underlying integral equation displays equivariance, then the discretized problem also displays some equivariance.

Let us now begin the discussion by assuming that the domain D displays symmetries, i.e., there is a non-trivial group Γ of orthogonal transformations in \mathbb{R}^N that map D onto itself. We will show that such symmetries can be exploited if they are also respected by the kernel function K . It turns out that the appropriate condition for K is the following:

Definition 2. Let the domain D have the symmetries Γ . Let $K : D \times D \rightarrow \mathbb{R}$ be a kernel. We call the kernel K or the associated integral operator *equivariant* with respect to Γ if the operator commutes with the actions of Γ on D , i.e.,

$$(5) \quad \int_D K(s, t)x(gt)d\mu(t) = \int_D K(gs, t)x(t)d\mu(t)$$

holds for all $s \in D$, $g \in \Gamma$, and for all permissible functions x .

Remark 3. We are considering only the standard volume and surface elements as measures for the integration. It is readily seen that they are invariant under the orthogonal transformations $g \in \Gamma$. This fact will be used in the next proof and in other parts of the paper.

Theorem 4. Let the domain D have the symmetries Γ . Let $K : D \times D \rightarrow \mathbb{R}$ be a kernel. Then K is equivariant if and only if

$$(6) \quad K(gs, gt) = K(s, t) \quad \text{for } g \in \Gamma \quad \text{and } s, t \in D.$$

Proof. We obtain the following identity:

$$\begin{aligned} \int_D K(s, g^{-1}t)x(t)d\mu(t) &= \int_D K(s, g^{-1}u)x(u)d\mu(u) \\ &= \int_D K(s, g^{-1}u)x(u)d\mu(g^{-1}u) = \int_D K(s, t)x(gt)d\mu(t). \end{aligned}$$

Hence, using (5), the integral operator is equivariant if and only if

$$\int_D K(s, g^{-1}t)x(t)d\mu(t) = \int_D K(gs, t)x(t)d\mu(t)$$

holds for all $s \in D$, $g \in \Gamma$ and all functions x (in some Sobolev space) which are permitted for the integral operator. It is easily seen (by using the appropriate Sobolev space and the appropriate assumptions on the kernel function!) that this is equivalent to

$$(7) \quad K(s, g^{-1}t) = K(gs, t) \quad \text{for } g \in \Gamma \quad \text{and } s, t \in D,$$

or equivalently, (6). □

Kernels that occur frequently in classical problems (such as potential theory) often have this equivariance property (6) with respect to all orthogonal transformations.

Theorem 5. *If the kernel depends only on the distance, i.e.,*

$$K(s, t) = F(\|s - t\|),$$

then (6) holds for all orthogonal transformations g .

Note that if not explicitly otherwise stated, $\|\cdot\|$ indicates the 2-norm.

In many typical examples, F may have a singularity at 0. Nevertheless, the proof is obvious, since orthogonal transformations leave the 2-norm invariant. The next theorem is significant for double layer potentials.

Theorem 6. *Let the $(N-1)$ -dimensional manifold $D \subset \mathbb{R}^N$ have the symmetries Γ . Let $K : D \times D \rightarrow \mathbb{R}$ be a Γ -equivariant kernel. Then the kernels*

$$L : (s, t) \mapsto \frac{\partial}{\partial \boldsymbol{\nu}(s)} K(s, t)$$

$$L : (s, t) \mapsto \frac{\partial}{\partial \boldsymbol{\nu}(t)} K(s, t)$$

are equivariant. Here $\boldsymbol{\nu}(t)$ denotes the outer unit normal to D at t .

Of course, here the right conditions for the existence of the outer normal have to be assumed, e.g., piecewise smooth.

Proof. We only show the first case. The second is analogous. Let $\partial_1 K$ denote the partial derivative of K with respect to the first argument. Note that the standard use of the derivative symbol in analysis implies that $\partial_1 K$ has to be seen as a row vector.

We use (7) to obtain

$$\begin{aligned} \partial_1 K(g^{-1}s, t)g^{-1}h + \mathcal{O}(\|h\|^2) &= K(g^{-1}s + g^{-1}h, t) - K(g^{-1}s, t) \\ &= K(s + h, gt) - K(s, gt) = \partial_1 K(s, gt)h + \mathcal{O}(\|h\|^2), \end{aligned}$$

and hence

$$\partial_1 K(s, gt) = \partial_1 K(g^{-1}s, t)g^{-1}.$$

From the invariance of D it is obvious that

$$\boldsymbol{\nu}(gs) = g \boldsymbol{\nu}(s).$$

Now, using the above two facts, we obtain

$$\begin{aligned} L(gs, gt) &= \frac{\partial}{\partial \boldsymbol{\nu}(gs)} K(gs, gt) = \partial_1 K(gs, gt) \cdot \boldsymbol{\nu}(gs) \\ &= \partial_1 K(s, t)g^{-1} \cdot \boldsymbol{\nu}(gs) = \partial_1 K(s, t) \cdot \boldsymbol{\nu}(g^{-1}gs) \\ &= \partial_1 K(s, t) \cdot \boldsymbol{\nu}(s) = L(s, t) \end{aligned}$$

□

Among the numerical methods which are generally employed to solve integral equations are the projection methods, e.g., collocation and Galerkin methods, and Nyström's method, which is based upon applying a quadrature method. Recent monographs which describe these numerical methods in detail are those of Atkinson [7], and of Hackbusch [18]. In the following two sections we examine these numerical methods in the context of integral equations having equivariant kernels. Our aim in each case is to derive linear systems of equations which are in turn equivariant and hence amenable to the general symmetry reduction method outlined in Section 7.

5. COLLOCATION AND GALERKIN METHODS

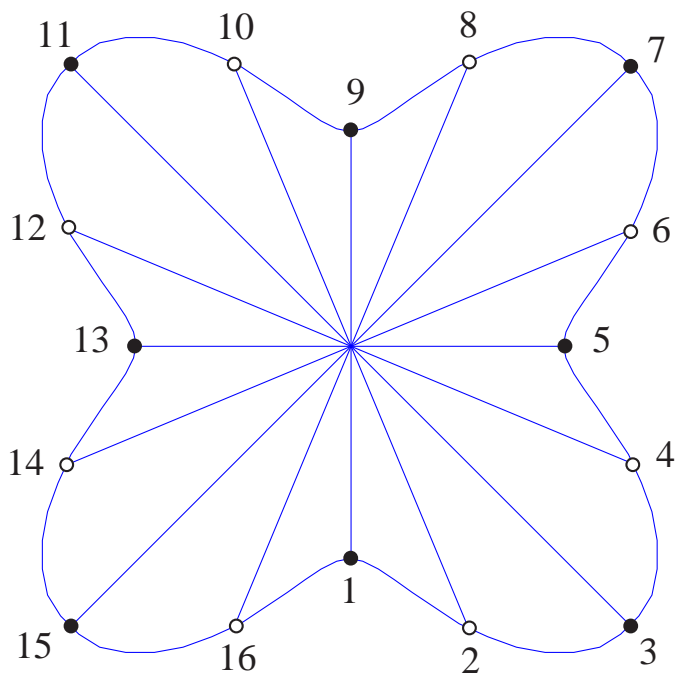


FIGURE 1. A Simple Symmetric Domain

We begin with a simple example. Let D be the closed curve displayed in Figure 1. Obviously, D exhibits the symmetries of a square: it is invariant under the reflection F about the y -axis and under the counterclockwise rotation R by $\pi/2$. By combining these two orthogonal transformations, we obtain the *dihedral group*

$$(8) \quad \Gamma = \mathcal{D}_4 = \{I, R, R^2, R^3, F, FR, FR^2, FR^3\}.$$

Table 1 gives a complete list of irreducible representations for \mathcal{D}_4 .

g	\mathbf{r}_1	\mathbf{r}_2	\mathbf{r}_3	\mathbf{r}_4	\mathbf{r}_5
1	1	1	1	1	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$
R	1	1	-1	-1	$\begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$
R^2	1	1	1	1	$\begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}$
R^3	1	1	-1	-1	$\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$
F	1	-1	1	-1	$\begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$
FR	1	-1	-1	1	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
FR^2	1	-1	1	-1	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
FR^3	1	-1	-1	1	$\begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}$

TABLE 1. Irreducible representations for \mathcal{D}_4

Assume further that we have an equivariant kernel $K : D \times D \rightarrow \mathbb{R}$. We discretize the equation (4) by a simple collocation method: the collocation points t_i , $i = 1 : n$ are shown in Figure 1 for $n = 16$, and we assume basis functions $\phi_i : D \rightarrow \mathbb{R}$, $i = 1 : n$, such that $\phi_i(t_j) = \delta_i^j$. In typical examples, the support of the ϕ_i 's is centered about the t_i 's. We thus obtain the following collocation equation

$$(9) \quad x[j] + \sum_{i=1}^n \int_D K(t_j, t) \phi_i(t) d\mu(t) x[i] = b(t_j).$$

We denote this linear system by $Ax = b$ with the system matrix A . After the equations have been solved for the n unknowns $x[i]$, the solution of (4) is approximated via

$$(10) \quad x(t) \approx \sum_{i=1}^n x[i] \phi_i(t).$$

Now obviously the action of the group Γ on \mathbb{R}^2 induces an action of Γ as a group of permutations on the indices $1 : n$ via

$$(11) \quad gt_i = t_{gi} \quad \text{for } i = 1 : n \quad \text{and } g \in \Gamma.$$

Note that we do not change the notation when a group element acts as a permutation on the indices $1 : n$ instead of as an orthogonal transformation on the vectors $t \in \mathbb{R}^2$. For example, in Figure 1,

$$(12) \quad \begin{aligned} F : i &\mapsto 18 - i \\ R : i &\mapsto i + 4 \pmod{16} \\ FR : i &\mapsto 14 - i \pmod{16}. \end{aligned}$$

Because of the symmetries of the domain, it is quite natural to assume (for practical purposes) that the choice of the basis functions reflects this symmetry:

$$(13) \quad g\phi_i = \phi_i \circ g^{-1} = \phi_{gi} \quad \text{for } i = 1 : 16 \quad \text{and } g \in \Gamma.$$

The definition of equivariance of a matrix with respect to a group of permutations Γ is similarly motivated by its equivariance as a linear transformation $\mathbb{R}^n \rightarrow \mathbb{R}^n$. It is straightforward to see that this is equivalent to the following

Definition 7. A square matrix A of size n is *equivariant* with respect to a group Γ of permutations on $1 : n$ if

$$(14) \quad A[i, j] = A[gi, gj] \quad \text{for all } i, j = 1 : n \quad \text{and } g \in \Gamma,$$

or equivalently,

$$(15) \quad A[gi, j] = A[i, g^{-1}j] \quad \text{for all } i, j = 1 : n \quad \text{and } g \in \Gamma,$$

We have adopted the notation that inputs into functions are surrounded by parentheses and indices of matrices or columns by square brackets.

The following theorem shows that appropriate collocation discretizations of integral equations involving equivariant kernels lead to equivariant matrices.

Theorem 8. Let $D \subset \mathbb{R}^N$ be a domain with symmetries Γ , let $K : D \times D \rightarrow \mathbb{R}$ be an equivariant kernel, let $t_i, i = 1 : n$ be collocation points and $\phi_i : D \rightarrow \mathbb{R}$ be basis functions such that

$$gt_i = t_{gi} \quad \text{and} \quad g\phi_i = \phi_i \circ g^{-1} = \phi_{gi} \quad \text{for } i = 1 : n \quad \text{and } g \in \Gamma,$$

where Γ acts as a group of permutations on the indices $1 : n$. Then the system matrix A of the collocation method for (4) is equivariant with respect to Γ .

Proof. Because of the invariance of the measure, see Remark 3, and the equivariance of the kernel we have

$$\begin{aligned}
A[gi, gj] &= \delta_{gj}^{gi} + \int_D K(t_{gi}, t) \phi_{gj}(t) d\mu(t) \\
&= \delta_j^i + \int_D K(gt_i, t) \phi_j(g^{-1}t) d\mu(t) \\
&= \delta_j^i + \int_D K(t_i, g^{-1}t) \phi_j(g^{-1}t) d\mu(t) \\
&= \delta_j^i + \int_D K(t_i, u) \phi_j(u) d\mu(gu) \\
&= \delta_j^i + \int_D K(t_i, u) \phi_j(u) d\mu(u) = A[i, j].
\end{aligned}$$

□

It is routine to modify the above theorem for Galerkin methods: An evaluation at a point has to be replaced by an additional integration using a basis function as a factor. The flux of the proof is the same.

6. NYSTRÖM METHOD

Given a quadrature formula

$$(16) \quad \int_D f(t) d\mu(t) \approx \sum_{i=1}^n \omega_i f(t_i)$$

with nodes $t_i \in D \subset \mathbb{R}^N$ and weights $\omega_i \in \mathbb{R}$, the Nyström discretization of (4) is obtained by solving the linear system of equations

$$(17) \quad x[j] + \sum_{i=1}^n \omega_i K(t_j, t_i) x[i] = b(t_j).$$

We denote this linear system by $Ax = b$ with A being the system matrix for the Nyström method. After the equations have been solved for the n unknowns $x[i]$, the solution of (4) is approximated via the interpolation formula

$$(18) \quad x(t) \approx b(t) - \sum_{i=1}^n \omega_i K(t, t_i) x[i].$$

If the kernel K is equivariant, see (6), and the nodes t_i are permuted under Γ and if the weights ω_i are invariant under the same permutations, then the system matrix A is equivariant under the same permutations. We explain this now in more detail:

Since the action of Γ leaves D invariant, it is reasonable to choose the quadrature nodes $t_i \in D$ in such a way that Γ also leaves the set of nodes invariant. In this way the elements g of the group Γ act as permutations on the indices $1 : n$ via

$$(19) \quad gt_i := t_{gi} \quad \text{for } i = 1 : n \quad \text{and } g \in \Gamma.$$

Note that we do not change the notation when a group element acts as a permutation on the indices $1 : n$ instead of as an orthogonal transformation on the vectors $t \in \mathbb{R}^N$.

Theorem 9. *Let D be a domain with symmetries Γ , let $K : D \times D \rightarrow \mathbb{R}$ be an equivariant kernel, and let $\int_D f(t) d\mu(t) \approx \sum_{i=1}^n \omega_i f(t_i)$ be a quadrature formula on D such that Γ acts as a group of permutations on the nodes, see (19), and such that the weights are fixed, i.e.,*

$$(20) \quad \omega_i = \omega_{gi} \quad \text{for } i = 1 : n \quad \text{and } g \in \Gamma.$$

Then the system matrix A of the Nyström method (17) is equivariant with respect to Γ .

Proof. We have

$$\begin{aligned} A[gi, gj] &= \delta_{gj}^{gi} + \omega_{gi} K(t_{gj}, t_{gi}) = \delta_j^i + \omega_i K(gt_j, gt_i) \\ &= \delta_j^i + \omega_i K(t_j, t_i) = A[i, j]. \quad \square \end{aligned}$$

An interesting example is taken from Atkinson's article [6]: Let D be a closed surface in \mathbb{R}^3 and let Σ be a finite collection of triangles represented by its vertices, i.e., for $\sigma \in \Sigma$ we have $\sigma = \{v_1, v_2, v_3\}$ where the $v_1, v_2, v_3 \in \mathbb{R}^3$ are affinely independent. We assume that all vertices are in D , and that Σ is a 3-dimensional piecewise linear manifold without boundary. This means that each edge $\{u, v\} \subset \sigma \in \Sigma$, $u \neq v$, belongs to precisely two triangles $\sigma, \sigma' \in \Sigma$. We view Σ as a triangulation approximating the surface D .

Let us further denote the set of all edges by \mathcal{T} . We assume that an approximate midpoint construction $\{u, v\} \in \mathcal{T} \mapsto q_{u,v} \in D$ is given, e.g., $q_{u,v}$ could be the point on D closest to the midpoint $\frac{1}{2}(u + v)$. Let us note in passing that in Atkinson's software [5] the function $\{u, v\} \in \mathcal{T} \mapsto q_{u,v}$ is required from the user.

Atkinson proposes a quadrature rule which is of order 4 for sufficiently smooth functions $f : D \rightarrow \mathbb{R}$. It is straightforward to see that this quadrature rule can be expressed in the following way:

$$(21) \quad \int_D f(t) d\mu(t) = \sum_{\{u,v\} \in \mathcal{T}} \omega_{u,v} f(q_{u,v}) + \mathcal{O}(h^4)$$

where h is the mesh size of the triangulation. The weights $\omega_{u,v}$ are determined in the following way: Let $\{u, v\} \in \mathcal{T}$. From the main properties of Σ (see above) it follows that there are uniquely defined vertices x, z such that $\{x, u, v\}, \{z, u, v\} \in \Sigma$. Then

$$(22) \quad \omega_{u,v} := \frac{1}{6} \left\| (u - v) \times (2q_{u,z} + 2q_{v,z} - z - \frac{1}{2}u - \frac{1}{2}v - 2q_{u,v}) \right\| \\ + \frac{1}{6} \left\| (u - v) \times (2q_{u,x} + 2q_{v,x} - x - \frac{1}{2}u - \frac{1}{2}v - 2q_{u,v}) \right\| .$$

Now, if a group Γ of symmetry transformations acts on the surface D , it is reasonable to assume that the group acts as a group of permutations on the vertices, edges, and triangles of the triangulation. It is further reasonable to assume that the approximate midpoint construction $\{u, v\} \in \mathcal{T} \mapsto q_{u,v}$ respects this symmetry in the following sense:

$$(23) \quad gq_{u,v} = q_{gu,gv} \quad \text{for } \{u, v\} \in \mathcal{T} \quad \text{and } g \in \Gamma.$$

It is then obvious from the form of the weights (22), that

$$(24) \quad \omega_{gu,gv} = \omega_{u,v} \quad \text{for } \{u, v\} \in \mathcal{T} \quad \text{and } g \in \Gamma.$$

Therefore the system matrix A in (17) is equivariant with respect to the group of permutations Γ (acting on the edges of the triangulation).

Remark 10. Any quadrature formula originally given over a triangle (or more generally: a simplex) can be modified to be used for the Nyström method. In this context, the formula needs to have certain (invariance) properties to yield a quadrature formula that satisfies the assumptions of Theorem 9. Such invariances are discussed in the survey [22]. The reader should be aware that some work still needs to be done in order to adapt such formulae to the present purpose. In particular, the approximation of the surface by local charts should be of the same order as the quadrature formula. Because of space limitations, we abstain from further discussions. The above discussion shows that Atkinson's method is such an example, which (in our opinion) is of practical importance.

7. THE SYMMETRY REDUCTION METHOD FOR EQUIVARIANT MATRICES

In the preceding two sections we have seen that appropriate versions of standard discretization methods for integral equations involving equivariant kernels lead to linear systems involving equivariant matrices. Let us now discuss the symmetry reduction method for solving $Ax = b$ with A equivariant. Let us assume hereafter that Γ is a group of permutations acting on the indices $\{1, \dots, n\}$, and that A is a square

matrix of size n which is equivariant with respect to Γ in the sense of Definition 7.

Definition 11 (Selection of Indices). Let Γ be a group of permutations acting on the indices $\{1, \dots, n\}$. Then clearly there is a minimal set $\mathbb{S} \subset \{1, 2, \dots, n\}$ such that

$$\{gi : g \in \Gamma, i \in \mathbb{S}\} = \{1, 2, \dots, n\}.$$

We call such a set of indices \mathbb{S} a *selection* with respect to the action of Γ .

From (14) or (15) it is immediately seen that all entries of A can be derived from a selection of columns or rows. Hence, for purposes of storing the matrix A , it is sufficient to store a selected number of its columns (or rows).

Another aspect arises in the connection with discretization methods. If A is a system matrix (e.g., of a Galerkin method), then only the entries of A for a selection of columns (or rows) need to be computed, and this can save a considerable amount of computational expense.

Definition 12 (Isotropy Subgroup). For $i = 1 : n$ we define the *isotropy subgroup* $\Gamma_i := \{g \in \Gamma : gi = i\}$. Obviously, i is not fixed under any (non-trivial) permutation $g \in \Gamma$ if and only if $|\Gamma_i| = 1$. We call the action of Γ on the indices $1, \dots, n$ *fixed point free* if $|\Gamma_i| = 1$ holds for all $i = 1 : n$.

Remark 13. It is immediately seen that the action of Γ is fixed point free if and only if $|\Gamma| \cdot |\mathbb{S}| = n$. Here $|\mathbb{S}|$ denotes the cardinality of \mathbb{S} , i.e., the number of selected indices. In discretization methods, $\Gamma_i = \{I\}$ is the case for almost all nodes: Nodes in $D \subset \mathbb{R}^N$ are fixed under some $g \in \Gamma$ if and only if they lie on a lower dimensional subset of D .

Example 14. In the discretization via collocation relating to Figure 1, the even numbered collocation points are fixed point free, whereas the isotropy subgroups for the remaining points are

$$\begin{aligned} \Gamma_1 = \Gamma_9 &= \{I, F\} & \Gamma_3 = \Gamma_{11} &= \{I, FR^3\} \\ \Gamma_5 = \Gamma_{13} &= \{I, FR^2\} & \Gamma_7 = \Gamma_{15} &= \{I, FR\}. \end{aligned}$$

For $\mathbf{r} \in \mathcal{R}$ and $i = 1 : n$ we introduce the projectors

$$(25) \quad \mathbf{P}_{\mathbf{r},i} := \frac{1}{|\Gamma_i|} \sum_{g \in \Gamma_i} \mathbf{r}(g).$$

It is easily seen that the $\mathbf{P}_{\mathbf{r},i}$ are orthogonal projectors which have rank

$$m_{\mathbf{r},i} := \text{rank } \mathbf{P}_{\mathbf{r},i} = \text{trace } \mathbf{P}_{\mathbf{r},i}.$$

Note that in practice, many of the $P_{\mathbf{r},i}$ will be identical, and this can be numerically exploited. Note also that for i such that $\Gamma_i = \{I\}$ is trivial the projector $P_{\mathbf{r},i}$ is the identity.

For each $\mathbf{r} \in \mathcal{R}$ and $i \in \mathbb{S}$ we introduce a matrix $u_{\mathbf{r},i}$ of size $(d_{\mathbf{r}}, m_{\mathbf{r},i})$ whose columns are an orthonormal basis of the range of the projectors $P_{\mathbf{r},i}$. Hence

$$(26) \quad u_{\mathbf{r},i} u_{\mathbf{r},i}^* = P_{\mathbf{r},i} \quad \text{and} \quad u_{\mathbf{r},i}^* u_{\mathbf{r},i} = I.$$

Note that for the symmetry groups corresponding to discretizations of three dimensional problems, $d_{\mathbf{r}}$ is very small and typically has values in $\{1, 2, 3\}$.

A symmetry adapted basis can be obtained by applying what is called in [3] the modified Fourier transform to the standard unit basis vectors and writing the result as a column in \mathbb{C}^n . If we view the symmetry adapted basis as a matrix of columns, then the formulas in [3] lead to the following

Definition 15. The matrix F describing the Fourier transform is obtained by

$$(27) \quad F[\tau(\mathbf{r}, j, k, i), l] := \sqrt{\frac{d_{\mathbf{r}}}{|\Gamma|}} \sum_{g \in \Gamma} \sum_{p=1}^{d_{\mathbf{r}}} \delta_{gl}^k u_{\mathbf{r},k}[p, i] \mathbf{r}_{p,j}(g)$$

where the index τ is defined in the following way:

$$(28) \quad \begin{array}{l} \text{counter} \leftarrow 0 \\ \text{for } \mathbf{r} \in \mathcal{R} \\ \quad \text{for } j = 1 : d_{\mathbf{r}} \\ \quad \quad \text{for } k \in \mathbb{S} \\ \quad \quad \quad \text{for } i = 1 : m_{\mathbf{r},k} \\ \quad \quad \quad \quad \text{counter} \leftarrow \text{counter} + 1 \\ \quad \quad \quad \quad \tau(\mathbf{r}, j, k, i) := \text{counter} \\ \quad \quad \quad \quad \text{end} \\ \quad \quad \quad \text{end} \\ \quad \quad \text{end} \\ \text{end} \end{array}$$

After the completion of all of the loops, the counter has the value n . Note that it is not difficult to implement the function τ as well as its inverse τ^{-1} in an efficient way (not indicated by (28)). Also note that for k such that $\Gamma_k = \{I\}$ is trivial, see Remark 13, the inner sum $i = 1 : m_{\mathbf{r},k}$ simplifies to $i = 1 : d_{\mathbf{r}}$ since $u_{\mathbf{r},k} = I_{d_{\mathbf{r}}}$.

The following theorem is a consequence of the orthogonality relation, see Theorem 1:

Theorem 16. F is a unitary matrix.

Note also that F is typically very sparse. In fact, it is immediately seen from (27) that each row of F has at most $|\Gamma|$ non-zero elements.

Symmetry Reduction Method. Consider a linear system $Ax = b$ where A is equivariant with respect to a group Γ of permutations. Let us denote the Fourier transform by $\hat{x} := Fx$. Then we transform the equation $Ax = b$ into $FAF^*\hat{x} = \hat{b}$. The point is that FAF^* has block diagonal structure, where the blocks are given in the following way:

For $\mathbf{r} \in \mathcal{R}$ and $j \in \{1 : d_{\mathbf{r}}\}$ we define the submatrix $F_{\mathbf{r},j}$ of F of size $(\sum_{k \in \mathbb{S}} m_{\mathbf{r},k}) \times n$ via

$$(29) \quad F_{\mathbf{r},j} := F[\tau(\mathbf{r}, j, :, :), :].$$

The colon denotes that an index ranges over all possibilities (as in MATLAB). The diagonal blocks of FAF^* of size $\sum_{k \in \mathbb{S}} m_{\mathbf{r},k}$ are given by

$$(30) \quad A_{\mathbf{r},j} := F_{\mathbf{r},j} A F_{\mathbf{r},j}^*$$

Furthermore blocks referring to the same irreducible representation \mathbf{r} are identical:

$$(31) \quad A_{\mathbf{r}} := A_{\mathbf{r},1} = A_{\mathbf{r},2} = \dots = A_{\mathbf{r},d_{\mathbf{r}}} \quad \text{for each } \mathbf{r} \in \mathcal{R}.$$

Hence, the system $Ax = b$ splits into the decoupled systems

$$(32) \quad A_{\mathbf{r}} \hat{x}_{\mathbf{r},j} = \hat{b}_{\mathbf{r},j} \quad \text{for } \mathbf{r} \in \mathcal{R} \quad \text{and } j \in \{1 : d_{\mathbf{r}}\}$$

Here we have used the notation $\hat{x}_{\mathbf{r},j} := F_{\mathbf{r},j} x$.

The method for solving $Ax = b$ consists of the following steps:

1. Generate the decoupled systems (32).
2. Solve the decoupled systems (32).
3. Reassemble x via $x = F^* \hat{x}$.

Remark 17 (Invertibility). Recall that F is unitary, see Theorem 16. Hence the block diagonalization FAF^* results from a similarity transformation. We see that the blocks $A_{\mathbf{r}}$ are all invertible if and only if the matrix A is invertible.

Remark 18 (Eigenvalues). If an eigenvalue problem with an equivariant matrix A has to be solved, the symmetry reduction method can be used similarly to (32):

$$(33) \quad Ax = \lambda x \quad \text{if and only if} \quad A_{\mathbf{r}} \hat{x}_{\mathbf{r},j} = \lambda \hat{x}_{\mathbf{r},j} \\ \text{for } \mathbf{r} \in \mathcal{R} \quad \text{and } j \in \mathbb{S}.$$

The eigenvalues of the original matrix A are distributed among the various blocks $A_{\mathbf{r}}$. Multiplicities of eigenvalues generated by the symmetries disappear. Eigenvectors are also easily obtained from the eigenvectors of the subproblems.

In fact, one sees from the repeated occurrence of submatrices $A_{\mathbf{r}}$ for irreducible representations of dimension greater than 1, that equivariant matrices generally have eigenvalues of higher multiplicity. If (λ, x) is an eigenvalue-eigenvector pair for A , then so also is (λ, gx) for all $g \in \Gamma$. Of course, since g corresponds to a permutation matrix, this is only of interest if $gx \neq x$. Thus if $Ax = \lambda x$, then the multiplicity of the eigenvalue λ is at least as large as the dimension of the span of the orbit $\{gx : g \in \Gamma\}$. In a related vein, one also easily sees that the quadratic form $Q(x) := x^*Ax$ is invariant with respect to Γ if A is equivariant with respect to Γ .

Let us return to our simple example of Figure 1, where the collocation method led to an equivariant system matrix of size 16. We list the block diagonal decomposition where the number of repetitions of a block is the same as the dimension of the corresponding irreducible representation and is given in the first row. The irreducible representations refer to Table 1:

dim \mathbf{r} :	1	1	1	1	2
Blocks:	$A_{\mathbf{r}_1}$	$A_{\mathbf{r}_2}$	$A_{\mathbf{r}_3}$	$A_{\mathbf{r}_4}$	$A_{\mathbf{r}_5}$
Size:	3	1	2	2	4

The symmetry reduction method has been studied in some detail by the authors and co-workers for the case that the domain under consideration displays the symmetry of the three dimensional cube, e.g., the boundary element method for an exterior boundary value problem, see [3, 4, 13, 14, 26, 27]. Let us mention one example of a discretization over the surface of a cube, namely collocation with quadratic elements. The numerical codes in [5] can be used to obtain the entries of the system matrix and right hand side.

The symmetry group Γ_c of the 3-cube has 48 elements, and a complete list of irreducible representations consists of 4 one-dimensional, 2 two-dimensional, and 4 three-dimensional representations.

The collocation points are indicated in Figure 2 where only a selection of collocation points is shown, i.e., the remaining points are obtained by applying the 48 symmetries of the cube. Note that only one selected point, namely the one numbered 7, is not fixed under any symmetry, i.e., has a trivial isotropy subgroup.

Note however that the fixed point free nodes become dominant if we refine the discretization, see Remark 13.

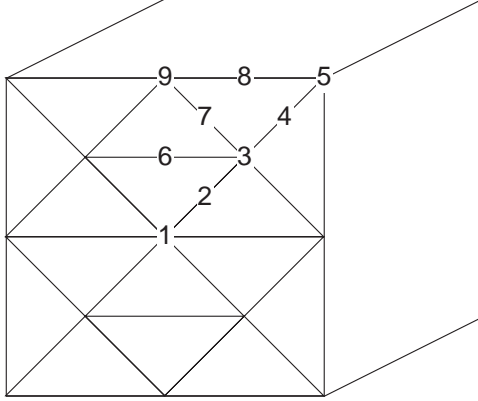


FIGURE 2. Cube Symmetry With Fixed Points

The system matrix for quadratic collocation referring to Figure 2 has size 194. We list the block diagonal decomposition where the number of repetitions of a block is the same as the dimension of the corresponding irreducible representation and is given in the first row:

dim \mathbf{r} :	1	1	1	1	2	2	3	3	3	3
Blocks :	$A_{\mathbf{r}_1}$	$A_{\mathbf{r}_2}$	$A_{\mathbf{r}_3}$	$A_{\mathbf{r}_4}$	$A_{\mathbf{r}_5}$	$A_{\mathbf{r}_6}$	$A_{\mathbf{r}_7}$	$A_{\mathbf{r}_8}$	$A_{\mathbf{r}_9}$	$A_{\mathbf{r}_{10}}$
Size :	9	1	2	6	10	6	16	8	10	14

8. OVERHEAD AND COMPUTATIONAL SAVINGS

Let us look at the overhead of the reduction method. In order to simplify the analysis, we assume a fixed point free situation (which is approximately true for all discretization methods, see Remark 13). The operations $\hat{b} \leftarrow Fb$ and $x \leftarrow F^*\hat{x}$ each cost $|\Gamma| \cdot n$ flops. However, the main overhead cost is generated by calculating the block diagonal matrices $A_{\mathbf{r}}$ for all $\mathbf{r} \in \mathcal{R}$. A straightforward application of the symmetry adapted basis, i.e., of applying the sparse matrix F , leads to an implementation of the formula $A_{\mathbf{r}} \leftarrow F_{\mathbf{r},1} A F_{\mathbf{r},1}^*$ which costs $n^2 (1 + \sum_{\mathbf{r} \in \mathcal{R}} d_{\mathbf{r}})$ flops. This cost can, however, be considerably reduced by avoiding the explicit use of the symmetry adapted basis. Namely, by exploiting the formulas in [3], it can be seen that

$$(34) \quad A_{\mathbf{r}}[\tau_{\mathbf{r}}(k, i), \tau_{\mathbf{r}}(k', i')] = \sqrt{\frac{|\Gamma|}{d_{\mathbf{r}}} \frac{1}{|\Gamma_{k'}|}} \sum_{p=1}^{d_{\mathbf{r}}} (F a_{k'})[\tau(\mathbf{r}, p, k, i)] u_{\mathbf{r}, k'}[p, i']$$

where $\tau_{\mathbf{r}}(k, i) := \tau(\mathbf{r}, 1, k, i) - \tau(\mathbf{r}, 1, 1, 1) + 1$. Here $a_{k'}$ denotes the k' -th column of A .

Also note that for k' such that $\Gamma_{k'} = \{I\}$ is trivial, see Remark 13, the above equation simplifies to

$$(35) \quad A_{\mathbf{r}}[\tau_{\mathbf{r}}(k, i), \tau_{\mathbf{r}}(k', i')] = \sqrt{\frac{|\Gamma|}{d_{\mathbf{r}} |\Gamma_{k'}|}} (F a_{k'})[\tau(\mathbf{r}, i', k, i)]$$

since $u_{\mathbf{r}, k'}[p, i'] = \delta_p^{i'}$.

It can be seen that an implementation of formula (34) leads to n^2 flops for generating all reduced matrices, as opposed to the above estimate $n^2 (1 + \sum_{\mathbf{r} \in \mathcal{R}} d_{\mathbf{r}})$, since essentially only a selection of columns of A needs to be transformed.

The savings in computational expense which can be effected by the symmetry reduction method are significant, especially in the context of the numerical solution of integral equations. Here the resulting system matrices A are generally full and are often solved by direct methods. For simplicity of the following discussion, let us assume that Γ is fixed point free. In this case the symmetry reduction yields $d_{\mathbf{r}}$ matrices $A_{\mathbf{r}}$ of size $d_{\mathbf{r}}|\mathbb{S}|$.

If the same direct solver is used for both the unreduced problem $Ax = b$ and the symmetry reduced subproblems (32), respectively, then asymptotically we have $f_1 := Cn^3 = C|\Gamma|^3|\mathbb{S}|^3$ flops as opposed to $f_2 := C \sum_{\mathbf{r} \in \mathcal{R}} |\mathbb{S}|^3 d_{\mathbf{r}}^3$. Hence the quotient which asymptotically describes the reduction factor in the number of flops is

$$\frac{f_2}{f_1} = \frac{\sum_{\mathbf{r} \in \mathcal{R}} d_{\mathbf{r}}^3}{|\Gamma|^3}.$$

In particular, for the group Γ_c of symmetries of the cube, there are four irreducible representations of dimension 1, two irreducible representations of dimension 2, and four irreducible representations of dimension 3. Hence if Γ is the symmetry group of the three dimensional cube, then $\frac{f_2}{f_1} = 128/48^3 \approx 0.116\%$.

Let us note that the symmetry reduction method can also lead to a significant reduction in computational cost in the context of iterative solution methods. Iterative methods generally are best used when the system matrix A is sparse. In [3] it was shown that to a large extent, sparsity carries over to the submatrices $A_{\mathbf{r}}$ arising in the symmetry reduction. It turns out that the symmetry reduction can also offer a computational reduction if an iterative method is employed for a full system. Many modern iterative methods in numerical linear algebra involve the repeated application of matrix-vector products Ax . Let us suppose that A and x are of size n and A is equivariant.

For simplicity assume again that Γ is fixed point free. Again the symmetry reduction yields $d_{\mathbf{r}}$ matrices $A_{\mathbf{r}}$ of size $d_{\mathbf{r}}|\mathbb{S}|$. Whereas a matrix-vector multiplication Ax for a full matrix A costs n^2 flops, each

of the multiplications $A_{\mathbf{r}}\hat{x}_{\mathbf{r}}$ costs $(d_{\mathbf{r}}|\mathbb{S}|)^2$ flops. Hence performing this latter multiplication for each block costs

$$|\mathbb{S}|^2 \sum_{\mathbf{r} \in \mathcal{R}} d_{\mathbf{r}}^3$$

flops. Neglecting the overhead for the symmetry reduction (which costs n^2 flops) the reduction factor per multiplication effected by the symmetry reduction is given by the following quotient

$$Q(\Gamma) := \left(\frac{|\mathbb{S}|}{n}\right)^2 \sum_{\mathbf{r} \in \mathcal{R}} d_{\mathbf{r}}^3 = \frac{1}{|\Gamma|^2} \sum_{\mathbf{r} \in \mathcal{R}} d_{\mathbf{r}}^3.$$

In particular, for the dihedral group \mathcal{D}_4 , there are four irreducible representations of dimension 1 and one of dimension 2, see Table 1. Hence $Q(\mathcal{D}_4) = \frac{12}{64} = 0.1875$.

In general, for a dihedral group \mathcal{D}_n , we consider two cases: If n is even, then there are 4 irreducible representations of dimension 1 and $n/2 - 1$ irreducible representations of dimension 2. Hence $Q(\mathcal{D}_n) = 1/n - 1/n^2$. If n is odd, then there are 2 irreducible representations of dimension 1 and $(n - 1)/2$ irreducible representations of dimension 2. Hence $Q(\mathcal{D}_n) = 1/n - 1/(2n^2)$.

For the group Γ_c of symmetries of the cube, $Q(\Gamma_c) = 1/18$.

An additional aspect of the symmetry reduction which bears mentioning is the fact that when the equivariant matrix A is reduced into the submatrices $A_{\mathbf{r}}$ the eigenvalues of A become distributed over the submatrices. Thus each block has a condition number which is generally smaller, and also the number of eigenvalues is reduced. These properties will further contribute to faster convergence and greater stability of an iterative process.

9. THE SYMMETRY REDUCTION METHOD AS A PRECONDITIONER

In applications it is often the case that an operator equation under investigation only displays approximate symmetries which may be flawed by either less important terms in the equation and/or imperfections in the geometrical shape.

In this case, it has been shown in the PhD thesis [26, 27] that an equivariant preconditioner can be constructed which is efficient and improves convergence drastically, in particular for equations with bad conditioning (such as integral equations of the first kind).

In such cases, the action of a permutation group is evident from the discretization, however the equivariance conditions, see Definition 7,

are not quite satisfied by the system matrix A . The *equivariant part*

$$A_{\Gamma}[i, k] := \frac{1}{|\Gamma|} \sum_{g \in \Gamma} A[gi, gk]$$

of A is a very good preconditioner in such cases. In fact, it is easily seen that A_{Γ} is the equivariant matrix nearest to A in the Frobenius norm. Our symmetry reduction method asserts that the action A_{Γ}^{-1} can be implemented at a low computational expense.

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