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Exploiting Permutation Symmetries with Fixed Points in Linear Equations

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Abstract. The basic problem discussed here is the exploitation of symmetry in solving linear systems of equations which are equivariant under a permutation of the indices. It is essentially an overview of the method given in [**11**] and [**10**], augmented by a careful discussion of the case of fixed points, which was left untreated in these articles.

1. Introduction

Let V be an N-dimensional vector space over $\mathbb{C}$, and let $\mathcal{L} : V \to V$ be a nonsingular linear map. Any vector $v \in V$ gives rise to a linear system

$$\mathcal{L}u = v \tag{1.1}$$

which typically one wants to solve for the unknown vector u.

Suppose that G is a finite group, acting linearly on V. We denote the action of a group element g on a vector v by gv. We say that $\mathcal{L}$ is *G-equivariant* if

$$\mathcal{L}(gv) = g\mathcal{L}(v)$$

for all $g \in G$ and all $v \in V$.

The main problem we wish to address in this article is how to use the equivariance of $\mathcal{L}$ to solve the system (1.1) more efficiently.

This problem has been addressed previously is such works as [**1**], [**2**], [**3**], [**5**], [**6**] [**7**], [**9**], [**11**], and [**10**]. Some of these, dealing with finite and boundary element methods, treat fundamental domain decomposition; others discuss the method of symmetry-adapted bases.

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In this article we will concentrate on the case of permutation symmetry. This is the assumption that the vector space V has a basis $\{e_i\}$ which is simply permuted by the action of G. That is, we have an index set $\mathcal{I}$, indexing the basis of V, and for every group element $g \in G$, we have a permutation (which we will also call g) of the index set. This induces a linear action of G on V by setting

$$ge_i = e_{gi}$$

and extending by linearity. This is called a *permutation representation* of the group G on V.

The basis $\{e_i\}$ for V allows us to identify V with a space of column vectors of length N. We will denote the i^{th} coordinate of a column vector v by $v[i]$. Note that this implies that the permutation action of G on V can be expressed as

$$(gv)[m] = v[g^{-1}m].$$

We will denote the ij^{th} entry of a matrix L by $L[i,j]$. If the operator $\mathcal{L}$ has the matrix L with respect to this basis $\{e_i\}$, then the G-equivariance of $\mathcal{L}$ when the representation of G is a permutation representation as described above is equivalent to the formula

$$L[m,n] = L[gm,gn]$$

holding for all $g \in G$ and all indices m,n.

We say that a permutation representation is *without fixed points* if no index m is fixed by any non-trivial group element g. In general, the *isotropy subgroup* of an index m is the subgroup $G_m = \{g \in G \mid gm = m\}$. If G acts without fixed points, then every isotropy subgroup is trivial. The *orbit* of an index n is the set $Gn = \{gn \mid g \in G\}$ of indices to which n is moved by the group elements in G.

If G acts without fixed points, we see that there are exactly $\#G$ elements in each orbit. In this case any two orbits are either identical or disjoint, so that there are exactly $M = N/\#G$ orbits.

A *selection* of indices is a subset $\mathcal{J}$ of $\mathcal{I}$ which consists of one index in each orbit of G.

2. Irreducible Representations and Projectors

Let $\rho : G \to \mathrm{GL}(d)$ be a homomorphism from G to the group $\mathrm{GL}(d)$ of invertible $d \times d$ matrices over $\mathbb{C}$. Such a homomorphism is called a *complex matrix representation* of G, of dimension d. It is said to be *irreducible* if the matrices of ρ cannot be simultaneously put into an upper triangular block form. We will also denote the matrix $\rho(g)$ by $\mathbf{A}^\rho(g)$.

Recall that two elements g_1 and g_2 of a group G are *conjugate* if $g_1 = gg_2g^{-1}$ for some $g \in G$; this is an equivalence relation on G, and the equivalence classes are called the *conjugacy classes* of G.

In the context of complex matrix representations, one usually uses the terminology that two complex matrix representations ρ_1 and ρ_2 are em equivalent if there is a fixed invertible matrix A such that $A\rho_1(g)A^{-1} = \rho_2(g)$ for all $g \in G$.

The following theorem contains some basic facts about irreducible complex matrix representations of a finite group; for a reference, see [**12**] or [**4**].

Theorem 2.1. *Let G be a finite group of order $\#G$, with R conjugacy classes.*

- 2.1.1: *There are R non-equivalent irreducible complex matrix representations $\rho_1, \ldots, \rho_R$ of dimensions $d_1, \ldots, d_R$ respectively, such that any irreducible matrix representation of G is equivalent to exactly one of the ρ_i's.*
- 2.1.2: *Any complex matrix representation is equivalent to a direct sum of the ρ_i's.*
- 2.1.3: $\sum_i d_i^2 = \#G$.
- 2.1.4: *The representations ρ_i can be taken to be unitary.*

We call a set of representations $\{\rho_i\}$ as in the above theorem a *full set of irreducible representations* for G.

Given an irreducible matrix representation ρ of G, we will write the ij^{th} element of the matrix $\mathbf{A}^\rho(g)$ as $A^\rho_{ij}(g)$.

Let V be any representation of G, and let ρ be an irreducible matrix representation of G. Following [**12**, section 2.7], define maps

$$P^\rho_{ij} : V \to V$$

by the formula

$$P^\rho_{ij}(v) = \frac{\dim \rho}{\#G} \sum_{g \in G} A^\rho_{ji}(g^{-1}) gv.$$

Note the reversal of indices and the use of the inverse element in the sum. Since the action operation sending v to gv is linear for each g, the map P^ρ_{ij} is a linear operator from V to V, and it is defined for each i and j between 1 and $\dim \rho$.

We have the following orthogonality relation (see [**12**, section 2.7])

Proposition 2.2. *Let ρ and τ be two irreducible complex matrix representations of G from a full set of irreducible representations. (I.e., ρ and τ are either identical or non-equivalent.) Then*

$$P^\rho_{ij} \circ P^\tau_{kl} = P^\tau_{il} \delta_{jk} \delta_{\rho\tau}.$$

Note that this implies that the "diagonal" operators P^ρ_{ii} are a set of mutually orthogonal projectors, defined on any vector space V on which G acts, as ρ ranges over a full set of irreducible representations for G, and as i runs from 1 to $\dim \rho$. Indeed, they form a complete set of projectors (see [**12**, section 2.7]):

Proposition 2.3. *Let G act linearly on a vector space V. Then*

$$\sum_\rho \sum_{i=1}^{\dim \rho} P^\rho_{ii} = \mathrm{Id}_V\,.$$

In the above sum, ρ ranges over a full set of irreducible representations for G.

We denote by V_i^ρ the image of the projector P_{ii}^ρ. The previous Proposition implies that the subspaces V_i^ρ completely decompose the original space V:

$$V = \bigoplus_{\rho} \bigoplus_{i=1}^{\dim \rho} V_i^\rho. \tag{2.4}$$

Given a vector $v \in V$, we denote by v_{ij}^ρ its image under P_{ij}^ρ:

$$v_{ij}^\rho = P_{ij}^\rho(v).$$

This gives the formula

$$v = \sum_{\rho} \sum_{i=1}^{\dim \rho} v_{ii}^\rho \tag{2.5}$$

for any vector $v \in V$, by Proposition 2.3.

Using this notation we may re-write the definition of the P_{ij}^ρ's as follows:

$$v_{ij}^\rho[m] = \frac{\dim \rho}{\#G} \sum_{g \in G} A_{ji}^\rho(g^{-1}) v[g^{-1}m], \tag{2.6}$$

3. The Reduction to the Sub-problems

Let the finite group G act as a group of permutations on the indices of a basis for the vector space V. Let $\mathcal{L}$ be a G-equivariant nonsingular operator on V, with matrix L in the permuted basis. Let ρ be an irreducible matrix representation of G. Since $\mathcal{L}$ commutes with the action of each group element $g \in G$, and the operators P_{ij}^ρ are simply linear combinations of the group elements, we see that $\mathcal{L}$ commutes with each P_{ij}^ρ; in particular, we have

$$\mathcal{L}(P_{ii}^\rho(v)) = P_{ii}^\rho(\mathcal{L}(v))$$

for every $v \in V$. Therefore we see that $\mathcal{L}$ maps V_i^ρ to itself, i.e., the subspace V_i^ρ is stable under the operator $\mathcal{L}$. Let us denote by $\mathcal{L}_i^\rho$ the restriction of $\mathcal{L}$ to V_i^ρ:

$$\mathcal{L}_i^\rho = \mathcal{L}|_{V_i^\rho} : V_i^\rho \to V_i^\rho.$$

Note that since $\mathcal{L}$ is nonsingular, so is each $\mathcal{L}_i^\rho$.

We now have the following plan for reducing the original system (1.1) into sub-problems:

To Solve $\mathcal{L}u = v$:

(i) Choose a full set $\{\rho\}$ of irreducible representations for G.

(ii) For each ρ and each $i = 1, \ldots, \dim\rho$, apply the projectors P^ρ_{ii} to both sides of the system, obtaining the sub-system $P^\rho_{ii}(v) = P^\rho_{ii}(\mathcal{L}(u)) = \mathcal{L}(P^\rho_{ii}(u))$ which we write as

$$\mathcal{L}^\rho_i(u^\rho_{ii}) = v^\rho_{ii} \tag{3.1}$$

(iii) Solve these sub-problems for the unknowns u^ρ_{ii}.
(iv) Reconstruct the solution

$$u = \sum_\rho \sum_{i=1}^{\dim\rho} u^\rho_{ii}.$$

4. The Method Without Fixed Points

It is now time to get specific about how to write down the matrices for the sub-problems, in the case of permutation symmetry.

There are two basic formulas which govern the construction of the matrices for the sub-operators $\mathcal{L}^\rho_i$. The first comes from the following equation relating the group action and the operators P^ρ_{ij} (see [**12**, section 2.7]):

Lemma 4.1. *If ρ is an irreducible matrix representation of G, then*

$$gP^\rho_{ij} = \sum_k A^\rho_{ki}(g)P^\rho_{kj}.$$

The above formula has as a special but important case the following, expressed in terms of the v^ρ_{ij}'s:

$$v^\rho_{kk}[gm] = \sum_{i=1}^{\dim\rho} A^\rho_{ik}(g^{-1})v^\rho_{ik}[m]. \tag{4.2}$$

¿From this we see the following principle: to determine all of the coordinates of the vector v^ρ_{kk}, it suffices to know the coordinates $v^\rho_{ik}[m]$, *for one m in each G-orbit of indices.*

Hence we have natural "coordinates" for a vector v in the space V^ρ_k consisting of the numbers $v^\rho_{ik}[m]$, as i goes from 1 to $\dim\rho$, and m ranges over a selection of indices, i.e., one from each G-orbit.

If G acts without fixed points, then there are $M = N/\#G$ elements in any selection; hence the number of these "coordinates" is $M\dim\rho$. This is exactly the dimension of the space V^ρ_k, and hence we have no duplication or relations among these "coordinates".

To see this, we view the introduction of the coordinates $v^\rho_{ik}[m]$ as showing that the dimension of V^ρ_k is at most the number of these coordinates, which is $M\dim\rho$:

$$\dim(V^\rho_k) \le M\dim\rho = N\dim\rho/\#G. \tag{4.3}$$

Now the total space V has dimension N, and decomposes as the direct sum of the spaces V_k^ρ, by (2.4). Therefore

$$N = \dim V \leq \sum_\rho \sum_{k=1}^{\dim \rho} (N \dim \rho / \#G) = \frac{N}{\#G} \sum_\rho \dim^2 \rho.$$

Now by Theorem 2.1.3, $\sum_\rho \dim^2 \rho = \#G$; hence the inequality in the previous formula must be an equality, which forces $\dim(V_k^\rho) = M \dim \rho = N \dim \rho / \#G$ for every ρ and k, in the case where G acts without fixed points.

Choose therefore once and for all a selection $\mathcal{J} \subset \mathcal{I}$ of M indices. We now want to write the matrix equation for the sub-operator $\mathcal{L}_k^\rho$ using these new "coordinates". Thus we seek a matrix L_k^ρ, whose rows and columns are indexed by pairs (i,m), (i goes from 1 to $\dim \rho$, and m ranges over the selection $\mathcal{J}$ of indices), which represents the matrix of the sub-operator $\mathcal{L}_k^\rho$. That is, we seek the entries $L_k^\rho[(i,m),(j,n)]$, such that

$$P_{ik}^\rho(\mathcal{L}_k^\rho(v_{kk}^\rho))[m] = \sum_{(j,n)} L_k^\rho[(i,m),(j,n)] v_{jk}^\rho[n].$$

These entries are readily worked out from the formulas for P_{ik}^ρ; we obtain the following.

$$L_k^\rho[(i,m),(j,n)] = \sum_{g \in G} L[g^{-1}m, n] A_{ji}^\rho(g^{-1}) \tag{4.4}$$

Notice now that these entries are independent of the index k! This means that we actually have a single matrix $L^\rho = L_k^\rho$. This shows that our method is a variant of the "symmetry-adapted basis" technique described in [**9**].

In addition, note that to determine these matrices, we do not need to know the entire original matrix L; we only need to know those columns of L indexed by elements in the given selection $\mathcal{J}$.

Now the specific application of the method in the case of permutation symmetry without fixed points can be described with the following algorithm.

To Solve $\mathcal{L}u = v$:

(i) Choose a full set $\{\rho\}$ of irreducible representations for G.
(ii) Choose a selection $\mathcal{J}$ of indices, one from each G-orbit.
(iii) Determine the entries $L[m,n]$ of the matrix for the operator $\mathcal{L}$, for all indices $m \in \mathcal{I}$ and all selected indices $n \in \mathcal{J}$.
(iv) For each irreducible matrix representation ρ:
  - a: Form the doubly-indexed matrices L^ρ using (4.4).
  - b: Using (2.6), determine the coordinates $v_{ik}^\rho[m]$ for all i and k from 1 to $\dim \rho$ and all selected indices $m \in \mathcal{J}$.
  - c: Solve the sub-problems

$$L^\rho u_{ik}^\rho = v_{ik}^\rho$$

for the unknowns $u^\rho_{ik}[m]$, again for $i, k = 1, \ldots, \dim \rho$ and all selected indices $m \in \mathcal{J}$.

d: For each $k = 1, \ldots, \dim \rho$, reconstruct every coordinate of the vector u^ρ_{kk} using (4.2).

(v) Reconstruct the solution $u = \sum_\rho \sum_{k=1}^{\dim \rho} u^\rho_{kk}$.

5. Complexity Reduction Factors

Suppose that one is using a direct linear system solver which has complexity $O(n^3)$ for an $n \times n$ problem, as is suitable for full problems. To solve our original system of size N which is considered to be full, would then require approximately cN^3 flops, for some constant c.

In using the above method, what is the reduction factor in the complexity? The work is done in the step 4(c) in the outline in the previous section, where the linear sub-problems are solved. For each irreducible matrix representation ρ, we must solve the system of step 4(c), which is of size $\dim \rho N/\#G$. This has computational cost approximately $c(\dim \rho N/\#G)^3$. Hence the total cost is approximately $\sum_\rho c(\dim \rho N/\#G)^3$; dividing by the cost of the original problem cN^3 gives a reduction factor

$$\frac{1}{(\#G)^3} \sum_\rho \dim^3 \rho.$$

Note that in the above computation we have neglected the overhead in the method, which is the work involved in constructing the matrices and right-hand sides of the sub-problems in steps 4(a) and 4(b) of the outline in the previous section. This overhead is not insignificant; we have computed it to be approximately N^2 flops, and the reader should consult [**13**] for numerical results using this method in a boundary element problem involving the unit cube.

6. Matrix Notation for the Projectors and Transfers

The double-indexing of the projectors P^ρ_{jj} and tranfers P^ρ_{ij} indicate that we may benefit from grouping these functions together and viewing the output as a matrix. In this section we would like to lay out the notation for this point of view.

Fix an irreducible representation ρ, and let $d = \dim \rho$ be its dimension. For any vector $v \in V$ and any index $n \in \mathcal{I}$, let $\mathbf{v}^\rho[n]$ denote the d-by-d matrix whose ij^{th} entry is $v^\rho_{ij}[n]$:

$$\mathbf{v}^\rho[n] = \begin{pmatrix} v^\rho_{11}[n] & \ldots & v^\rho_{1d}[n] \\ \vdots & \ddots & \vdots \\ v^\rho_{d1}[n] & \ldots & v^\rho_{dd}[n] \end{pmatrix} \tag{6.1}$$

We will also use the notation $\mathbf{P}^\rho$ to denote the matrix of operators

$$\mathbf{P}^\rho = \left(P^\rho_{ij}\right),$$

so that for a vector $v \in V$, $\mathbf{P}^\rho(v)[n] = \mathbf{v}^\rho[n]$. In particular, we think of $\mathbf{P}^\rho(v)$ as a column vector of $d \times d$ matrices, not as a $d \times d$ matrix of vectors.

Using the formula (2.6), we see that the definition of $\mathbf{v}^\rho[m]$ can be expressed as a linear combination of transposes of the matrices $\mathbf{A}^\rho$ which define the representation ρ:

$$\mathbf{v}^\rho[m] = \frac{\dim\rho}{\#G} \sum_{g\in G} v[g^{-1}m]\mathbf{A}^\rho(g^{-1})^\top. \tag{6.2}$$

Proposition 2.2 and Lemma 4.1 can be expressed in the following succinct way.

PROPOSITION 6.3.

6.3.1: *Let $g \in G$, $n \in \mathcal{I}$, and $v \in V$. If ρ is an irreducible matrix representation of G, then*

$$\mathbf{v}^\rho[gn] = \mathbf{A}^\rho(g^{-1})^\top \mathbf{v}^\rho[n].$$

6.3.2: *Let ρ and τ be two irreducible complex matrix representations of G from a full set of irreducible representations. (I.e., ρ and τ are either identical or non-equivalent.) Then*

$$\mathbf{P}^\rho \circ \mathbf{P}^\tau = \dim\tau \mathbf{P}^\tau \delta_{\rho\tau}.$$

The formula (6.2) expresses the matrices $\mathbf{v}^\rho[m]$ in terms of the original vector v. Inverting this procedure is also straightforward. Fix an index n. Then by (2.5), we have

$$v[n] = \sum_\rho \operatorname{trace}(\mathbf{v}^\rho[n]). \tag{6.4}$$

In fact, the image v^ρ of v in the canonical space V^ρ is

$$v^\rho[n] = \operatorname{trace}(\mathbf{v}^\rho[n]). \tag{6.5}$$

The final bit of organization for these matrices $\mathbf{v}^\rho[n]$ is to make a "vector of matrices" out of them. Specifically, let $\mathbf{v}^\rho$ be defined as the column vector whose n^{th} entry is the matrix $\mathbf{v}^\rho[n]$:

$$\mathbf{v}^\rho = \begin{pmatrix} \mathbf{v}^\rho[1] \\ \mathbf{v}^\rho[2] \\ \vdots \\ \mathbf{v}^\rho[N] \end{pmatrix}. \tag{6.6}$$

Denote by $\mathbf{V}^\rho_\mathcal{I}$ the vector space of such columns of matrices. It is a complex vector space of dimension Nd^2, where $d = \dim \rho$.

Given a selection $\mathcal{J}$ of indices, we will denote by $\mathbf{V}^\rho_\mathcal{J}$ the vector space of columns of matrices $\mathbf{v}^\rho[m]$ where we only have selected coordinates $m \in \mathcal{J}$. The corresponding "vector" in $\mathbf{V}^\rho_\mathcal{J}$ will be denoted by $\mathbf{v}^\rho_\mathcal{J}$:

$$\mathbf{v}^\rho_\mathcal{J} = \begin{pmatrix} \mathbf{v}^\rho[m_1] \\ \mathbf{v}^\rho[m_2] \\ \vdots \\ \mathbf{v}^\rho[m_M] \end{pmatrix}. \tag{6.7}$$

The space $\mathbf{V}^\rho_\mathcal{J}$ is a complex vector space of dimension Md^2, where $d = \dim \rho$ and M is the number of orbits of the action of G on the indices $\mathcal{I}$.

Finally fix a selection $\mathcal{J}$ and let $d = \dim \rho$. Denote by $\mathbf{U}^\rho_\mathcal{J}$ the vector space with coordinates indexed by $\mathcal{J}$ and whose entries are column vectors of length d. We are thinking of this space as the space of "column vectors" for elements of $\mathbf{V}^\rho_\mathcal{J}$. The space $\mathbf{U}^\rho_\mathcal{J}$ is a complex vector space of dimension Md.

The use of the "coordinates" $v^\rho_{ik}[m]$ for vectors in the subspace V^ρ_k can be expressed in the matrix notation very nicely. View the matrix of operators $\mathbf{P}^\rho$ as a linear map from the space of ordinary vectors V to the space of vectors of matrices $\mathbf{V}^\rho_\mathcal{I}$:

$$\mathbf{P}^\rho : V \to \mathbf{V}^\rho_\mathcal{I}$$

sending a vector $v \in V$ to the column vector $\mathbf{v}^\rho$ of matrices. Given the selection $\mathcal{J}$, we have the natural projection of $\mathbf{V}^\rho_\mathcal{I}$ onto $\mathbf{V}^\rho_\mathcal{J}$ given by keeping only those M coordinates in $\mathcal{J}$; let us denote this projection by $\pi^\rho_\mathcal{J}$:

$$\pi^\rho_\mathcal{J} : \mathbf{V}^\rho_\mathcal{I} \to \mathbf{V}^\rho_\mathcal{J}.$$

Finally let $\mathbf{U}^\rho_\mathcal{J}$ be the space of "vectors of vectors" as described above. For any fixed $j = 1, \ldots, \dim \rho$, we have a natural projection $\pi^\rho_{\mathcal{J},j}$ of $\mathbf{V}^\rho_\mathcal{J}$ onto $\mathbf{U}^\rho_\mathcal{J}$, sending a vector of matrices $\mathbf{v}^\rho_\mathcal{J}$ to the vector of j^{th} columns $\mathbf{v}^\rho_{\mathcal{J},j}$ (i.e., the m^{th} entry of $\mathbf{v}^\rho_{\mathcal{J},j}$ is the j^{th} column of the m^{th} entry of $\mathbf{v}^\rho_\mathcal{J}$):

$$\pi^\rho_{\mathcal{J},j} : \mathbf{V}^\rho_\mathcal{J} \to \mathbf{U}^\rho_\mathcal{J}.$$

The composition $\pi^\rho_{\mathcal{J},j} \circ \pi^\rho_\mathcal{J} \circ \mathbf{P}^\rho$ can be restricted to the symmetry subspace V^ρ_j to give a linear map

$$\phi^\rho_j = \pi^\rho_{\mathcal{J},j} \circ \pi^\rho_\mathcal{J} \circ \mathbf{P}^\rho : V^\rho_j \to \mathbf{U}^\rho_\mathcal{J}.$$

Proposition 6.8. *With the above notation, if G acts without fixed points, the linear map $\phi^\rho_j : V^\rho_j \to \mathbf{U}^\rho_\mathcal{M}$ is an isomorphism of complex vector spaces.*

PROOF. We can easily write down the inverse map, guided by the formula (4.2). Fix an index j, and let $(\underline{w})$ be a vector of vectors in $\mathbf{U}^\rho_{\mathcal{J}}$ (so that $\underline{w}[m]$ is a column vector of length $d = \dim \rho$, whose i^{th} coordinate is $w_i[m]$, say). Define $\psi : \mathbf{U}^\rho_{\mathcal{J}} \to V^\rho_j$ by

$$\psi(\underline{w})[n] = \sum_{k=1}^{\dim \rho} A^\rho_{kj}(g^{-1}) w_k[m]$$

if $n = gm$. (Under the assumption of no fixed points, there is a unique selected index $m \in \mathcal{J}$ and a unique group element $g \in G$ such that $n = gm$.) We leave it to the reader to check that ψ maps $\mathbf{V}^\rho_{\mathcal{J},j}$ into V^ρ_j, and that it is an inverse to ϕ^ρ_j. $\square$

An alternate proof of the above proposition is obtained by noting that, in the case where G acts without fixed points, these spaces have the same dimension. Hence it suffices to show that the linear map ϕ^ρ_j is 1-1, which is elementary.

As a corollary, we see that we have a similar isomorphism for the canonical subspaces. Let ϕ^ρ be the composition $\pi^\rho_{\mathcal{J}} \circ \mathbf{P}^\rho$ restricted to the canonical subspace $V^\rho = \bigoplus_i V^\rho_i$.

COROLLARY 6.9. *With the above notation, if G acts without fixed points, the linear map $\phi^\rho : V^\rho \to \mathbf{V}^\rho_{\mathcal{J}}$ is an isomorphism of complex vector spaces.*

With this use of matrix notation, the linear system for the subproblem (3.1) can now be written as

$$\mathbf{L}^\rho \, \mathbf{u}^\rho = \mathbf{v}^\rho \tag{6.10}$$

where $\mathbf{L}^\rho$ is an appropriately-indexed version of the matrix $L^\rho[(i,m),(j,n)]$ constructed in Section 4. This matrix $\mathbf{L}^\rho$ is an Md-by-Md matrix, which because of the double-indexing, can be viewed naturally as an M-by-M matrix whose mn^{th} entry is a d-by-d matrix. Indeed, using the definition (4.4) of $L^\rho[(i,m),(j,n)]$, we see that the mn^{th} entry is the matrix $\sum_{g \in G} L[g^{-1}m, n] \mathbf{A}^\rho(g^{-1})^\top$. Thus $\mathbf{L}^\rho$ in this form is naturally *a sum of tensor product matrices.*

Recall that the tensor product of two matrices X and Y which are d-by-d and e-by-e respectively is the de-by-de matrix $X \otimes Y$ which breaks naturally into a d-by-d matrix with e-by-e matrix entries: the matrix in the rs^{th} block is $X_{rs}Y$.

To write our matrix $\mathbf{L}^\rho$ with this notation, one more definition is useful. Specifically, for $g \in G$ define the M-by-M matrix $\mathbf{L}_g$ by

$$\mathbf{L}_g[m,n] = L[g^{-1}m, n]. \tag{6.11}$$

Then

$$\mathbf{L}^\rho = \sum_{g \in G} \mathbf{L}_g \otimes \mathbf{A}^\rho(g^{-1})^\top. \tag{6.12}$$

The overview of the method given in this article can now be written with this notation as follows:

Given: a vector v of V.
To Solve: $\mathcal{L}(u) = v$ for the unknown vector u.

1: Choose a selection $\mathcal{J}$ of indices.
2: Find a full set of irreducible complex matrix representations for G.
3: Determine the entries $L[m,n]$ of the matrix for $\mathcal{L}$ in the selected columns, find the matrices $\mathbf{L}_g$ for each group element g, and form the matrix $\mathbf{L}^\rho$ for each complex matrix representation ρ.
4: For each ρ in the full set of irreducible complex matrix representations, perform steps 4a - b:
 4a: Form the column vector (with matrix entries) $\mathbf{v}^\rho$ from the given vector v, using (6.2):

$$\mathbf{v}^\rho[m] = \frac{\dim\rho}{\#G}\sum_{g\in G} v[g^{-1}m]\mathbf{A}^\rho(g^{-1})^\top$$

 4b: Solve the subproblems (6.10) for the column vector (with matrix entries) $\mathbf{u}^\rho$:

$$\mathbf{L}^\rho\mathbf{u}^\rho = \left[\sum_{g\in G}\mathbf{L}_g \otimes \mathbf{A}^\rho(g^{-1})^\top\right]\mathbf{u}^\rho = \mathbf{v}^\rho.$$

5: Reconstruct the solution vector u from the $\mathbf{u}^\rho$'s using (6.5) and (2.5):

$$u[gm] = \sum_\rho \operatorname{trace}(\mathbf{A}^\rho(g^{-1})^\top\mathbf{u}^\rho[m]).$$

7. Variations in the Case of Fixed Points

How does the preceding discussion change if there are fixed points for the permutation action of G on the indices? The alteration in the method comes from the fact that the coordinates $v^\rho_{ik}[m]$ no longer are independent coordinates for the subspaces V^ρ_k. One sees this by analyzing the formula (4.2) in the case where m is a fixed index under a group element g, i.e., when $gm = m$; one obtains

$$v^\rho_{kk}[m] = \sum_{i=1}^{\dim\rho}\mathbf{A}^\rho_{ik}(g^{-1})v^\rho_{ik}[m]. \tag{7.1}$$

which gives a relation among the coordinates $v^\rho_{ik}[m]$ whenever we have a non-trivial element g fixing an index m.

Expressed in the matrix notation, using Proposition 6.3.1 this becomes

$$\mathbf{v}^\rho[m] = \mathbf{A}^\rho(g^{-1})^\top\mathbf{v}^\rho[m] \tag{7.2}$$

for any group element g in the isotropy subgroup G_m.

We claim that these are the only conditions on the coordinates. To be precise, let $\widehat{\mathbf{V}^\rho_\mathcal{J}}$ be the subspace of $\mathbf{V}^\rho_\mathcal{J}$ consisting of those "vectors of $d \times d$ matrices" $(\mathbf{w}[-])$ indexed by $m \in \mathcal{J}$ satisfying (7.2), i.e.,

$$\mathbf{w}[m] = \mathbf{A}^\rho(g^{-1})^\top \mathbf{w}[m] \tag{7.3}$$

for every $m \in \mathcal{J}$ and every g in the isotropy subgroup G_m. Then we have immediately that the linear map ϕ^ρ defined above maps the canonical space V^ρ into the subspace $\widehat{\mathbf{V}^\rho_\mathcal{J}}$.

Proposition 7.4. *With the above notation, the linear map*

$$\phi^\rho : V^\rho \to \widehat{\mathbf{V}^\rho_\mathcal{J}}$$

is an isomorphism of complex vector spaces.

Proof. Again we will proceed by constructing an inverse map ψ for ϕ^ρ. Fix an element $(\mathbf{w}[-])$ in $\widehat{\mathbf{V}^\rho_\mathcal{J}}$, i.e., $(\mathbf{w}[-]) \in \mathbf{V}^\rho_\mathcal{J}$ and satisfies (7.3) for every $m \in \mathcal{J}$ and every $g \in G_m$. Fix an index $n \in \mathcal{I}$, and write $n = gm$ for some $g \in G$ and $m \in \mathcal{J}$. Define $\psi((\mathbf{w}[-]))$ to be the vector v with n^{th} coordinate

$$v[n] = \mathrm{trace}(\mathbf{A}^\rho(g^{-1})^\top \mathbf{w}[m]).$$

The reader can easily check that this assignment is well-defined, independent of the choice of the group element g. (In the case of non-trivial isotropy, more than one group element can send m to n.) Moreover, one next checks that ψ actually maps to the canonical subspace V^ρ.

Finally it is an easy matter to verify that ψ is an inverse for ϕ^ρ. $\square$

The corresponding statement for the symmetry subspaces $\mathbf{V}^\rho_j$ can be obtained as a corollary of the above, since the j^{th} symmetry space V^ρ_j exactly corresponds under the above isomorphism to the j^{th} columns of the associated vector of matrices.

To be specific, let $\widehat{\mathbf{U}^\rho_\mathcal{J}}$ be the subspace of $\mathbf{U}^\rho_\mathcal{J}$ consisting of those "vectors of vectors" $(\mathbf{u}[-])$ indexed by $m \in \mathcal{J}$ satisfying the vector version of (7.2), i.e.,

$$\mathbf{u}[m] = \mathbf{A}^\rho(g^{-1})^\top \mathbf{u}[m] \tag{7.5}$$

for every $m \in \mathcal{J}$ and every $g \in G_m$. Then we have immediately that the linear map ϕ^ρ_j defined above maps the symmetry space V^ρ_j into the subspace $\widehat{\mathbf{U}^\rho_\mathcal{J}}$.

Corollary 7.6. *With the above notation, the linear map*

$$\phi^\rho_j : V^\rho_j \to \widehat{\mathbf{U}^\rho_\mathcal{J}}$$

is an isomorphism of complex vector spaces.

If indeed G acts without fixed points, then $\widehat{\mathbf{V}^\rho_{\mathcal{J}}} = \mathbf{V}^\rho_{\mathcal{J}}$ and $\widehat{\mathbf{U}^\rho_{\mathcal{J}}} = \mathbf{U}^\rho_{\mathcal{J}}$, so that Proposition 6.8 and Corollary 6.9 are actually trivial consequences of Proposition 7.4 and Corollary 7.6.

Using a bit of character theory, we can develop a formula for the dimension of the vector spaces $\widehat{\mathbf{U}^\rho_{\mathcal{J}}}$ and $\widehat{\mathbf{V}^\rho_{\mathcal{J}}}$ (and therefore, by the above results, for the symmetry spaces V^ρ_j and the canonical spaces V^ρ).

Proposition 7.7. *Let the irreducible matrix representation ρ have character function χ^ρ. Then*

$$\dim V^\rho_j = \dim \widehat{\mathbf{U}^\rho_{\mathcal{J}}} = \sum_{m \in \mathcal{J}} \frac{1}{\#G_m} \sum_{g \in G_m} \chi^\rho(g)$$

and

$$\dim V^\rho = \dim \widehat{\mathbf{V}^\rho_{\mathcal{J}}} = \dim \rho \sum_{m \in \mathcal{J}} \frac{1}{\#G_m} \sum_{g \in G_m} \chi^\rho(g)$$

Proof. By considering every component of a "vector of vectors" in $\widehat{\mathbf{U}^\rho_{\mathcal{J}}}$ separately, it is clear that

$$\dim \widehat{\mathbf{U}^\rho_{\mathcal{J}}} = \sum_{m \in \mathcal{J}} \dim\{u \in \mathbb{C}^{\dim \rho} \mid u = \mathbf{A}^\rho(g^{-1})^\top u \text{ for all } g \in G_m\}$$

and so the task is to compute the dimension of this last vector space. This space is exactly the subspace of vectors, in the space of the inverse transpose representation τ to ρ, where G_m acts trivially. I.e., it is the "trivial part" of the restricted representation $\tau|_{G_m}$. The restricted representation $\tau|_{G_m}$ has the character function $\overline{\chi^\rho|_{G_m}}$. Moreover, the trivial part of any representation of any group H has dimension $\sum_{h \in H} \chi(h)/\#H$, where χ is the character of the representation. Therefore the desired dimension in our case is the quantity $(1/\#G_m)\sum_{g \in G_m} \overline{\chi^\rho(g)}$; since this quantity must be an integer, we may dispense with the complex conjugation in the sum, proving the first part of the proposition. The second equation follows since all the spaces V^ρ_j are isomorphic to each other, and so by Corollary 7.6, so are the spaces $\widehat{\mathbf{U}^\rho_{\mathcal{J}}}$; hence their direct sum $\widehat{\mathbf{V}^\rho_{\mathcal{J}}}$ has dimension equal to $\dim \rho$ times the dimension for $\widehat{\mathbf{U}^\rho_{\mathcal{J}}}$. $\square$

It is instructive to check that in the case where G acts without fixed points, the above formulas give the expected answer. Specifically, in this case, for every $m \in \mathcal{J}$, $G_m = \{I\}$; since $\chi^\rho(I) = \dim \rho$, the above reduces to the value $M \dim \rho$ found in the discussion following (4.3).

Now the method proceeds in a similar manner to the fixed-point-free case. First, one chooses, for each ρ, a basis for the space $\widehat{\mathbf{U}^\rho_{\mathcal{J}}}$. Then one transports the linear operator L from V^ρ_j to $\widehat{\mathbf{U}^\rho_{\mathcal{J}}}$ via the isomorphism ϕ^ρ_j. Actually, at this point one can transport the entire canonical space V^ρ to $\widehat{\mathbf{V}^\rho_{\mathcal{J}}}$ via ϕ^ρ; it is the same in principle.

The isomorphisms ϕ^ρ and $\phi^\rho_{\mathcal{J}}$ are sufficiently explicit to easily transport the right-hand-side vector v into the space. Thus a good choice of basis for the fixed-point space $\widehat{\mathbf{U}^\rho_{\mathcal{J}}}$ essentially finishes the variation in the method. This we have done by hand in simple cases. The interested reader should also consult [**8**] for a classification and construction of the symmetry-adapted bases for all permutation representations of the point groups in dimensions 2 and 3. It is a subject of ongoing study to efficiently determine a useful basis for this space in general, and thus to give a complete algorithm in the fixed-point case. The interested reader should also consult [**8**] for a classification and construction of the symmetry-adapted bases for all permutation representations of the point groups in dimensions 2 and 3.

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