Exploiting Symmetry in Numerical Solving[3,4]

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Abstract: It has recently been seen that the cost of numerically solving linear systems of equations in which the coefficient matrix is equivariant with respect to a permutation group Γ can be significantly reduced via the method of symmetry reduction. For systems in which the coefficient matrix is not equivariant, the numerical solving can be accelerated by using the Γ-equivariant part of the coefficient matrix as a preconditioner. In the present paper the equivariant part of a general linear transformation is studied for general finite groups Γ.

For finding the Γ-invariant zero points of Γ-equivariant nonlinear maps, the Jacobian map can be replaced by its equivariant part in Newton-type methods. This increases the numerical efficiency of a Newton step significantly. For this modification, it is shown that the familiar local convergence behavior to solutions is generally preserved. We give two examples. It is shown how these techniques can be used in numerical continuation and bifurcation.

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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.

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The first numerical symmetry reduction approaches along these lines have been given by Stiefel and Fässler [19, 31]. They introduced symmetry adapted bases to analyze equivariant linear maps. This tool has been exploited in many papers on bifurcation theory under group actions in the spirit of [23, 24, 34] for numerical purposes, see, e.g., [15, 20, 25, 26, 27, 35].

In the context of partial differential equations under group actions, a different approach for exploiting the symmetry structure has been to effect a domain reduction. The same PDE has to be repeatedly solved over a reduced domain (symmetry cell) with varying boundary conditions on the new boundaries, see, e.g., [1, 10, 11, 12, 13, 16, 17].

In a series of papers [2, 7, 8, 21, 22, 32, 33] the authors and collaborators have discussed efficient methods to exploit permutation symmetries in linear systems of equations. Such systems often arise naturally when discretizing equivariant operator equations. Our methods avoid the explicit use of symmetry adapted bases to gain higher efficiency. Most proofs relating to our methods for linear systems can be found in [8]. A systematic approach to our symmetry reduction method has been implemented and is available via the net:

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ftp        ftp.math.colostate.edu
login:     anonymous
password:  your_email_address
cd         pub/georg
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The present paper is concerned with incorporating the numerical symmetry reduction methods for linear systems of equations into methods of Newton type for solving discretizations of nonlinear operator equations and particularly into numerical continuation methods. In the latter application the aim is to follow a branch of solutions which are invariant under the action of some group. The hindrance to making an immediate incorporation of the symmetry reduction method into the numerical continuation method is that at points which are not in the solution set, e.g., at points arising in the corrector process, the Jacobians with respect to the state variables are in general not equivariant and hence the symmetry reduction method is not directly applicable. The novelty investigated here deals with replacing the Jacobian of a map in the Newton method by its equivariant part. It is shown that in making this replacement there is no loss in the asymptotic convergence behavior.

The paper is organized as follows. In Section 2 some of the group theoretical background required for our discussions is given. Section 3 contains a brief review of the most important aspects of the symmetry reduction method for linear systems of equations which was developed by the authors and collaborators. In Section 4 we introduce the idea of the equivariant part of a linear operator and characterize its properties. Section 5 deals with Newton type methods which incorporate the equivariant part of the Jacobian in place of the actual Jacobian. In Section 6 we analyse possibilities for numerically exploiting equivariant structure in continuation methods. Section 7 can be viewed as an appendix to Section 6: we furnish some relevant theorems and proofs.

2. Group Theoretical Background

Let us begin with a review of some group theoretical ideas of which we will make use. Let H be a complex Hilbert space, and let Γ be a finite group. By $\mathcal{U}(H)$ we denote the unitary linear operators on H, and by $\mathcal{L}(H)$ the bounded linear operators from H into H.

Definition 1. A map $T : \Gamma \to \mathcal{U}(H)$ is called a (unitary) *representation* of Γ on H if and only if:

1. T is a homomorphism of groups,
2. T maps the unit $e \in \Gamma$ onto the identity $\mathrm{I} \in \mathcal{U}(H)$.

We also say that the group Γ *acts* on H. We note that by the above assumptions $T(g^{-1}) = T(g)^{-1} = T(g)^*$ is the adjoint of $T(g)$ for $g \in \Gamma$.

A typical example is the following

Example 2. Let Γ be a finite group of orthogonal linear transformations on $\mathbb{R}^N$. Let $H := L^2(\mathbb{R}^N)$ denote the Hilbert space of square integrable functions on $\mathbb{R}^N$. Then $T(g)x = x \circ g^{-1}$, $g \in \Gamma$, $x \in H$, defines a representation of Γ on H. We call Γ the *canonical* action of Γ on H.

Definition 3. Let T be a representation of Γ on H. We call T *reducible* if and only if there exists a splitting of H into a non-trivial direct sum $H = H_1 \oplus H_2$ such that $T(g)H_1 \subset H_1$ and (consequently) $T(g)H_2 \subset H_2$ for all $g \in \Gamma$. We then have that T splits into $T = T_1 \oplus T_2$ where T_1 acts on H_1 and T_2 on H_2.

A representation is called *irreducible* if and only if it is not reducible.

Two of the celebrated theorems in representation theory of groups state:

Theorem 4. *Each irreducible representation T acts on a finite dimensional space, the dimension of which is called the* dimension $\dim(T)$.

Hence, we will denote an irreducible representation T as a unitary square matrix $T(g)[i, j]$ where the elements depend on $g \in \Gamma$.

Theorem 5. *Each representation splits into a direct sum of irreducible representations:*

$$T = \bigoplus_i T_i \quad \textit{where} \quad H = \bigoplus_i H_i$$

and T_i acts on H_i.

Remark 6. Two irreducible representations T_1, T_2 are called *equivalent* if they are obtained from each other via a similarity transformation (which is independent of $g \in \Gamma$). Let us call a list of irreducible representations *complete* if any two members of the list are non-equivalent, and if the list is maximal. Complete lists of important groups have been studied in great detail and can be found in the standard literature on group theory, see, e.g., [30]. We emphasize that for the symmetry groups occuring in typical discretizations of equivariant operator equations such complete lists are well-known.

Definition 7. Assume that T is a representation of Γ on H.

1. Let $F : H \times \mathbb{R} \to H$ be a (nonlinear) map. We call F Γ-*equivariant* if and only if $T(g)F(x, \lambda) = F(T(g)x, \lambda)$ holds for all $g \in \Gamma$, $x \in H$ and $\lambda \in \mathbb{R}$.
2. Similarly, a linear operator $A \in \mathcal{L}(H)$ is Γ-equivariant if and only if $T(g)A = AT(g)$ for all $g \in \Gamma$,
3. also a (nonlinear) map $G : H \to H$ is called Γ-equivariant if and only if $T(g)G(x) = G(T(g)x)$ holds for all $g \in \Gamma$ and all $x \in H$.
4. Finally, $x \in H$ is called Γ-*invariant* if and only if $T(g)x = x$ for all $g \in \Gamma$,

If geometric symmetries are present, then many classical operators induced by differential or integral equations are Γ-equivariant. Typical nonlinear differential operators which exhibit equivariance are many of the mildly nonlinear elliptic differential operators defined on domains which are invariant with respect to a group. The following examples illustrate how equivariance manifests itself in integral equations.

Example 8. Let Γ be a finite group of orthogonal linear transformations on $\mathbb{R}^N$, and let $\Omega \subset \mathbb{R}^N$ be a measurable subset. We denote $H := L^2(\Omega)$. Let Ω be *invariant* under Γ, i.e., $g(\Omega) = \Omega$ for all $g \in \Gamma$. Let $K : \Omega \times \Omega$ be a kernel such that the induced integral operator $(\tilde{K}x)(s) = \int_\Omega K(s,t)x(t)dt$, $x \in H$, $s \in \Omega$ has the property that $\tilde{K} \in \mathcal{L}(H)$. Consider the canonical action T of Γ on H introduced in Example 2. Then $\tilde{K}$ is Γ-equivariant if and only if $K(gs, gt) = K(s,t)$ holds for all $g \in \Gamma$, $s, t \in \Omega$. For a proof, see [5].

Example 9. Let Γ be a finite group of orthogonal linear transformations on $\mathbb{R}^N$, and let $\Omega \subset \mathbb{R}^N$ be an open bounded domain with sufficiently regular boundary $\partial\Omega$. We denote $H := L^2(\partial\Omega)$. Let Ω be invariant under Γ, i.e., $g(\Omega) = \Omega$ for all $g \in \Gamma$. Let $K : \partial\Omega \times \partial\Omega$ be a kernel such that the induced boundary integral operator $(\tilde{K}x)(s) = \int_{\partial\Omega} K(s,t)x(t)\mu(dt)$, $x \in H$, $s \in \partial\Omega$ has the property that $\tilde{K} \in \mathcal{L}(H)$. Here μ denotes the measure obtained from the so-called surface element. Consider the canonical action T of Γ on H introduced in Example 2. Then $\tilde{K}$ is Γ-equivariant if and only if $K(gs, gt) = K(s,t)$ holds for all $g \in \Gamma$, $s, t \in \partial\Omega$. For a proof, see [5].

Typical examples for the latter equivariant kernels K are those arising in potential theory and boundary integral equations.

3. A brief Sketch of our Symmetry Reduction Method

Let Γ be a subgroup of the permutation group S_n of the n indices $\{1:n\}$. We define a natural action T of Γ on the vector space $\mathbb{C}^n$ via

$$(T(g)x)[k] := x[g^{-1}k] \quad \text{for} \quad g \in \Gamma,\ x \in \mathbb{C}^n,\ k \in \{1:n\} .$$

If A is a square matrix of size n, we can view A as a linear map $A \in \mathcal{L}(\mathbb{C}^n)$, and hence Γ-equivariance of A is defined via Definiton 7. It is easy to see that the following holds:

Lemma 10. *The square matrix A of size n is Γ-equivariant if and only if:*

$$A[gk, gl] = A[k,l] \quad \textit{for} \quad k,l \in \{1:n\},\ g \in \Gamma ,$$

or equivalently

$$A[gk, l] = A[k, g^{-1}l] \quad \textit{for} \quad k,l \in \{1:n\},\ g \in \Gamma . \tag{1}$$

Example 11. Consider an action T of a finite group Γ on a Hilbert space H, and assume that a linear operator equation $Lu = f$ has to be solved where L is Γ-equivariant. Galerkin's method is based on a choice of basis functions u_k. It is reasonable to assume that T permutes the basis functions u_k. Hence we can view the group Γ as a group of permutations on the indices k according to the following formula:

$$T(g)u_k = u_{gk} \quad \text{for} \quad g \in \Gamma.$$

If we approximate the solution $u = \sum_k x[k]u_k$ and set

$$A[k,l] = \langle Lu_k\, ,\, u_l\rangle \text{ and } b[l] = \langle f\, ,\, u_l\rangle,$$

then Galerkin's method means that we have to solve the linear system $Ax = b$. It is easy to see that the system matrix A is Γ-equivariant in the sense of (1). See [3, 4, 5] for more details and examples.

Let us illustrate how a linear equation $Ax = b$ with a Γ-equivariant matrix A can be efficiently solved. For proofs we refer to [8]. Hence in the following we consider a linear system $Ax = b$ where the square matrix A of size n is Γ-equivariant in the sense of Lemma 10.

Let $\mathbb{S} \subset \{ 1 : n \}$ be a *selection* of indices. By that we mean that

$$\{ g(\mathbb{S}) \}_{g \in \Gamma} \quad \text{is a partition of } \{ 1 : n \}.$$

Indices that are fixed under some of the permutations $g \in \Gamma$ need special attention. We therefore define for $i \in \{ 1 : n \}$ the *isotropy subgroup*

$$\Gamma_i := \{ g \in \Gamma \ : \ gi = i \} \ . \tag{2}$$

Obviously, i is not fixed under any (non-trivial) permutation $g \in \Gamma$ if and only if $|\Gamma_i| = 1$, i.e., Γ is trivial. Let us call such an index *free*.

Discretizations of Γ-equivariant operator equations often generate a few indices that are fixed, though the majority of indices typically are free.

Note that for computer implementations, only a selection of columns $\{ a_l \ : \ l \in \mathbb{S} \}$ of a Γ-equivariant matrix A has to be generated and stored. The other entries are easily obtained via (1).

Let us denote by $\mathcal{R}$ a complete list of irreducible representations of Γ, see Remark 6. We denote the elements of $\mathcal{R}$ by r.

For each $\mathrm{r} \in \mathcal{R}$ and $i \in \{ 1 : n \}$ we define the orthogonal projection matrix

$$\mathrm{P}_{r,i} := \tfrac{1}{|\Gamma_i|} \sum_{g \in \Gamma_i} r(g) \tag{3}$$

$$\text{which has rank} \quad m_{r,i} := \operatorname{rank} \mathrm{P}_{r,i} = \operatorname{trace} \mathrm{P}_{r,i} \ .$$

Let us denote by d_r the dimension of r. Hence $m_{r,i} \leq d_\mathrm{r}$. Note that $\mathrm{P}_{r,i} = \mathrm{I}$ if i is free. Also note that for the symmetry groups corresponding to discretizations of three dimensional problems, d_r is very small and typically has values in $\{ 1, 2, 3 \}$.

We further introduce a matrix $u_{\mathrm{r},i}$ of size $(d_\mathrm{r}\, ,\, m_{\mathrm{r},i})$ whose columns are an orthonormal basis of the range of the projectors $\mathrm{P}_{\mathrm{r},i}$. Hence

$$u_{\mathrm{r},i} u_{\mathrm{r},i}^* = \mathrm{P}_{\mathrm{r},i} \quad \text{and} \quad u_{\mathrm{r},i}^* u_{\mathrm{r},i} = \mathrm{I}\, . \tag{4}$$

Note again that $u_{r,i} = \mathrm{I}$ if i is free.

The main tool for our symmetry reduction method consists of the following transformation which can be viewed as a generalization of the discrete Fourier transform:

Definition 12 (Generalized Fourier Transform (GFT))**.**
Let $w \in \mathbb{C}^n$. Then for each $r \in \mathcal{R}$ and each $i \in \{ 1 : n \}$ we define

$$\hat{w}[\mathrm{r}, i] := \sqrt{\tfrac{d_\mathrm{r}}{|\Gamma|}}\; u_{\mathrm{r},i}^* \sum_{g \in \Gamma} w[gi]\; \mathrm{r}(g^{-1}) \;. \tag{5}$$

Note that the entries of $\hat{w}$ are small rectangular block matrices of varying size $(d_\mathrm{r}\,,\, m_{\mathrm{r},i})$. It is important that we can easily retrieve w from $\hat{w}$:

Lemma 13 (Inverse GFT)**.**

$$w[gk] = \sum_{\mathrm{r} \in \mathcal{R}} \sqrt{\tfrac{d_\mathrm{r}}{|\Gamma|}}\, \mathrm{trace}\left(r(g) u_{r,k} \hat{w}[\mathrm{r}, k]\right) \;. \tag{6}$$

Note that according to the above formula the GFT $\hat{w}[\mathrm{r}, k]$ needs to be known only for a selection $k \in \mathbb{S}$ of indices in order to retrieve the column w completely.

Let us denote the l-th column of A by a_l. Our symmetry reduction method is based on the following formula:

$$\sqrt{\tfrac{|\Gamma|}{d_\mathrm{r}}} \sum_{l \in \mathbb{S}} \tfrac{1}{|\Gamma_l|} \hat{a}_l[\mathrm{r}, k] u_{\mathrm{r},l}\; \hat{x}[\mathrm{r}, l] = \hat{b}[\mathrm{r}, k], \quad \mathrm{r} \in \mathcal{R},\; k \in \mathbb{S}\,. \tag{7}$$

Note that for each fixed irreducible representation $\mathrm{r} \in \mathcal{R}$, these are linear equations for the $\sum_{l \in \mathbb{S}} m_{\mathrm{r},l} \cdot d_\mathrm{r}$ unknowns $\hat{x}[\mathrm{r}, l]$, $l \in \mathbb{S}$, involving the matrix

$$\mathcal{A}_\mathrm{r}[k, l] := \sqrt{\tfrac{|\Gamma|}{d_\mathrm{r}}}\; \tfrac{1}{|\Gamma_l|} \hat{a}_l[\mathrm{r}, k] u_{\mathrm{r},l}, \quad k, l \in \mathbb{S}\,. \tag{8}$$

Thus, the linear system $Ax = b$ is transformed into the block-diagonal form

$$\boxed{\sum_{l \in \mathbb{S}} \mathcal{A}_\mathrm{r}[k, l]\; \hat{x}[\mathrm{r}, l] = \hat{b}[\mathrm{r}, k], \quad k, l \in \mathbb{S}, \quad \mathrm{r} \in \mathcal{R},} \tag{9}$$

where each square block $\mathcal{A}_\mathrm{r}$ has size $\sum_{l \in \mathbb{S}} m_{\mathrm{r},l}$ and appears d_r times.

Let us summarize our symmetry reduction method for solving the Γ-equivariant linear system $Ax = b$:

1. Calculate the GFT $\hat{b}$ of b.
2. Calculate the GFT $\hat{a}_l$ of a selection of columns a_l to generate the submatrices $\mathcal{A}_\mathrm{r}$ in (8).
3. Solve the reduced problems (9) for a complete list of irreducible representations $\mathrm{r} \in \mathcal{R}$.
4. Use the inverse Fourier transform (6) to retrieve x from $\hat{x}$.

Since the method generates a block diagonalization of A, it is also well suited to numerically handle eigenvalue problems. Thus the eigenvalues of the original matrix A are distributed among the various blocks $\mathcal{A}_{\mathrm{r}}$. Multiplicities of eigenvalues generated by the symmetries disappear.

In general, if A is a sparse matrix, the symmetry reduced submatrices $\mathcal{A}_{\mathrm{r}}$ are still sparse. For further details and examples, see [3, 4, 5, 7, 8, 9, 21, 22, 33].

Our approach can be easily used to *automatically* generate symmetry adapted bases of discretized problems which have often been used in the context of bifurcation and eigenvalue analysis. This is important for standard discretizations of operator equations which will typically contain nodes that are fixed under some of the symmetries, so that the generation of symmetry adapted bases is not very simple. Our reduction procedures actually sidestep the need to generate and make use of such symmetry adapted bases.

On the other hand, we argue that by avoiding the explicit use of a symmetry adapted basis in the above way we reduce the computational effort considerably. For details, see the section *Overhead and Computational Savings* in [5].

4. The Equivariant Part of an Operator

When analyzing bifurcation problems with symmetry via numerical methods, some path-following (predictor-corrector) method has to be employed which traces a branch of solutions that are fixed under the action of some group, say Γ. At bifurcation points, the symmetry (i.e., group) may switch. Such points are called *symmetry breaking bifurcation points.*

Numerically, it is important to have efficient methods for following the branch. While a predictor step along the branch is usually inexpensive, Newton type corrector steps are usually computationally very expensive and contain the main cost of the continuation process. If $F : H \times \mathbb{R} \to H$ is the nonlinear map characterizing the bifurcation scenario, then a typical Newton type step would involve the solving of a linear system involving a linear operator B approximating derivatives of F, see Section 6.

In Section 3 we have seen that symmetry can be exploited to drastically reduce the computational expense if B is Γ-equivariant. This is the motivation for the following discussion.

Definition 14. Let T be an action of Γ on H. Let $B \in \mathcal{L}(H)$. Then we call

$$B_\Gamma := \tfrac{1}{|\Gamma|} \sum_{g \in \Gamma} T(g) B T(g)^* \tag{10}$$

the Γ-*equivariant part* of B. Here $|\Gamma|$ denotes the number of elements in Γ, i.e., the order of the group Γ.

It is straightforward to verify that $B = B_\Gamma$ if and only if B is Γ-equivariant.

We also note that

$$B_\Gamma = \tfrac{1}{|\Gamma|} \sum_{g \in \Gamma} T(g)^* B T(g) \tag{11}$$

since with g also g^{-1} runs through Γ and since $T(g^{-1}) = T(g)^*$ holds.

Let us now show that the Γ-equivariant part of B is the Γ-equivariant operator *nearest* to B. To show this, we introduce some facts about Hilbert-Schmidt operators, see, e.g., [18, Section XI.6].

Remark 15. Let u_α be a Hilbert basis of H, and let $B \in \mathcal{L}(H)$. We call B a *Hilbert-Schmidt operator* if and only if

$$||B||_{\mathrm{HS}}^2 := \sum_\alpha ||Bu_\alpha||^2 < \infty\,.$$

In this case $||B||_{\mathrm{HS}}$ is called the *Hilbert-Schmidt norm* of B. The Hilbert-Schmidt operators form a Hilbert space $\mathcal{L}_{\mathrm{HS}}(H)$ with the scalar product

$$\langle A\,,\, B\rangle_{\mathrm{HS}} := \sum_\alpha \langle Au_\alpha\,,\, Bu_\alpha\rangle \;\;.$$

It is important to note that the above definitions are independent of the choice of the basis u_α.

Example 16. Continuing our Example 8, it can be shown that

$$||\tilde{K}||_{\mathrm{HS}}^2 = \int_\Omega \int_\Omega |K(s,t)| ds\, dt \;.$$

Example 17. If $H = \mathbb{C}^n$ with the usual scalar product, then $\mathcal{L}(H)$ consists of the square matrices B of size n, and since we have

$$||B||_{\mathrm{HS}}^2 = \sum_{k,l=1}^{n} |B[k,l]|^2,$$

the Hilbert-Schmidt norm for matrices is the Frobenius norm.

The following theorem was shown in [32, 33] for the special case that T is a permutation representation of Γ on $\mathbb{C}^n$.

Theorem 18. *Let T be an action of Γ on H, and let $B \in \mathcal{L}_{\mathrm{HS}}(H)$. Then B_Γ is the Γ-equivariant operator in $\mathcal{L}_{\mathrm{HS}}(H)$ which is closest to B in the $||\cdot||_{\mathrm{HS}}$-norm.*

Proof. In the proof below we will need that along with u_α that also $T(g)^* u_\alpha$ for fixed $g \in \Gamma$ is a Hilbert basis. We define the map $\mathcal{P} : \mathcal{L}_{\mathrm{HS}}(H) \to \mathcal{L}_{\mathrm{HS}}(H)$ by $\mathcal{P}B = B_\Gamma$. It is obvious that $\mathcal{P}$ is linear, $\mathcal{P}^2 = \mathcal{P}$, and that

$$\operatorname{range} \mathcal{P} = \{\, A \in \mathcal{L}_{\mathrm{HS}}(H) \,:\, A \text{ is } \Gamma\text{-equivariant} \,\}\,.$$

Let us show that $\mathcal{P}$ is self-adjoint (with respect to the Hilbert space $\mathcal{L}_{\mathrm{HS}}(H)$), i.e., that

$$\langle \mathcal{P}A\,,\, B\rangle_{\mathrm{HS}} = \langle A\,,\, \mathcal{P}B\rangle_{\mathrm{HS}} \quad \text{for all } A, B \in \mathcal{L}_{\mathrm{HS}}(H)\ .$$

In fact, this follows from

$$\begin{aligned}
\langle A_\Gamma\,,\, B\rangle_{\mathrm{HS}} &= \tfrac{1}{|\Gamma|} \sum_{g\in\Gamma} \sum_{\alpha} \langle T(g)AT(g)^* u_\alpha\,,\, Bu_\alpha\rangle \\
&= \tfrac{1}{|\Gamma|} \sum_{g\in\Gamma} \sum_{\alpha} \langle AT(g)^* u_\alpha\,,\, T(g)^* Bu_\alpha\rangle \\
&= \tfrac{1}{|\Gamma|} \sum_{g\in\Gamma} \sum_{\alpha} \langle AT(g)^* u_\alpha\,,\, T(g)^* BT(g)T(g)^* u_\alpha\rangle \\
&= \tfrac{1}{|\Gamma|} \sum_{g\in\Gamma} \langle A\,,\, T(g)^* BT(g)\rangle_{\mathrm{HS}} \\
&= \langle A\,,\, B_\Gamma\rangle_{\mathrm{HS}}\ .
\end{aligned}$$

Hence $\mathcal{P}$ is an orthogonal projector from $\mathcal{L}_{\mathrm{HS}}(H)$ onto

$$\{\, A \in \mathcal{L}_{\mathrm{HS}}(H) \,:\, A \text{ is } \Gamma\text{-equivariant} \,\}\,,$$

and the assertion follows. □

If instead of the Hilbert-Schmidt norm the usual (induced) operator norm is considered, then the following simple inequality will be useful:

Theorem 19. *Let T be an action of Γ on H, and let $B \in \mathcal{L}(H)$. Then $||B_\Gamma|| \le ||B||$.*

Proof. From $B_\Gamma = \frac{1}{|\Gamma|} \sum_{g\in\Gamma} T(g)BT(g)^*$ it follows that

$$||B_\Gamma|| \le \tfrac{1}{|\Gamma|} \sum_{g\in\Gamma} ||T(g)BT(g)^*|| = \tfrac{1}{|\Gamma|} \sum_{g\in\Gamma} ||B|| = ||B||$$

□

In a similar but much simpler way we can also study the Γ-invariant part of a vector $x \in H$:

$$x_\Gamma := \tfrac{1}{|\Gamma|} \sum_{g \in \Gamma} T(g)x \ . \tag{12}$$

It is readily seen that $x \mapsto x_\Gamma$ is an orthogonal projector onto the subspace $\{\, v \in H \ : \ T(g)v = v \text{ for } g \in \Gamma \,\}$ of Γ-invariant vectors in H.

5. Equivariant Newton's Method

In the following let H be a real Hilbert space. Hence actions of Γ on H are orthogonal transformations.

The following well-known fact can be used to exploit symmetry:

Example 20. Let T be an action of Γ on H, and let the sufficiently smooth (nonlinear) map $G : H \to H$ be Γ-equivariant. Let $\bar{x} \in H$ be Γ-invariant. Then the Jacobian $G'(\bar{x})$ is a Γ-equivariant linear operator in $\mathcal{L}(H)$.

Proof. Taylor's formula implies

$$\begin{aligned} &T(g)G(\bar{x}) + T(g)G'(\bar{x})h + \mathcal{O}(||h||^2) \\ =\ &T(g)G(\bar{x}+h) = G(\bar{x} + T(g)h) \\ =\ &G(\bar{x}) + G'(\bar{x})T(g)h + \mathcal{O}(||h||^2). \end{aligned}$$

Comparing the coefficients of h finishes the proof. □

The preceding example describes a special case of an operator G such that $G'(\bar{x})$ is Γ-equivariant with respect to some group action. Let us now investigate Newton like methods under the general assumption that $G(\bar{x}) = 0$ and $G'(\bar{x})$ is Γ-equivariant. Note that we do *not* assume in the following that G is equivariant and $\bar{x}$ is invariant. We begin with a simple situation:

Theorem 21. *Let T be an action of Γ on H, and let $G : H \to H$ three times continuously differentiable. Let $\bar{x}$ be a zero point of G such that $G'(\bar{x})$ is bijective and Γ-equivariant. Then the following modification of Newton's method*

$$G'(x_k)_\Gamma\, s_k + G(x_k) = 0 \qquad x_{k+1} := x_k + s_k \tag{13}$$

is locally quadratically convergent.

Proof. Define the map Φ via $\Phi(x) = x - G'(x)_\Gamma^{-1} G(x)$. Then Φ is defined on some neighborhood of $\bar{x}$, and (13) is the fixed point iteration with respect to Φ. We have $\Phi(\bar{x}) = \bar{x}$. Differentiating gives

$$\Phi'(x) = \mathrm{I} - G'(x)_\Gamma^{-1} G'(x) + \mathcal{O}(||G(x)||).$$

Since $G'(\bar{x})$ is Γ-equivariant and hence $G'(\bar{x})_\Gamma = G'(\bar{x})$. This implies that $\Phi'(\bar{x}) = 0$, and Φ is twice continuously differentiable. The result now follows from standard arguments in numerical analysis, e.g., [29]. □

In the same way, other theorems and proofs on the convergence of Newton like methods can be modified in such a way that an approximation of the Jacobian is replaced by its Γ-equivariant part. The following is an example. In order to keep the technicalities to a minimum, we make global (instead of local) assumptions and use the Landau symbol (instead of giving estimates with constants).

Theorem 22 (Inexact Newton Method)**.** *Let T be an action of Γ on H, and let $G : H \to H$ be such that G' exists and is Lipschitz continuous. Let $\bar{x}$ be a zero point of G such that $G'(\bar{x})$ is bijective and Γ-equivariant. Consider the iteration:*

$$\begin{aligned} \textit{Find } s_k \textit{ such that} \quad & ||G'(x_k)_\Gamma\, s_k + G(x_k)|| \le \eta_k \, \|G(x_k)\| \\ \textit{and set} \quad & x_{k+1} := x_k + s_k \,. \end{aligned}$$

Then

$$||x_{k+1} - \bar{x}|| \le (||x_k - \bar{x}|| + \eta_k)\, \mathcal{O}(||x_k - \bar{x}||).$$

for sufficiently small $||x_k - \bar{x}||$.

Typically, $\eta_k > 0$ is a sequence chosen so that $\lim_{k\to\infty} \eta_k = 0$.

Proof. From Taylors's formula

$$G(x_k) = G(\bar{x}) + \int_0^1 G'(\bar{x} + t(x_k - \bar{x}))dt(x_k - \bar{x})$$

we obtain

$$||G(x_k)|| = \mathcal{O}(||x_k - \bar{x}||). \tag{14}$$

From Theorem 19 we obtain

$$||G'(x_k)_\Gamma - G'(\bar{x})|| \le ||G'(x_k) - G'(\bar{x})|| = \mathcal{O}(||x_k - \bar{x}||)$$

and since G' is Lipschitz continuous,

$$\begin{aligned} ||G'(x_k)_\Gamma - G'(x_k)|| &\le ||G'(x_k)_\Gamma - G'(\bar{x})|| + ||G'(\bar{x}) - G'(x_k)|| \\ &= \mathcal{O}(||x_k - \bar{x}||). \end{aligned} \tag{15}$$

Now

$$x_{k+1} - \bar{x} = x_k - \bar{x} + s_k = x_k - \bar{x} + G'(x_k)_\Gamma^{-1} G(x_k) + \eta_k\, \mathcal{O}(||G(x_k)||)$$

From (14) and (15) it follows that

$$x_{k+1} - \bar{x} = x_k - \bar{x} + G'(x_k)^{-1} G(x_k) + (||x_k - \bar{x}|| + \eta_k)\, \mathcal{O}(||x_k - \bar{x}||)$$

Finally from the standard Newton estimate

$$x_k - \bar{x} + G'(x_k)^{-1} G(x_k) = \mathcal{O}(||x_k - \bar{x}||^2)$$

the assertion follows. □

Remark 23. Even if the map G is slightly perturbed from an equivariant map, due, e.g., to imperfections in the domain and/or lower order terms in a differential operator, the efficiency of the Newton method can be significantly improved by using the Γ-equivariant part in place of the actual Jacobian.

A different approach (which has been seen to be very successful, see [32, 33]) would be to use the Γ-equivariant part as a preconditioner.

6. Numerical Continuation and Equivariance

In many bifurcation problems one studies the solution sets of operator equations of the form $F(x, \lambda) = 0$ where $F : H \times \mathbb{R} \to H$ is a sufficiently smooth Fredholm operator of index one and H (for simplicity) is a Hilbert space. Typically, the solution set is approximated by making a discretization and subsequently numerically tracing the solution set of the discretized analogue $F(x, \lambda) = 0$ where H now is finite dimensional. Note that in the finite dimensional setting F is automatically Fredholm of index one.

The numerical tracing of curves in the solution set $F^{-1}(0)$ is performed via a numerical continuation method. A recent survey of numerical continuation methods has been given in [6]. We briefly sketch the main ideas of these methods. In doing so, we simultaneously analyse possibilities for numerically exploiting equivariance structure. To facilitate the reading, we leave the technical details and proofs to the next section.

Numerical continuation methods generally are of predictor-corrector type in which for an accepted solution $(\bar{x}_0, \bar{\lambda}_0)$ satisfying $F(\bar{x}_0, \bar{\lambda}_0) \approx 0$ a new solution $(\tilde{x}, \tilde{\lambda})$ is predicted in a chosen direction for tracing the solution set. A frequently used predictor step is the *tangent predictor*

$$(\tilde{x}_0, \tilde{\lambda}_0) = (\bar{x}_0, \bar{\lambda}_0) + h t(F'(\bar{x}_0, \bar{\lambda}_0))$$

where

$$t(F'(\bar{x}_0, \bar{\lambda}_0)) = \Big(t_1(F'(\bar{x}_0, \bar{\lambda}_0))\ ,\ t_2(F'(\bar{x}_0, \bar{\lambda}_0))\Big) \in H \times \mathbb{R}$$

denotes the unit null-vector of the Jacobian $F'(\bar{x}_0, \bar{\lambda}_0)$ in the desired direction of tracing, provided that $(\bar{x}_0, \bar{\lambda}_0)$ is a regular point of F, and $h > 0$ is a chosen *step length*.

The corrector process is carried out by performing a Newton type process starting from $(\tilde{x}_0, \tilde{\lambda}_0)$ applied to an augmented system

$$G(x, \lambda) := \begin{bmatrix} F(x, \lambda) \\ N(x, \lambda) \end{bmatrix}$$

where $N : H \times \mathbb{R} \to \mathbb{R}$ is generally an additional smooth constraint. Various constraint maps have been employed in the numerical continuation literature. For the sake of simplicity, we only consider the (most frequently used) constraint

$$N(x, \lambda) = \left\langle t_1(F'(\bar{x}_0, \bar{\lambda}_0))\, ,\, x - \tilde{x} \right\rangle + t_2(F'(\bar{x}_0, \bar{\lambda}_0)) \cdot (\lambda - \tilde{\lambda}).$$

This constraint restricts the corrector points to the affine space through the predictor point which is orthogonal to the tangent $t(F'(\bar{x}_0, \bar{\lambda}_0))$. This corresponds to a local parametrization with respect to a pseudo arc length.

Numerous important aspects of numerical continuation have been treated in the literature. One of them concerns the incorporation of fast efficient linear solvers into the corrector steps for large structured systems such as those deriving from discretizations of operator equations. The symmetry reduction method for equivariant matrices falls into this category. One of the approaches for incorporating fast linear solvers is the bordering algorithm using the Schur complement. We briefly review this approach below.

Another important topic in numerical continuation concerns the detection of bifurcation points and the switching of branches. This topic can also be considered under the aspect of equivariance, however it will not be handled here.

In the pseudo arc length parametrization, the calculation of the unit tangent vector $t(F'(\bar{x}_0, \bar{\lambda}_0))$ can be performed by solving the equation

$$\partial_1 F(\bar{x}_0, \bar{\lambda}_0) u = -\partial_2 F(\bar{x}_0, \bar{\lambda}_0)$$

for u and setting

$$t(F'(\bar{x}_0, \bar{\lambda}_0)) = \pm \frac{1}{\sqrt{||u||^2 + 1}} \begin{bmatrix} u \\ 1 \end{bmatrix} \; .$$

If F is Γ-equivariant and $\bar{x}_0$ is Γ-invariant, then according to Lemma 24 $\partial_1 F(\bar{x}_0, \bar{\lambda}_0)$ is also Γ-equivariant. Hence a fast symmetry exploiting solver can be used.

In the corrector process of the numerical continuation one has to perform Newton type iterations. For illustration purposes let us consider an inexact Newton method:

$$
\begin{aligned}
&\text{Find } s_k \text{ such that} \quad ||G'(\tilde{x}_k, \tilde{\lambda}_k)\, s_k + G(\tilde{x}_k, \tilde{\lambda}_k)|| \le \eta_k \left\| G(\tilde{x}_k, \tilde{\lambda}_k) \right\| \\
&\text{and set} \quad (\tilde{x}_{k+1}, \tilde{\lambda}_{k+1}) := (\tilde{x}_k, \tilde{\lambda}_k) + s_k \ , \qquad (16)
\end{aligned}
$$

which we assume to converge to a solution $(\bar{x}_1, \bar{\lambda}_1)$.

Again, if F is Γ-equivariant and $\bar{x}_1$ is Γ-invariant, then, according to Theorem 27, $G'(\bar{x}_1, \bar{\lambda}_1)$ is Γ-equivariant, and according to Theorem 22, $G'(\tilde{x}_k, \tilde{\lambda}_k)$ can be replaced by its Γ-equivariant part $G'(\tilde{x}_k, \tilde{\lambda}_k)_\Gamma$ in the iteration (16). In this way, we can exploit the symmetry reduction method for the Newton type iteration (16).

Using the equations (17) and Lemma 26, it is easily seen that

$$
G'(\tilde{x}_k, \tilde{\lambda}_k)_\Gamma = \begin{bmatrix} \Big(\partial_1 F(\tilde{x}_k, \tilde{\lambda}_k)\Big)_\Gamma & \Big(\partial_2 F(\tilde{x}_k, \tilde{\lambda}_k)\Big)_\Gamma \\ \Big\langle \cdot \,,\, t_1(F'(\bar{x}_0, \bar{\lambda}_0)) \Big\rangle & t_2(F'(\bar{x}_0, \bar{\lambda}_0)) \end{bmatrix} .
$$

It is also reasonable to regard $A := G'(\tilde{x}_k, \tilde{\lambda}_k)_\Gamma$ as a bordered linear operator:

$$
A =: \begin{bmatrix} B & b \\ \langle \cdot \,,\, c \rangle & d \end{bmatrix} .
$$

Note that B is Γ-equivariant and b, c are Γ-invariant.

The corrector process can now be facilitated by employing the bordering algorithm involving the Schur complement, see, e.g., [14, 28]:

$$
\sigma := d - \big\langle c \,,\, B^{-1} b \big\rangle .
$$

If A is invertible, then

$$
A^{-1} \begin{bmatrix} u \\ \tau \end{bmatrix} = \frac{1}{\sigma} \begin{bmatrix} \sigma B^{-1} u + \langle c \,,\, B^{-1} u \rangle\, B^{-1} b - \tau B^{-1} b \\ - \langle c \,,\, B^{-1} u \rangle + \tau \end{bmatrix} .
$$

We note that one action of A^{-1} amounts to performing two actions with the linear operator B^{-1} and two inner products. In typical applications, B would not only be equivariant, but also sparse, and hence the action of B^{-1} can be implemented very efficiently. Furthermore, since b is Γ-invariant, the action $B^{-1}b$ is reduced to solving with respect to just one block in (9), namely the one corresponding to the trivial irreducible representation $r(g) = 1$, $g \in \Gamma$.

7. Appendix to: Numerical Continuation and Equivariance

In the following let H be a real Hilbert space. Hence actions of Γ on H are orthogonal transformations. The theorems and proofs in this section are given as a reference and completion for the previous section.

The following is just a restatement of example 20:

Lemma 24. *Let T be an action of Γ on H, and let $F : H \times \mathbb{R} \to H$ be (sufficiently) smooth and Γ-equivariant. Let $\bar{x}$ be Γ-invariant. Then $\partial_1 F(\bar{x}, \bar{\lambda}) \in \mathcal{L}(H)$ is Γ-equivariant.*

Lemma 25. *Let T be an action of Γ on H, and let $F : H \times \mathbb{R} \to H$ be (sufficiently) smooth and Γ-equivariant. Let $\bar{x}$ be Γ-invariant. Then $\partial_2 F(\bar{x}, \bar{\lambda})$ is Γ-invariant.*

Proof. Taylor's formula implies

$$\begin{aligned} & T(g)F(\bar{x}, \bar{\lambda}) + T(g)\partial_2 F(\bar{x}, \bar{\lambda})h + \mathcal{O}(h^2) \\ = {} & T(g)F(\bar{x}, \bar{\lambda} + h) = F(\bar{x}, \bar{\lambda} + h) \\ = {} & F(\bar{x}) + \partial_2 F(\bar{x})h + \mathcal{O}(h^2). \end{aligned}$$

Comparing the coefficients of h finishes the proof. □

Lemma 26. *Let T be an action of Γ on H, and let $F : H \times \mathbb{R} \to H$ be a sufficiently smooth Γ-equivariant Fredholm operator of index one. Let $\bar{x}$ be Γ-invariant. Assume that $(\bar{x}, \bar{\lambda})$ is a regular point of F. Let $(u, s) \in H \times \mathbb{R}$ with $s \neq 0$ be such that*

$$\partial_1 F(\bar{x}, \bar{\lambda})u + \partial_2 F(\bar{x}, \bar{\lambda})s = 0 \quad \textit{and} \quad ||u||^2 + |s|^2 = 1.$$

Then u is Γ-invariant.

Proof. Let $g \in \Gamma$. By Lemmas 24-25 we have

$$\partial_1 F(\bar{x}, \bar{\lambda})T(g)u + \partial_2 F(\bar{x}, \bar{\lambda})s = T(g)\Big(\partial_1 F(\bar{x}, \bar{\lambda})u + \partial_2 F(\bar{x}, \bar{\lambda})s\Big) = 0$$

Since the kernel of $F'(\bar{x}, \bar{\lambda})$ is one-dimensional, and since $||T(g)u|| = ||u||$, this implies $T(g)u = u$. □

The following theorem refers to a corrector iteration while following a solution branch of Γ-invariant points.

Theorem 27. *Let T be an action of Γ on H, and let $F : H \times \mathbb{R} \to H$ be a sufficiently smooth Γ-equivariant Fredholm operator of index one. Define an action $\tilde{T}$ of Γ on $H \times \mathbb{R}$ by setting $\tilde{T}(g)(x, \lambda) = (T(g)x, \lambda)$. Let zero be a regular value of F and $F(\bar{x}_0, \bar{\lambda}_0) = 0$ where $\bar{x}_0$ is Γ-invariant. Let $(u, s) \in H \times \mathbb{R}$ with $s \neq 0$ be such that*

$$\partial_1 F(\bar{x}_0, \bar{\lambda}_0)u + \partial_2 F(\bar{x}_0, \bar{\lambda}_0)s = 0 \quad \textit{and} \quad ||u||^2 + |s|^2 = 1.$$

Consider a predictor point $(\tilde{x}_0, \tilde{\lambda}_0) = (\bar{x}_0 + hu, \bar{\lambda}_0 + hs)$ for some step size $h > 0$. Define an augmented map $G : H \times \mathbb{R} \to H \times \mathbb{R}$ via

$$G(x, \lambda) = \begin{bmatrix} F(x, \lambda) \\ \langle x - \tilde{x}_0 \,,\, u\rangle + (\lambda - \tilde{\lambda}_0)s \end{bmatrix} .$$

Let $G(\bar{x}_1, \bar{\lambda}_1) = 0$, where $\bar{x}_1$ is Γ-invariant. Then the Jacobian $G'(\bar{x}_1, \bar{\lambda}_1)$ is Γ-equivariant.

Proof. Let $g \in \Gamma$. By using Lemmas 24–26, we see that

$$\begin{aligned} \tilde{T}(g)G'(\bar{x}_1, \bar{\lambda}_1)\tilde{T}(g)^* &= \begin{bmatrix} T(g)\partial_1 F(\bar{x}_1, \bar{\lambda}_1)T(g)^* & T(g)\partial_2 F(\bar{x}_1, \bar{\lambda}_1) \\ \langle \cdot \,,\, T(g)u\rangle & s \end{bmatrix} \\ &= \begin{bmatrix} \partial_1 F(\bar{x}_1, \bar{\lambda}_1) & \partial_2 F(\bar{x}_1, \bar{\lambda}_1) \\ \langle \cdot \,,\, u\rangle & s \end{bmatrix} \qquad (17) \\ &= G'(\bar{x}_1, \bar{\lambda}_1) \end{aligned}$$

□

Remark 28. So far, we are considering finite or infinite dimensional Hilbert spaces H. Of course, for a numerical setting of Newton's method, H will usually be finite dimensional after some appropriate discretization step.

Let us point out here that the assumption $s \neq 0$ in Lemma 26 and Theorem 27 is purely technical. It is needed to guarantee that $T(g)u \neq -u$ at the end of the proof of Lemma 26. For finite dimensional H, this assumption can be dropped, since $T(g)u \neq -u$ can be guaranteed by an orientation argument as follows:

$$\begin{aligned} &\begin{bmatrix} T(g) & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \partial_1 F(\bar{x}, \bar{\lambda}) & \partial_2 F(\bar{x}, \bar{\lambda}) \\ u^* & s \end{bmatrix} \begin{bmatrix} T(g)^* & 0 \\ 0 & 1 \end{bmatrix} \\ = &\begin{bmatrix} T(g)\partial_1 F(\bar{x}, \bar{\lambda})T(g)^* & T(g)\partial_2 F(\bar{x}, \bar{\lambda}) \\ (T(g)u)^* & s \end{bmatrix} = \begin{bmatrix} \partial_1 F(\bar{x}, \bar{\lambda}) & \partial_2 F(\bar{x}, \bar{\lambda}) \\ (T(g)u)^* & s \end{bmatrix} \end{aligned}$$

and hence

$$\det \begin{bmatrix} \partial_1 F(\bar{x}, \bar{\lambda}) & \partial_2 F(\bar{x}, \bar{\lambda}) \\ u^* & s \end{bmatrix} = \det \begin{bmatrix} \partial_1 F(\bar{x}, \bar{\lambda}) & \partial_2 F(\bar{x}, \bar{\lambda}) \\ (T(g)u)^* & s \end{bmatrix} .$$

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