SUPPLEMENT TO "MODEL SELECTION IN THE SPACE OF GAUSSIAN MODELS INVARIANT BY SYMMETRY"

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Supplement contains proofs and examples. We provide proofs of Theorems 1, 5, 6 along with a background on representation theory that is needed to understand proofs. Moreover, we present proofs of Proposition 7 and Theorems 8 and 9, an example to Section 2.3, proof of Lemma 13 and the real data example considered in Miller et al. (2005) and Højsgaard and Lauritzen (2008).

In this document, references to equations are sometimes to the main file and sometimes to this supplementary file. For the reader's convenience we put a subindex $(\ )_{mf}$ to equation, section and theorem numbers referring to the main file.

1. Basics of representation theory over reals. Representation theory has long been known to be very useful in statistics, cf. Diaconis (1988). However, the representation theory over $\mathbb{R}$ that we need in our work, is less known to the statisticians than the standard one over $\mathbb{C}$ (see Subsection 2.3 for a contrast between the theories over $\mathbb{R}$ and $\mathbb{C}$). In this section we recall some basic notions and results of the representation theory of groups over the reals. We intend to introduce the reader with all background needed to understand proofs of Theorem 1_{mf} as well as Theorems 5_{mf} and 6_{mf}. For further details, the reader is referred to Serre (1977).

For a real vector space V, we denote by $\mathrm{GL}(V)$ the group of linear automorphisms on V. Let G be a finite group.

DEFINITION 1. A function $\rho\colon G \to \mathrm{GL}(V)$ is called a representation of G over $\mathbb{R}$ if it is a homomorphism, that is

$$\rho(g\,g') = \rho(g)\,\rho(g') \qquad (g, g' \in G).$$

The vector space V is called the representation space of ρ.

If $\dim V = n$, taking a basis $\{v_1, \ldots, v_n\}$ of V, we can identify $\mathrm{GL}(V)$ with the group $\mathrm{GL}(n;\mathbb{R})$ of all $n \times n$ non-singular real matrices. Then a representation $\rho\colon G \to \mathrm{GL}(V)$ corresponds to a group homomorphism $B\colon G \to \mathrm{GL}(n;\mathbb{R})$ for which

$$\rho(g)v_j = \sum_{i=1}^{n} B_{ij}(g)v_i. \tag{1}$$

We call B the matrix expression of ρ with respect to the basis $\{v_1, \ldots, v_n\}$.

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DEFINITION 2. A linear subspace $W \subset V$ is said to be G-invariant if

$$\rho(g)w \in W \qquad (w \in W,\, g \in G).$$

A representation ρ is said to be irreducible if the only G-invariant subspaces are non-proper, that is, whole V and $\{0\}$. A restriction of ρ to a G-invariant subspace W is a subrepresentation. Two representations, $\rho\colon G \to \mathrm{GL}(V)$ and $\rho'\colon G \to \mathrm{GL}(V')$ are equivalent if there exists an isomorphism of vector spaces $\ell\colon V \mapsto V'$ with

$$\ell(\rho(g)v) = \rho'(g)\ell(v) \qquad (v \in V,\, g \in G).$$

We note that a group homomorphism $B\colon G \to \mathrm{GL}(n;\mathbb{R})$ defines a representation of G on $\mathbb{R}^n$ naturally. We see that B is a matrix expression of a representation (ρ, V) if and only if B and ρ are equivalent via the map $\ell\colon \mathbb{R}^n \ni (x_i)_{i=1}^n \mapsto \sum_{i=1}^n x_i v_i \in V$, that is, $\ell(B(g)\underline{x}) = \rho(g)\ell(\underline{x})$ for $\underline{x} \in \mathbb{R}^n$. Here $\{v_1, \dots, v_n\}$ denotes a fixed basis of V. Therefore, two representations (ρ, V) and (ρ', V') are equivalent if and only if they have the same matrix expressions with respect to appropriately chosen bases. We shall write $\rho \sim B$ if ρ has a matrix expression B with respect to some basis.

Let (ρ, V) be a representation of G, and $B\colon G \to \mathrm{GL}(n;\mathbb{R})$ be a matrix expression of ρ with respect to a basis $\{v_1, \dots, v_n\}$ of V. Then it is known that the function $\chi_\rho\colon G \ni g \mapsto \operatorname{Tr} B(g) = \sum_{i=1}^n B_{ii}(g) \in \mathbb{R}$ is independent of the choice of the basis $\{v_1, \dots, v_n\}$. The function χ_ρ is called a character of the representation ρ. The function χ_ρ characterizes the representation ρ in the following sense.

LEMMA 1. *Two representations (ρ, V) and (ρ', V') of a group G are equivalent if and only if $\chi_\rho = \chi_{\rho'}$.*

We apply this lemma in practice to know whether two given representations are equivalent or not.

It is known that, for a finite group G, the set $\Lambda(G)$ of equivalence classes of irreducible representations of G is a finite set. We fix the group homomorphisms $B_\alpha\colon G \to \mathrm{GL}(k_\alpha;\mathbb{R})$, $\alpha \in A$, indexed by a finite set A so that $\Lambda(G) = \{\, [B_\alpha]\,;\, \alpha \in A \,\}$, where $[B_\alpha]$ denotes the equivalence class of B_α.

Let (ρ, V) be a representation of G. Then there exists a G-invariant inner product on V. In fact, from any inner product $\langle \cdot, \cdot \rangle_0$ on V, one can define such an invariant inner product $\langle \cdot, \cdot \rangle$ by $\langle v, v' \rangle := \sum_{g \in G} \langle \rho(g)v, \rho(g)v' \rangle_0$ for $v, v' \in V$. In what follows, we fix a G-invariant inner product on V.

If W is a G-invariant subspace, the orthogonal complement $W^\perp$ is also a G-invariant subspace. Thus, any representation ρ can be decomposed into a finite number of irreducible subrepresentations

$$\rho = \rho_1 \oplus \ldots \oplus \rho_K \tag{2}$$

along the orthogonal decomposition $V = V_1 \oplus \cdots \oplus V_K$, where ρ_i is the restriction of ρ to the G-invariant subspace V_i, $i = 1, \dots, K$. Let r_α be the number of subrepresentations ρ_i such that $\rho_i \sim B_\alpha$. Although the irreducible decomposition (2) of V is not unique in general, r_α is uniquely determined. We have

$$\rho \sim \bigoplus_{r_\alpha > 0} B_\alpha^{\oplus r_\alpha}, \tag{3}$$

where $\sum_{r_\alpha > 0} r_\alpha = K$. To see this, let $V(B_\alpha)$ be the direct sum of subspaces V_i for which $\rho_i \sim B_\alpha$. The space $V(B_\alpha)$ is called the B_α-component of V. If $r_\alpha > 0$, gathering an appropriate basis of each V_i, the matrix expression of the subrepresentation of ρ on $V(B_\alpha)$ becomes (recall that $B_\alpha(g) \in \mathrm{GL}(k_\alpha;\mathbb{R})$)

$$B_\alpha(g)^{\oplus r_\alpha} = \begin{pmatrix} B_\alpha(g) & & & \\ & B_\alpha(g) & & \\ & & \ddots & \\ & & & B_\alpha(g) \end{pmatrix} = I_{r_\alpha} \otimes B_\alpha(g) \in \mathrm{GL}(r_\alpha k_\alpha;\mathbb{R}) \qquad (g \in G).$$

Moreover, V is decomposed as $V = \bigoplus_{r_\alpha > 0} V(B_\alpha)$. Therefore, taking a basis of V by gathering the bases of $V(B_\alpha)$, we obtain (3).

2. The proof of Theorem 1_{mf}. In this section we apply general results on representation theory from previous section to the mapping $\sigma \mapsto R(\sigma)$ defined in $(3)_{mf}$.

Let Γ be a subgroup of the symmetric group $\mathfrak{S}_p$. By definition, we have $R\colon \Gamma \to \mathrm{GL}(p;\mathbb{R})$ and $R(\sigma \circ \sigma') = R(\sigma) \cdot R(\sigma')$ for all $\sigma, \sigma' \in \Gamma$. Thus, R is a representation of Γ over $\mathbb{R}$.

We will show, in this section, that for R, as for all representations of a finite group, through an appropriate change of basis, matrices $R(\sigma)$, $\sigma \in \Gamma$, can be simultaneously written as block diagonal matrices with the number and dimensions of these block matrices being the same for all $\sigma \in \Gamma$. This, in turn, will imply that any matrix in $\mathcal{Z}_\Gamma$ can be written under the form described by Theorem 1_{mf}. For readerâĂŹs convenience we repeat its statement below.

THEOREM 1. *Fix a permutation subgroup $\Gamma \subset \mathfrak{S}_p$. Then, there exist constants $L \in \mathbb{N}$, $(k_i, d_i, r_i)_{i=1}^L$ and orthogonal matrix U_Γ such that if $X \in \mathcal{Z}_\Gamma$, i.e. $X \in \mathrm{Sym}(p;\mathbb{R})$ and*

$$X_{ij} = X_{\sigma(i)\sigma(j)} \qquad (\sigma \in \Gamma,\, i,j \in \{1,\ldots,p\}),$$

then

$$X = U_\Gamma \cdot \begin{pmatrix} M_{\mathbb{K}_1}(x_1) \otimes I_{k_1/d_1} & & & \\ & M_{\mathbb{K}_2}(x_2) \otimes I_{k_2/d_2} & & \\ & & \ddots & \\ & & & M_{\mathbb{K}_L}(x_L) \otimes I_{k_L/d_L} \end{pmatrix} \cdot U_\Gamma^\top, \tag{4}$$

where $M_{\mathbb{K}_i}(x_i)$ is a real matrix representation of an $r_i \times r_i$ Hermitian matrix x_i with entries in $\mathbb{K}_i = \mathbb{R}, \mathbb{C}$ or $\mathbb{H}$, $i = 1, \ldots, L$, and $A \otimes B$ denotes the Kronecker product of matrices A and B.

2.1. *Irreducible decomposition of representation R.* Regarding $\rho(\sigma) = R(\sigma) \in \mathrm{GL}(\mathbb{R}^p)$ as an operator on $V = \mathbb{R}^p$ via the standard basis $v_i = e_i \in \mathbb{R}^p$, $i = 1, \ldots, p$, we see that (1) holds trivially with $B = R$.

We will apply (3) to $G = \Gamma \subset \mathfrak{S}_p$ and $(\rho, V) = (R, \mathbb{R}^p)$. If we let $\{\,\alpha \in A\,;\, r_\alpha > 0\,\} =: \{\alpha_1, \alpha_2, \ldots, \alpha_L\}$ and if we denote by U_Γ an orthogonal matrix whose column vectors form orthonormal bases of $V(B_{\alpha_1}), \ldots, V(B_{\alpha_L})$ successively, then for $\sigma \in \Gamma$, we have

$$U_\Gamma^\top \cdot R(\sigma) \cdot U_\Gamma = \begin{pmatrix} I_{r_1} \otimes B_{\alpha_1}(\sigma) & & & \\ & I_{r_2} \otimes B_{\alpha_2}(\sigma) & & \\ & & \ddots & \\ & & & I_{r_L} \otimes B_{\alpha_L}(\sigma) \end{pmatrix}. \tag{5}$$

Note that, since the left hand side of (5) is an orthogonal matrix, matrices $B_\alpha(\sigma)$, $\alpha \in A$, are orthogonal. In the general case, $B_\alpha(g)$ are orthogonal if we work with a G-invariant inner product. Note that the usual inner product on $V = \mathbb{R}^p$ is clearly Γ-invariant.

Example below gives an illustration of the representation R and also an illustration of all the notions and results we already stated.

EXAMPLE 3. Let $p=4$ and let $\Gamma=\{\mathrm{id},(1,2)(3,4)\}$ be the subgroup of $\mathfrak{S}_4$ generated by $\sigma=(1,2)(3,4)$. The matrix representation of σ in the standard basis $(e_i)_i$ of $\mathbb{R}^4$ is

$$R(\sigma)=\begin{pmatrix}0&1&0&0\\1&0&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix},$$

which has the two eigenvalues 1 and -1 with multiplicity 2 for each. We choose the following orthonormal eigenvectors of $R(\sigma)$:

$$u_1=\frac{1}{\sqrt{2}}(e_1+e_2),u_2=\frac{1}{\sqrt{2}}(e_3+e_4),u_3=\frac{1}{\sqrt{2}}(e_1-e_2),u_4=\frac{1}{\sqrt{2}}(e_3-e_4)$$

and let $U_\Gamma=(u_1,u_2,u_3,u_4)$. The corresponding eigenspaces $V_i=\mathbb{R}u_i$ are invariant under $R(\sigma)$ and $R(\mathrm{id})=I_4$. As V_i, $i=1,\dots,4$, are 1-dimensional, the subrepresentations defined by

$$\rho_i(\gamma)=R(\gamma)|_{V_i}\qquad(\gamma\in\Gamma)$$

are irreducible. We have the decomposition (2) of R:

$$R=\rho_1\oplus\rho_2\oplus\rho_3\oplus\rho_4.$$

The matrix expressions of ρ_1 and ρ_2 are equal to $B_1(\gamma)=(1)$ for all $\gamma\in\Gamma$, since $\rho_i(\gamma)v=v$ for $v\in V_i$, $i=1,2$. We have $r_1=2$.

The matrix expressions of ρ_3 and ρ_4 are both equal to $B_2(\gamma)=\mathrm{sign}(\gamma)$ for all $\gamma\in\Gamma$, since $\rho_i(\mathrm{id})v=v$ and $\rho_i(\sigma)v=-v$ for $v\in V_i$ for $i=3,4$. We have $r_2=2$.

The representations ρ_1 and ρ_3 are not equivalent, which can be seen by looking at the characters: $\chi_{\rho_1}=1$, $\chi_{\rho_3}(\gamma)=\mathrm{sign}(\gamma)$, which are not equal.

In the basis u_1,u_2,u_3,u_4, the matrix of $R(\gamma)$ is (compare with (5))

$$\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&\mathrm{sign}(\gamma)&0\\0&0&0&\mathrm{sign}(\gamma)\end{pmatrix}=B_1(\gamma)^{\oplus 2}\oplus B_2(\gamma)^{\oplus 2}=U_\Gamma^\top\cdot R(\gamma)\cdot U_\Gamma.$$

This is the decomposition (3) of R in the basis (u_1,u_2,u_3,u_4).

2.2. *Block diagonal decomposition of* $\mathcal{Z}_\Gamma$. So far, we have shown that through an appropriate change of basis, the representation $(R,\mathbb{R}^p)$ of Γ can be expressed as the direct sum (3) of irreducible subrepresentations. We now want to turn our attention to the elements of $\mathcal{Z}_\Gamma$.

A linear operator $T\colon V\to V$ is said to be an intertwining operator of the representation (ρ,V) if $T\circ\rho(g)=\rho(g)\circ T$ holds for all $g\in G$. In our context, since $(4)_{mf}$ can be rewritten as

(6) $$\mathcal{Z}_\Gamma=\{\,x\in\mathrm{Sym}(p;\mathbb{R})\,;\,x\cdot R(\sigma)=R(\sigma)\cdot x\text{ for all }\sigma\in\Gamma\,\},$$

$\mathcal{Z}_\Gamma$ is the set of symmetric intertwining operators of the representation $(R,\mathbb{R}^p)$.

Let $\mathrm{End}_\Gamma(\mathbb{R}^p)$ denote the set of all intertwining operators of the representation $(R,\mathbb{R}^p)$ of Γ. Recall that the set A enumerates the elements of $\Lambda(\Gamma)$, the finite set of all equivalence classes of irreducible representations of Γ. From (3) and (5), it is clear that to study $\mathrm{End}_\Gamma(\mathbb{R}^p)$, it is sufficient to study the sets,

$$\mathrm{End}_\Gamma(V_\alpha)=\{\,T\in\mathrm{Mat}(k_\alpha,k_\alpha;\mathbb{R})\,;\,T\cdot B_\alpha(\sigma)=B_\alpha(\sigma)\cdot T\text{ for all }\sigma\in\Gamma\,\},$$

$\alpha \in A$, of all intertwining operators of the irreducible representation B_α, where $V_\alpha := \mathbb{R}^{k_\alpha}$ is the representation space of B_α equipped with a Γ-invariant inner product. Indeed, we have $V(B_\alpha) = I_{r_\alpha} \otimes V_\alpha$.

The actual formula for $B_\alpha(\sigma)$ obviously depends on the choice of U_Γ and hence, on the choice of orthonormal basis of $\mathbb{R}^p$. To ensure simplicity of formulation of our next result (Lemma 2), we will work with special orthonormal bases of $V(B_{\alpha_1}), \dots, V(B_{\alpha_L})$, which together constitute a basis of $\mathbb{R}^p$. Such bases always exist and will be defined in the next section. Usage of these bases is not indispensable for the proof of Theorem 1, but simplifies it greatly.

The result from (Serre, 1977, Page 108) implies that, since the representation B_α is irreducible, the space $\mathrm{End}_\Gamma(V_\alpha)$ is isomorphic either to $\mathbb{R}$, $\mathbb{C}$, or the quaternion algebra $\mathbb{H}$. Let

$$f_\alpha \colon \mathbb{K}_\alpha \to \mathrm{End}_\Gamma(V_\alpha),$$

denote this isomorphism, where $\mathbb{K}_\alpha$ is $\mathbb{R}$, $\mathbb{C}$, or $\mathbb{H}$. Let

$$d_\alpha := \dim_{\mathbb{R}} \mathrm{End}_\Gamma(V_\alpha) = \dim_{\mathbb{R}} \mathbb{K}_\alpha \in \{1, 2, 4\}.$$

The representation space V_α becomes a vector space over $\mathbb{K}_\alpha$ of dimension k_α/d_α via

$$q \cdot v := f_\alpha(q)v \qquad (q \in \mathbb{K}_\alpha,\, v \in V_\alpha).$$

Clearly the space $\mathbb{R}I_{k_\alpha}$ of scalar matrices is contained in $\mathrm{End}_\Gamma(V_\alpha)$. If $d_\alpha = 1 = \dim_{\mathbb{R}} \mathbb{R}I_{k_\alpha}$, we have $\mathrm{End}_\Gamma(V_\alpha) = \mathbb{R}I_{k_\alpha}$. Further, if $d_\alpha = 2$, take a $\mathbb{C}$-basis $\{v_1, \dots, v_{k_\alpha/2}\}$ of V_α in such a way that $\{v_1, \dots, v_{k_\alpha/2}, i \cdot v_1, \dots, i \cdot v_{k_\alpha/2}\}$ is an orthonormal $\mathbb{R}$-basis of V_α. We identify $\mathbb{R}^{k_\alpha}$ and V_α via this $\mathbb{R}$-basis. Then, the action of $q = a + bi \in \mathbb{C}$ on $w \in \mathbb{R}^{k_\alpha} \simeq V_\alpha$ is expressed as

$$q \cdot w = \begin{pmatrix} aI_{k_\alpha/2} & -bI_{k_\alpha/2} \\ bI_{k_\alpha/2} & aI_{k_\alpha/2} \end{pmatrix} w = \left\{ M_{\mathbb{C}}(a + bi) \otimes I_{k_\alpha/2} \right\} w.$$

Thus, if $d_\alpha = 2$, then

$$\mathrm{End}_\Gamma(V_\alpha) = \left\{ M_{\mathbb{C}}(q) \otimes I_{k_\alpha/2} \,;\, q \in \mathbb{C} \right\} = M_{\mathbb{C}}(\mathbb{C}) \otimes I_{k_\alpha/2}.$$

Similarly, when $\mathbb{K}_\alpha = \mathbb{H}$, take an $\mathbb{H}$-basis $\{v_1, \dots, v_{k_\alpha/4}\}$ of V_α so that

$$\{v_1, \dots, v_{k_\alpha/4}, i \cdot v_1, \dots, i \cdot v_{k_\alpha/4}, j \cdot v_1, \dots, j \cdot v_{k_\alpha/4}, k \cdot v_1, \dots, k \cdot v_{k_\alpha/4}\}$$

is an orthonormal $\mathbb{R}$-basis of V_α. The action of $Q \in \mathbb{H}$ on V_α is expressed as $M_{\mathbb{H}}(Q) \otimes I_{k_\alpha/4}$ with respect to this basis.

In this way we have proved the following result.

LEMMA 2. *For each $\alpha \in A$, one has*

$$\mathrm{End}_\Gamma(V_\alpha) = M_{\mathbb{K}_\alpha}(\mathbb{K}_\alpha) \otimes I_{k_\alpha/d_\alpha}. \tag{7}$$

For the proof of Theorem 1, we will need the following result.

LEMMA 3. *Let $i, j = 1, 2, \dots, L$, and assume that $Y \in \mathrm{Mat}(r_i k_i,\, r_j k_j; \mathbb{R})$ satisfies the condition*

$$[I_{r_i} \otimes B_i(\sigma)] \cdot Y = Y \cdot [I_{r_j} \otimes B_j(\sigma)] \qquad (\sigma \in \Gamma). \tag{8}$$

If $i = j$, then there exists $C \in \mathrm{Mat}(r_i, r_i; \mathbb{K}_i)$ such that $Y = M_{\mathbb{K}_i}(C) \otimes I_{k_i/d_i}$. On the other hand, if $i \neq j$, then $Y = 0$.

PROOF. Let us consider a block decomposition of Y as

$$Y=\begin{pmatrix} Y_{11} & Y_{12} & \dots & Y_{1,r_j} \\ Y_{21} & Y_{22} & \dots & Y_{2,r_j} \\ \vdots & \vdots & \ddots & \vdots \\ Y_{r_i,1} & Y_{r_i,2} & \dots & Y_{r_i,r_j} \end{pmatrix},$$

where each Y_{ab} is a $k_i \times k_j$ matrix. Then (8) implies that

$$B_i(\sigma)\cdot Y_{ab} = Y_{ab}\cdot B_j(\sigma) \qquad (\sigma\in\Gamma) \tag{9}$$

for all a,b. If $i=j$, then $Y_{ab}\in \mathrm{End}_\Gamma(\mathbb{R}^{k_i})$, so that there exists $C_{ab}\in\mathbb{K}_i$ for which $Y_{ab}=M_{\mathbb{K}_i}(C_{ab})\otimes I_{k_i/d_i}$ thanks to Lemma 2. Let us consider the case $i\neq j$. Eq. (9) tells us that $\mathrm{Ker}\, Y_{ab}\subset\mathbb{R}^{k_j}$ is a Γ-invariant subspace, which then equals $\{0\}$ or $\mathbb{R}^{k_j}$ because of the irreducibility of B_j. Similarly, since $\mathrm{Image}\, Y_{ab}\subset\mathbb{R}^{k_i}$ is a Γ-invariant subspace by (9), $\mathrm{Image}\, Y_{ab}$ equals $\{0\}$ or $\mathbb{R}^{k_i}$. Now suppose that $Y_{ab}\neq 0$. Then $\mathrm{Ker}\, Y_{ab}=\{0\}$ and $\mathrm{Image}\, Y_{ab}=\mathbb{R}^{k_i}$ by the argument above, and it means that Y_{ab} induces an isomorphism from $(B_j,\mathbb{R}^{k_j})$ onto $(B_i,\mathbb{R}^{k_i})$. But this contradicts the fact that the representations B_i and B_j are not equivalent for $i\neq j$. Hence we get $Y_{ab}=0$. □

PROOF OF THEOREM 1. Take $y\in U_\Gamma^\top\cdot\mathcal{Z}_\Gamma\cdot U_\Gamma$ and consider the block decomposition of y as

$$y=\begin{pmatrix} Y_{11} & Y_{12} & \dots & Y_{1L} \\ Y_{21} & Y_{22} & \dots & Y_{2L} \\ \vdots & \vdots & \ddots & \vdots \\ Y_{L1} & Y_{L2} & \cdots & Y_{LL} \end{pmatrix}$$

with $Y_{ij}\in\mathrm{Mat}(r_ik_i,\, r_jk_j;\mathbb{R})$. Then $x:=U_\Gamma\cdot y\cdot U_\Gamma^\top$ belongs to $\mathcal{Z}_\Gamma$, so that (6) implies

$$R(\sigma)\cdot U_\Gamma\cdot y\cdot U_\Gamma^\top\cdot R(\sigma)^\top = U_\Gamma\cdot y\cdot U_\Gamma^\top$$

for $\sigma\in\Gamma$, and this equality is rewritten as

$$[U_\Gamma^\top\cdot R(\sigma)\cdot U_\Gamma]\cdot y = y\cdot[U_\Gamma^\top\cdot R(\sigma)\cdot U_\Gamma].$$

By (5), we have

$$[I_{r_i}\otimes B_i(\sigma)]\cdot Y_{ij} = Y_{ij}\cdot[I_{r_j}\otimes B_j(\sigma)].$$

Lemma 3 tells us that $Y_{ij}=0$ if $i\neq j$, and that $Y_{ii}=M_{\mathbb{K}_i}(x_i)\otimes I_{k_i/d_i}$ with some $x_i\in\mathrm{Mat}(r_i,\, r_i;\mathbb{K}_i)$. Since y is a symmetric matrix, the block Y_{ii} is also symmetric, which implies that $x_i\in\mathrm{Herm}(r_i;\mathbb{K}_i)$. Actually, the map $\iota\colon\ \bigoplus_{i=1}^L \mathrm{Herm}(r_i;\mathbb{K}_i)\ni(x_i)_{i=1}^L\mapsto X\in\mathcal{Z}_\Gamma$ given by (4) gives a Jordan algebra isomorphism. □

2.3. *A comparison to the representation theory over the complex number field.* Theorem 1 has a much simpler counterpart in the representation theory over $\mathbb{C}$, which we state in a spirit of Shah and Chandrasekaran (2012) and Shah and Chandrasekaran (2013). Let Γ be a subgroup of $\mathfrak{S}_p$. We regard the natural representation R of Γ as a complex representation $R\colon\Gamma\to\mathrm{GL}(p;\mathbb{C})$. Assume that R is decomposed as $R\sim\bigoplus_{k=1}^K\vartheta_k^{\oplus s_k}$, where $\vartheta_k\colon\Gamma\to\mathrm{GL}(m_k;\mathbb{C})$, $k=1,\dots,K$, are mutually inequivalent irreducible complex representations. Let $W_\Gamma^{\mathbb{C}}$ be the vector space consisting of $A\in\mathrm{Mat}(p,p;\mathbb{C})$ such that $A\cdot R(\sigma)=R(\sigma)\cdot A$

for all $\sigma \in \Gamma$. Then there exists a unitary $p \times p$ matrix T_Γ for which all the matrices $A \in W_\Gamma^{\mathbb{C}}$ are simultaneously diagonalized as

$$T_\Gamma^* \cdot A \cdot T_\Gamma = \begin{pmatrix} a_1 \otimes I_{m_1} & & & \\ & a_2 \otimes I_{m_2} & & \\ & & \ddots & \\ & & & a_K \otimes I_{m_K} \end{pmatrix}, \quad \begin{array}{l} a_k \in \mathrm{Mat}(s_k, \mathbb{C}), \\ k = 1, \dots, K. \end{array} \tag{10}$$

Precisely, the diagonal blocks in the right-hand side are of the form $I_{m_k} \otimes a_k$ in Shah and Chandrasekaran (2013), but the difference can be made up by an appropriate permutation of the columns of T_Γ. Clearly the constants $(m_k, s_k)_k$ correspond to our structure constants $(k_i, r_i)_i$, while we can consider that a complex counterpart for d_i takes always the value 1. Since T_Γ is a unitary matrix, we see that if A is Hermitian, then the corresponding matrices a_k, $k = 1, \dots, K$, are also Hermitian. This fact together with (10) is efficiently utilized in a study of complex covariance matrices with group symmetry in Soloveychik, Trushin and Wiesel (2016). On the other hand, even though $A \in W_\Gamma^{\mathbb{C}}$ is a real matrix, the matrices a_k are not necessarily real, as Shah and Chandrasekaran (2012) seem to misunderstand implicitly. For instance, let us consider the case where $p = 3$ and $\Gamma \subset \mathfrak{S}_3$ is a cyclic group generated by $(1\,2\,3)$. Then $A \in W_\Gamma^{\mathbb{C}}$ is of the form $\begin{pmatrix} a & b & c \\ c & a & b \\ b & c & a \end{pmatrix}$ with $a, b, c \in \mathbb{C}$. Taking $T_\Gamma := \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 1 & 1 \\ 1 & \omega & \overline{\omega} \\ 1 & \overline{\omega} & \omega \end{pmatrix}$ with $\omega := e^{2\pi i/3}$, we have

$$T_\Gamma^* \begin{pmatrix} a & b & c \\ c & a & b \\ b & c & a \end{pmatrix} T_\Gamma = \begin{pmatrix} a_1 & & \\ & a_2 & \\ & & a_3 \end{pmatrix},$$

where $a_1 := a + b + c$, $a_2 := a + b\omega + c\overline{\omega}$, and $a_3 := a + b\overline{\omega} + c\omega$. In this case $m_k = s_k = 1$ for $k = 1, 2, 3$ (confer (Shah and Chandrasekaran, 2012, Remark 3.1)). Even if a, b, c are real, the right-hand side above is not necessarily real but of the form $\mathrm{diag}(a_1, a_2, \overline{a_2})$ with $a_1 \in \mathbb{R}$ and $a_2 \in \mathbb{C}$. Furthermore, if the matrix A is symmetric, that is, real and Hermitian, then right-hand side becomes $\mathrm{diag}(a_1, a_2, a_2)$ with $a_1, a_2 \in \mathbb{R}$ as is seen from Theorem 1 with $(k_1, k_2) = (1, 2)$, $(r_1, r_2) = (1, 1)$ and $(d_1, d_2) = (1, 2)$. This observation tells us that the constants $(m_k, s_k)_k$ from complex representation theory are not sufficient for the description of the simultaneous diagonalization of real symmetric matrices with group symmetry.

3. Additions to Section 2_{mf}.

3.1. *Example to Section 2.3_{mf}.*

EXAMPLE 4. In this example we present a colored space $\mathcal{Z}_\Gamma \subset \mathrm{Sym}(16; \mathbb{R})$, which has a component $\mathrm{Herm}(2; \mathbb{H})$. Let $\Gamma = \langle \sigma_1, \sigma_2 \rangle$ be the subgroup of $\mathfrak{S}_{16}$ generated by the two permutations

$$\sigma_1 = (1, 2, 5, 6)(3, 4, 7, 8)(9, 10, 13, 14)(11, 12, 15, 16),$$
$$\sigma_2 = (1, 3, 5, 7)(2, 8, 6, 4)(9, 11, 13, 15)(10, 16, 14, 12).$$

The space $\mathcal{Z}_\Gamma$ consists of matrices of the form

$$X = \begin{pmatrix}
\alpha_1 & \alpha_2 & \alpha_3 & \alpha_4 & \alpha_5 & \alpha_2 & \alpha_3 & \alpha_4 & \gamma_1 & \gamma_2 & \gamma_3 & \gamma_4 & \gamma_5 & \gamma_6 & \gamma_7 & \gamma_8 \\
\alpha_2 & \alpha_1 & \alpha_4 & \alpha_3 & \alpha_2 & \alpha_5 & \alpha_4 & \alpha_3 & \gamma_6 & \gamma_1 & \gamma_8 & \gamma_3 & \gamma_2 & \gamma_5 & \gamma_4 & \gamma_7 \\
\alpha_3 & \alpha_4 & \alpha_1 & \alpha_2 & \alpha_3 & \alpha_4 & \alpha_5 & \alpha_2 & \gamma_7 & \gamma_4 & \gamma_1 & \gamma_6 & \gamma_3 & \gamma_8 & \gamma_5 & \gamma_2 \\
\alpha_4 & \alpha_3 & \alpha_2 & \alpha_1 & \alpha_4 & \alpha_3 & \alpha_2 & \alpha_5 & \gamma_8 & \gamma_7 & \gamma_2 & \gamma_1 & \gamma_4 & \gamma_3 & \gamma_6 & \gamma_5 \\
\alpha_5 & \alpha_2 & \alpha_3 & \alpha_4 & \alpha_1 & \alpha_2 & \alpha_3 & \alpha_4 & \gamma_5 & \gamma_6 & \gamma_7 & \gamma_8 & \gamma_1 & \gamma_2 & \gamma_3 & \gamma_4 \\
\alpha_2 & \alpha_5 & \alpha_4 & \alpha_3 & \alpha_2 & \alpha_1 & \alpha_4 & \alpha_3 & \gamma_2 & \gamma_5 & \gamma_4 & \gamma_7 & \gamma_6 & \gamma_1 & \gamma_8 & \gamma_3 \\
\alpha_3 & \alpha_4 & \alpha_5 & \alpha_2 & \alpha_3 & \alpha_4 & \alpha_1 & \alpha_2 & \gamma_3 & \gamma_8 & \gamma_5 & \gamma_2 & \gamma_7 & \gamma_4 & \gamma_1 & \gamma_6 \\
\alpha_4 & \alpha_3 & \alpha_2 & \alpha_5 & \alpha_4 & \alpha_3 & \alpha_2 & \alpha_1 & \gamma_4 & \gamma_3 & \gamma_6 & \gamma_5 & \gamma_8 & \gamma_7 & \gamma_2 & \gamma_1 \\
\gamma_1 & \gamma_6 & \gamma_7 & \gamma_8 & \gamma_5 & \gamma_2 & \gamma_3 & \gamma_4 & \beta_1 & \beta_2 & \beta_3 & \beta_4 & \beta_5 & \beta_2 & \beta_3 & \beta_4 \\
\gamma_2 & \gamma_1 & \gamma_4 & \gamma_7 & \gamma_6 & \gamma_5 & \gamma_8 & \gamma_3 & \beta_2 & \beta_1 & \beta_4 & \beta_3 & \beta_2 & \beta_5 & \beta_4 & \beta_3 \\
\gamma_3 & \gamma_8 & \gamma_1 & \gamma_2 & \gamma_7 & \gamma_4 & \gamma_5 & \gamma_6 & \beta_3 & \beta_4 & \beta_1 & \beta_2 & \beta_3 & \beta_4 & \beta_5 & \beta_2 \\
\gamma_4 & \gamma_3 & \gamma_6 & \gamma_1 & \gamma_8 & \gamma_7 & \gamma_2 & \gamma_5 & \beta_4 & \beta_3 & \beta_2 & \beta_1 & \beta_4 & \beta_3 & \beta_2 & \beta_5 \\
\gamma_5 & \gamma_2 & \gamma_3 & \gamma_4 & \gamma_1 & \gamma_6 & \gamma_7 & \gamma_8 & \beta_5 & \beta_2 & \beta_3 & \beta_4 & \beta_1 & \beta_2 & \beta_3 & \beta_4 \\
\gamma_6 & \gamma_5 & \gamma_8 & \gamma_3 & \gamma_2 & \gamma_1 & \gamma_4 & \gamma_7 & \beta_2 & \beta_5 & \beta_4 & \beta_3 & \beta_2 & \beta_1 & \beta_4 & \beta_3 \\
\gamma_7 & \gamma_4 & \gamma_5 & \gamma_6 & \gamma_3 & \gamma_8 & \gamma_1 & \gamma_2 & \beta_3 & \beta_4 & \beta_5 & \beta_2 & \beta_3 & \beta_4 & \beta_1 & \beta_2 \\
\gamma_8 & \gamma_7 & \gamma_2 & \gamma_5 & \gamma_4 & \gamma_3 & \gamma_6 & \gamma_1 & \beta_4 & \beta_3 & \beta_2 & \beta_5 & \beta_4 & \beta_3 & \beta_2 & \beta_1
\end{pmatrix}.$$

The irreducible factorization of the determinant is given by

$$\begin{aligned}
\mathrm{Det}\,(X) = \Big((\gamma_1-\gamma_5)^2 + (\gamma_2-\gamma_6)^2 + (\gamma_3-\gamma_7)^2 + (\gamma_4-\gamma_8)^2 - (\alpha_1-\alpha_5)(\beta_1-\beta_5)\Big)^4 \\
\cdot \Big((\alpha_1 - 2(\alpha_2+\alpha_3-\alpha_4)+\alpha_5)(\beta_1 - 2(\beta_2+\beta_3-\beta_4)+\beta_5) - (\gamma_1-\gamma_2-\gamma_3+\gamma_4+\gamma_5-\gamma_6-\gamma_7+\gamma_8)^2\Big) \\
\cdot \Big((\alpha_1 - 2(\alpha_2-\alpha_3+\alpha_4)+\alpha_5)(\beta_1 - 2(\beta_2-\beta_3+\beta_4)+\beta_5) - (\gamma_1-\gamma_2+\gamma_3-\gamma_4+\gamma_5-\gamma_6+\gamma_7-\gamma_8)^2\Big) \\
\cdot \Big((\alpha_1 + 2(\alpha_2-\alpha_3-\alpha_4)+\alpha_5)(\beta_1 + 2(\beta_2-\beta_3-\beta_4)+\beta_5) - (\gamma_1+\gamma_2-\gamma_3-\gamma_4+\gamma_5+\gamma_6-\gamma_7-\gamma_8)^2\Big) \\
\cdot \Big((\alpha_1 + 2(\alpha_2+\alpha_3+\alpha_4)+\alpha_5)(\beta_1 + 2(\beta_2+\beta_3+\beta_4)+\beta_5) - (\gamma_1+\gamma_2+\gamma_3+\gamma_4+\gamma_5+\gamma_6+\gamma_7+\gamma_8)^2\Big).
\end{aligned}$$

Thus, Lemma 4_{mf} gives us that $L = 5$ and

$$r = (2,2,2,2,2), \quad k = (4,1,1,1,1), \quad d = (4,1,1,1,1).$$

This in turn implies

$$\mathcal{Z}_\Gamma \simeq \mathrm{Herm}(2;\mathbb{H}) \oplus \mathrm{Sym}(2;\mathbb{R})^{\oplus 4}.$$

As a matter of fact, the group Γ has four 1-dimensional representations and one 4-dimensional real irreducible representation, and each representation appears twice in $\mathbb{R}^{16}$.

3.2. *Proofs of Theorem 5_{mf} and Theorem 6_{mf}.*

PROOF OF THEOREM 5_{mf} AND THEOREM 6_{mf}. Let $M := \lfloor \frac{N}{2} \rfloor$ and denote the irreducible representations of Γ by

$$\begin{aligned}
B_0 &\colon \Gamma \ni \sigma^k \mapsto 1 \in \mathrm{GL}(1;\mathbb{R}), \\
B_\alpha &\colon \Gamma \ni \sigma^k \mapsto \mathrm{Rot}\left(\frac{2\pi\alpha k}{N}\right) \in \mathrm{GL}(2;\mathbb{R}) \quad (1 \le \alpha < N/2), \\
B_{N/2} &\colon \Gamma \ni \sigma^k \mapsto (-1)^k \in \mathrm{GL}(1;\mathbb{R}) \quad (\text{if } N \text{ is even}),
\end{aligned}$$

where $\mathrm{Rot}(\theta)$ denotes the rotation matrix $\begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$ for $\theta \in \mathbb{R}$. Then all the equivalence classes of the irreducible representations of Γ are $[B_0], [B_1], \ldots, [B_M]$ whether $N = 2M$ or $N = 2M+1$. We have $k_\alpha = d_\alpha = \begin{cases} 1 & (\alpha = 0 \text{ or } N/2), \\ 2 & (\text{otherwise}). \end{cases}$

Recall that $\{i_1, \dots, i_C\}$ is a complete system of representatives of the Γ-orbits, and, for each $c = 1, \dots, C$, p_c is the cardinality of the Γ-orbit through i_c. Let $\zeta_c := \exp(2\pi\sqrt{-1}/p_c)$. When $1 \le \beta < p_c/2$, we have

$$v_{2\beta}^{(c)} + \sqrt{-1}v_{2\beta+1}^{(c)} = \sqrt{\frac{2}{p_c}} \sum_{k=0}^{p_c-1} \zeta_c^{\beta k} e_{\sigma^k(i_c)}.$$

Thus

$$\begin{aligned} R(\sigma)(v_{2\beta}^{(c)} + \sqrt{-1}v_{2\beta+1}^{(c)}) &= \sqrt{\frac{2}{p_c}} \sum_{k=0}^{p_c-1} \zeta_c^{\beta k} e_{\sigma^{k+1}(i_c)} = \sqrt{\frac{2}{p_c}} \sum_{k=0}^{p_c-1} \zeta_c^{\beta(k-1)} e_{\sigma^k(i_c)} \\ &= \zeta_c^{-\beta}(v_{2\beta}^{(c)} + \sqrt{-1}v_{2\beta+1}^{(c)}) \\ &= \left\{\cos\left(\frac{2\pi\beta}{p_c}\right)v_{2\beta}^{(c)} + \sin\left(\frac{2\pi\beta}{p_c}\right)v_{2\beta+1}^{(c)}\right\} + \sqrt{-1}\left\{-\sin\left(\frac{2\pi\beta}{p_c}\right)v_{2\beta}^{(c)} + \cos\left(\frac{2\pi\beta}{p_c}\right)v_{2\beta+1}^{(c)}\right\}, \end{aligned}$$

where we have used $\sigma^{p_c}(i_c) = i_c$ and $\zeta_c^{p_c} = 1$ at the second equality. It follows that

$$R(\sigma)\left(v_{2\beta}^{(c)}\ v_{2\beta+1}^{(c)}\right) = \left(v_{2\beta}^{(c)}\ v_{2\beta+1}^{(c)}\right) \mathrm{Rot}\left(\frac{2\pi\beta}{p_c}\right) = \left(v_{2\beta}^{(c)}\ v_{2\beta+1}^{(c)}\right) B_\alpha(\sigma) \tag{11}$$

with $\beta/p_c = \alpha/N$. Similarly, we have

$$\begin{aligned} &R(\sigma)v_1^{(c)} = v_1^{(c)} = B_0(\sigma)v_1^{(c)}, \\ &R(\sigma)v_{p_c}^{(c)} = -v_{p_c}^{(c)} = B_{N/2}(\sigma)v_{p_c}^{(c)} \quad \text{(if } p_c \text{ and } N \text{ are even)}. \end{aligned}$$

Therefore, for $\alpha = 0, \dots, \lfloor N/2 \rfloor$, the multiplicity r_α of the representation B_α of Γ in $(R, \mathbb{R}^p)$ is equal to the number of c such that $\beta/p_c = \alpha/N$ with some $\beta \in \mathbb{N}$. In other words,

$$r_\alpha = \#\{\, c\,;\ \alpha p_c \text{ is a multiple of } N \,\} \quad (0 \le \alpha \le \lfloor N/2 \rfloor). \tag{12}$$

Then we have

$$\mathscr{Z}_\Gamma \simeq \bigoplus_{r_\alpha > 0} \mathrm{Herm}(r_\alpha; \mathbb{K}_\alpha).$$

□

3.3. *Finding structure constants when* Γ *is not cyclic.* In Section 2.3$_{mf}$, we gave a general algorithm for determining the structure constants as well as the invariant measure φ_Γ. In principle, the factorization of a determinant can be done e.g. in PYTHON, however there are some limitations regarding the dimension of a matrix. If the $p \times p$ matrix is not sparse, then the number of terms in the usual Laplace expansion of a determinant produces a polynomial with $p!$ terms. The RAM memory requirements for calculating such a polynomial would be in excess of $p!$, which cannot be handled on a standard PC even for moderate p. Depending on the subgroup and the method of calculating the determinant, we were able to obtain the determinant for models of dimensions up to 10-20. In order to factorize the determinant for moderate to high dimensions, we want to find an orthogonal matrix U such that $U^\top \cdot X \cdot U$ is sparse enough for a computer to calculate its determinant $\mathrm{Det}\left(U^\top \cdot X \cdot U\right) = \mathrm{Det}\,(X)$. The matrix U_Γ from (4) is in general very hard to obtain, but we propose an easy surrogate.

PROPOSITION 2. *Assume that* Γ *be a subgroup of* $\mathfrak{S}_p$. *Take* $\sigma_0 \in \mathfrak{S}_p$ *for which the cyclic group* $\Gamma_0 := \langle \sigma_0 \rangle$ *generated by* σ_0 *has the same orbits in* V *as* Γ. *Then, for any* $X \in \mathcal{Z}_\Gamma$ *one has*

$$U_{\Gamma_0}^\top \cdot X \cdot U_{\Gamma_0} = \begin{pmatrix} x_1 & 0 \\ 0 & y \end{pmatrix} \tag{13}$$

with $x_1 \in \mathrm{Sym}(C;\mathbb{R})$ *and* $y \in \mathrm{Sym}(p-C;\mathbb{R})$, *where* C *is the number of cycles of* σ_0. *Matrix* U_{Γ_0} *is the orthogonal matrix constructed in Theorem* 6_{mf} *for the cyclic subgroup* Γ_0.

PROOF. We observe that a vector $v \in \mathbb{R}^p$ is Γ-invariant (i.e. $R(\sigma)v = v$ for all $\sigma \in \Gamma$) if and only if $R(\sigma_0)v = v$ if and only if v is constant on Γ-orbits (i.e. $v_i = v_j$ if i and j belong to the same orbit of Γ). The first C column vectors of U_{Γ_0} are $v_1^{(1)}, v_1^{(2)}, \ldots, v_1^{(C)}$, which are Γ-invariant. The space $V_1 := \mathrm{span}\left\{ v_1^{(c)}\,;\, c = 1, \ldots, C \right\} \subset \mathbb{R}^p$ is the trivial-representation-component of Γ as explained after (3). Therefore, if α_1 is the trivial representation of Γ, then $r_1 = C$ and $d_1 = k_1 = 1$.

The orthogonal complement $V_1^\perp$ of V_1 is spanned by the rest of $v_\beta^{(c)}$, $1 \le c \le C$, $1 < \beta \le 2\lfloor p_c/2 \rfloor$. For $X \in \mathcal{Z}_\Gamma$, we see that $X \cdot v \in V_1$ for $v \in V_1$ and that $X \cdot w \in V_1^\perp$ for $w \in V_1^\perp$. In this way we obtain (13). □

We note that in general, there are no inclusion relations between groups Γ and Γ_0. Moreover, the correspondence $\phi_1 \colon \mathcal{Z}_\Gamma \ni X \mapsto x_1 \in \mathrm{Sym}(C;\mathbb{R})$ is exactly the Jordan algebra homomorphism defined before Corollary 3_{mf}. By Proposition 2 we obtain

$$\mathrm{Det}\,(X) = \mathrm{Det}\,(x_1)\,\mathrm{Det}\,(y)\,, \tag{14}$$

while the factor $\mathrm{Det}\,(x_1) = \det(\phi_1(X))$ is an irreducible polynomial of degree $r_1 = C$. In this way, for any subgroup Γ, we are able to factor out the polynomial of degree equal to the number of Γ-orbits in V easily. On the other hand, the factorization of $\mathrm{Det}\,(y)$ requires study of the subrepresentation R of Γ on $V_1^\perp$, where the group Γ_0 is useless in general.

EXAMPLE 5. Let $\Gamma = \langle (1,2,3),\, (4,5,6) \rangle \subset \mathfrak{S}_6$, which is not a cyclic group. The space $\mathcal{Z}_\Gamma$ consists of symmetric matrices of the form

$$X = \begin{pmatrix} a & b & b & e & e & e \\ b & a & b & e & e & e \\ b & b & a & e & e & e \\ e & e & e & c & d & d \\ e & e & e & d & c & d \\ e & e & e & d & d & c \end{pmatrix}$$

and moreover, $\mathcal{Z}_\Gamma$ does not coincide with $\mathcal{Z}_{\langle\sigma\rangle}$ for any $\sigma \in \mathfrak{S}_6$. Noting that the group Γ has two orbits: $\{1,2,3\}$ and $\{4,5,6\}$, we define $\sigma_0 := (1,2,3)(4,5,6)$. Taking $i_1 = 1$ and $i_2 = 4$, we have

$$U_{\Gamma_0} = \begin{pmatrix} 1/\sqrt{3} & 0 & \sqrt{2/3} & 0 & 0 & 0 \\ 1/\sqrt{3} & 0 & -1/\sqrt{6} & 1/\sqrt{2} & 0 & 0 \\ 1/\sqrt{3} & 0 & -1/\sqrt{6} & -1/\sqrt{2} & 0 & 0 \\ 0 & 1/\sqrt{3} & 0 & 0 & \sqrt{2/3} & 0 \\ 0 & 1/\sqrt{3} & 0 & 0 & -1/\sqrt{6} & 1/\sqrt{2} \\ 0 & 1/\sqrt{3} & 0 & 0 & -1/\sqrt{6} & -1/\sqrt{2} \end{pmatrix}.$$

Note that the first two column vectors $\left(1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3}, 0, 0, 0\right)^\top$ and $\left(0, 0, 0, 1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3}\right)^\top$ of U_{Γ_0} are Γ-invariant. By direct calculation we verify that $U_{\Gamma_0}^\top \cdot X \cdot U_{\Gamma_0}$ is of the form

$$\begin{pmatrix} A & B & 0 & 0 & 0 & 0 \\ B & C & 0 & 0 & 0 & 0 \\ 0 & 0 & D & 0 & 0 & 0 \\ 0 & 0 & 0 & D & 0 & 0 \\ 0 & 0 & 0 & 0 & E & 0 \\ 0 & 0 & 0 & 0 & 0 & E \end{pmatrix},$$

where $A, B, \cdots, E$ are linear functions of $a, b, \cdots, e$. The matrices x_1 and y are $\begin{pmatrix} A & B \\ B & C \end{pmatrix}$ and $\begin{pmatrix} D & 0 & 0 & 0 \\ 0 & D & 0 & 0 \\ 0 & 0 & E & 0 \\ 0 & 0 & 0 & E \end{pmatrix}$ respectively. The matrix y is of such simple form, because Γ_0 is a subgroup of Γ in this case.

We cannot expect that the matrix y in (13) is always of a nice form, as in the example above. However, we note that in many examples we considered, the matrix y was sparse, which also makes the problem of calculating $\mathrm{Det}\,(X)$ much more feasible on a standard PC.

In general Γ_0 defined above is not a subgroup of Γ. As we argue below, valuable insight about the factorization of $\mathcal{Z}_\Gamma$ can be obtained by studying cyclic subgroups of Γ. The argument is based on the following easy result.

LEMMA 4. *Let Γ_1 be a subgroup of Γ. Then $\mathcal{Z}_\Gamma \subset \mathcal{Z}_{\Gamma_1}$.*

Let Γ_1 be a cyclic subgroup of Γ. Then using Theorem 5_{mf}, we can easily calculate structure constant corresponding to Γ_1. Let U_{Γ_1} be the orthogonal matrix constructed in Theorem 6_{mf}. By Lemma 4 and (4), for any $X \in \mathcal{Z}_\Gamma$ the matrix $U_{\Gamma_1}^\top \cdot X \cdot U_{\Gamma_1}$ is of the form

$$\begin{pmatrix} M_{\mathbb{K}_1}(x_1') \otimes I_{\frac{k_1}{d_1}} & & & \\ & M_{\mathbb{K}_2}(x_2') \otimes I_{\frac{k_2}{d_2}} & & \\ & & \ddots & \\ & & & M_{\mathbb{K}_L}(x_L') \otimes I_{\frac{k_L}{d_L}} \end{pmatrix},$$

where $x_i' \in \mathrm{Herm}(r_i; \mathbb{K}_i)$, $i = 1, \ldots, L$. In particular, we have $k_1 = d_1 = 1$ and r_1 is the number of Γ_1-orbits in $\{1, \ldots, p\}$. Thus, we have $M_{\mathbb{K}_1}(x_1') \otimes I_{k_1/d_1} = x_1' \in \mathrm{Sym}(r_1; \mathbb{R})$. In contrast to (13), x_1' in general can be further factorized and we know that $\mathrm{Det}\,(x_1)$ from (14) is an irreducible factor of $\mathrm{Det}\,(x_1')$. In conclusion, each cyclic subgroup of the general group Γ brings various information about the factorization.

EXAMPLE 6. We continue Example 5. Let $\Gamma_1 = \langle(1,2,3)\rangle$, which is a subgroup of Γ. There are four Γ_1-orbits in V, that is, $\{1,2,3\}$, $\{4\}$, $\{5\}$, and $\{6\}$. We have

$$U_{\Gamma_1} = \begin{pmatrix} 1/\sqrt{3} & 0 & 0 & 0 & \sqrt{2/3} & 0 \\ 1/\sqrt{3} & 0 & 0 & 0 & -1/\sqrt{6} & 1/\sqrt{2} \\ 1/\sqrt{3} & 0 & 0 & 0 & -1/\sqrt{6} & -1/\sqrt{2} \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}.$$

For $X \in Z_\Gamma$, we see that $U_{\Gamma_1}^\top \cdot X \cdot U_{\Gamma_1}$ is of the form

$$\begin{pmatrix} A_{11} & A_{21} & A_{31} & A_{41} & 0 & 0 \\ A_{21} & A_{22} & A_{32} & A_{42} & 0 & 0 \\ A_{31} & A_{32} & A_{33} & A_{43} & 0 & 0 \\ A_{41} & A_{42} & A_{43} & A_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & D & 0 \\ 0 & 0 & 0 & 0 & 0 & D \end{pmatrix},$$

where A_{ij} are linear functions of $a, b, \ldots, e$, but they are not linearly independent. Indeed, we have

$$\operatorname{Det} \begin{pmatrix} A_{11} & A_{21} & A_{31} & A_{41} \\ A_{21} & A_{22} & A_{32} & A_{42} \\ A_{31} & A_{32} & A_{33} & A_{43} \\ A_{41} & A_{42} & A_{43} & A_{44} \end{pmatrix} = E^2 \det \begin{pmatrix} A & B \\ B & C \end{pmatrix},$$

which exemplifies the fact that $\operatorname{Det}(x_1)$ is an irreducible factor of $\operatorname{Det}(x_1')$.

3.4. *Gamma integrals.* In this section we prove Proposition 7_{mf}, Theorem 8_{mf} and Theorem 9_{mf}. Proofs of these results are based on Lemma 5 below.

The key ingredient to compute the Gamma integral on $\mathcal{P}_\Gamma$ is the block decomposition of $\mathcal{Z}_\Gamma$. We assume that $\mathcal{Z}_\Gamma$ is in the form of (4). Let Ω_i denote the symmetric cone of the simple Jordan algebra $\mathcal{A}_i = \mathrm{Herm}(r_i; \mathbb{K}_i)$ and $d_i = \dim_{\mathbb{R}} \mathbb{K}_i$, $i = 1, \ldots, L$. We have $\dim \Omega_i = r_i + r_i(r_i-1)d_i/2$. Recall that, for $X \in \mathcal{Z}_\Gamma$ represented as in (4), we write $\phi_i(X) = x_i \in \mathcal{A}_i$ for $i = 1, \ldots, L$.

LEMMA 5. *For any $Y \in \mathcal{P}_\Gamma$ and $\lambda_i > -1$, $i = 1, \ldots, L$, we have*

(15)
$$\int_{\mathcal{P}_\Gamma} \prod_{i=1}^L \det(\phi_i(X))^{\lambda_i} e^{-\operatorname{Tr}[Y \cdot X]} \,\mathrm{d}X = e^{-B_\Gamma} \left(\prod_{i=1}^L k_i^{-r_i\lambda_i} \right) \prod_{i=1}^L \frac{\Gamma_{\Omega_i}(\lambda_i + \dim\Omega_i/r_i)}{\det(\phi_i(Y))^{\lambda_i + \dim\Omega_i/r_i}},$$

where B_Γ is defined in $(15)_{mf}$.

PROOF OF LEMMA 5. Denote the left hand side of (15) by I. Let us change variables $x_i = \phi_i(X)$ for $i = 1, \ldots, L$. By $(10)_{mf}$ and $(14)_{mf}$ we obtain

$$I = e^{B_\Gamma} \prod_{i=1}^L \int_{\Omega_i} \det(x_i)^{\lambda_i} e^{-k_i \operatorname{tr}[\phi_i(Y) \cdot x_i]} m_i(\mathrm{d}x_i).$$

Each integral can be calculated using $(13)_{mf}$ for $\lambda_i > -1$ and $\phi_i(Y) \in \Omega_i$, $i = 1, \ldots, L$. Hence,

$$\begin{aligned} I &= e^{B_\Gamma} \prod_{i=1}^{L} \Gamma_{\Omega_i}(\lambda_i + \dim\Omega_i/r_i) \det(k_i\,\phi_i(Y))^{-\lambda_i - \dim\Omega_i/r_i} \\ &= e^{B_\Gamma} \left(\prod_{i=1}^{L} k_i^{-r_i\lambda_i - \dim\Omega_i}\right) \prod_{i=1}^{L} \frac{\Gamma_{\Omega_i}(\lambda_i + \dim\Omega_i/r_i)}{\det(\phi_i(Y))^{\lambda_i + \dim\Omega_i/r_i}} \\ &= e^{-B_\Gamma} \left(\prod_{i=1}^{L} k_i^{-r_i\lambda_i}\right) \prod_{i=1}^{L} \frac{\Gamma_{\Omega_i}(\lambda_i + \dim\Omega_i/r_i)}{\det(\phi_i(Y))^{\lambda_i + \dim\Omega_i/r_i}} \end{aligned}$$

and so we obtain (15). □

PROOF OF PROPOSITION 7_{mf}. Recall that $\mathcal{P}_\Gamma$ is a symmetric cone, so that it coincides with its dual cone, $\mathcal{P}_\Gamma^*$. Thus,

$$\varphi_\Gamma(Y) = e^{B_\Gamma} \left(\prod_{i=1}^{L} \frac{1}{\Gamma_{\Omega_i}(\dim\Omega_i/r_i)}\right) \int_{\mathcal{P}_\Gamma} e^{-\mathrm{Tr}[Y\cdot X]}\,\mathrm{d}X \qquad (Y \in \mathcal{P}_\Gamma).$$

Setting $\lambda_1 = \ldots = \lambda_L = 0$ in (15) we obtain the expression for $\varphi_\Gamma(Y)$. □

PROOF OF THEOREM 8_{mf} AND THEOREM 9_{mf}. Recall that for $X \in \mathcal{P}_\Gamma$ we have $\mathrm{Det}\,(X) = \prod_{i=1}^{L} \det(\phi_i(X))^{k_i}$, where the map $\phi_i : \mathcal{Z}_\Gamma \to \mathrm{Herm}(r_i; \mathbb{K}_i)$ is a Jordan algebra homomorphism, $i = 1, \ldots, L$.

If $\lambda_i = k_i\lambda - \dim\Omega_i/r_i$ with $\lambda > \max_{i=1,\ldots,L}\{(r_i - 1)d_i/(2k_i)\}$, then (15) implies

$$\prod_{i=1}^{L} k_i^{-r_i\lambda_i} = e^{-A_\Gamma\lambda + 2B_\Gamma} \quad \text{and} \quad \prod_{i=1}^{L} \det(\phi_i(Y))^{-\lambda_i - \dim\Omega_i/r_i} = \left(\prod_{i=1}^{L} \det(\phi_i(Y))^{k_i}\right)^{-\lambda}$$

If $\lambda_i = k_i\lambda$ with $\lambda > \max_{i=1,\ldots,L}\{-1/k_i\}$, then by (15) we obtain

$$\prod_{i=1}^{L} k_i^{-r_i\lambda_i} = e^{-A_\Gamma\lambda} \quad \text{and} \quad \prod_{i=1}^{L} \det(\phi_i(Y))^{-\lambda_i - \dim\Omega_i/r_i} = \left(\prod_{i=1}^{L} \det(\phi_i(Y))^{k_i}\right)^{-\lambda} \varphi_\Gamma(Y).$$

□

3.5. *Jacobian.*

PROOF OF LEMMA 13_{mf}. First observe that

$$(X+h)^{-1} - X^{-1} = (X+h)^{-1} \cdot [X - (X+h)] \cdot X^{-1} = -X^{-1} \cdot h \cdot X^{-1} + o(h),$$

so that, the Jacobian of $\mathcal{P}_\Gamma \ni X \mapsto X^{-1} \in \mathcal{P}_\Gamma$ equals $\mathrm{Det}_{\mathrm{End}}(\mathbb{P}_{X^{-1}})$, where $\mathrm{Det}_{\mathrm{End}}$ is the determinant in the space of endomorphisms of $\mathcal{Z}_\Gamma$ and for any $X \in \mathcal{Z}_\Gamma$ by $\mathbb{P}_X$ we denote the linear map on $\mathcal{Z}_\Gamma$ to itself defined by $\mathbb{P}_X Y = X \cdot Y \cdot X$. It is easy to see that for any $X \in \mathcal{P}_\Gamma$ we have $\mathbb{P}_X \in \mathrm{G}(\mathcal{P}_\Gamma)$. Indeed, since $\mathbb{P}_X Y$ is positive definite for $Y \in \mathcal{P}_\Gamma$, it is enough to verify that

$$R(\sigma) \cdot [\mathbb{P}_X Y] = [\mathbb{P}_X Y] \cdot R(\sigma) \qquad (\sigma \in \Gamma).$$

This follows quickly by the fact that $X, Y \in \mathcal{P}_\Gamma$. Further, by the $\mathrm{G}(\mathcal{P}_\Gamma)$ invariance of φ_Γ, we have

$$\varphi_\Gamma(gX) = |\mathrm{Det}_{\mathrm{End}}(g)|^{-1}\varphi_\Gamma(X) \qquad (g \in \mathrm{G}(\mathcal{P}_\Gamma)).$$

Taking $g = \mathbb{P}_{X^{-1}}$, we eventually obtain

$$\mathrm{Det}_{\mathrm{End}}(\mathbb{P}_{X^{-1}}) = \frac{\varphi_\Gamma(X)}{\varphi_\Gamma(X^{-1})} = [\varphi_\Gamma(X)]^2,$$

where the latter inequality can be easily verified by $(16)_{mf}$. □

4. Additions to Section 6_{mf}.

4.1. *Real data example.* We applied our procedure to the breast cancer data set considered in Section 7 of Højsgaard and Lauritzen (2008), see also Miller et al. (2005). Following approach of Højsgaard and Lauritzen, we consider set of $p = 150$ genes (designations of these genes can be read from (Højsgaard and Lauritzen, 2008, Fig. 11)) and $n = 58$ samples with mutation in the p53 sequence. We numbered the variables alphabetically. Since $p > n$, only parsimonious models can be fitted at all.

In Højsgaard and Lauritzen (2008), the variables were standardized to have zero mean and unit variance. As the authors write, due to "an issue of scaling of the variables", model selection within RCOR models (a superclass of RCOP models) was performed. However, when the search is done among RCOP models, the scaling ensuring unit variances favors transitive subgroups. Recall that a cyclic subgroup is transitive if it is generated by a permutation consisting of one big cycle. Therefore we only centered the data.

We run the Metropolis-Hastings algorithm (Algorithm 13_{mf}) with hyper-parameters $D = I_p$ and $\delta = 3$ for $150\,000$ iterations. Cardinality of the search space is not easy to compute, but already for $p = 130$, the number of cyclic subgroups is of magnitude 10^{217}, see OEIS sequence A051625. The cyclic subgroup with highest estimated posterior probability (7.1%) is given by $\hat{\Gamma} = \langle\sigma^*\rangle$, where

$$\begin{aligned}\sigma^* = &(1,2,139,149,61,52,8,145)(3,11,9,89,6,102,120,4)(5,47,90)(7,13,138,91,117,142,143,72,146,50,136,22,57,87,124,\\ &114,84,30)(10,99,39,21,101,26,37,73)(12,77,100,133,122)(14,19,76,147)(15,71,127,110)(16,92,83,34,140,27,49,137)\\ &(17,98,69)(18,65,134,88,107,75,108,106,82,109,123,68)(20,51,135,105,38,96,25,45)(23,111,24,42,67,43,131,112)\\ &(31,58,66,94,81)(32,33)(35,93,64,86,128,148,132,103,60,150,144,129,118,70,97,121)(36,85,141)(44,56,119,126,104,\\ &78,79,48)(46,130,115,74,116,59,113,125,95).\end{aligned}$$

The order of $\hat{\Gamma}$ is 720. The structure constants of $\mathcal{Z}_{\hat{\Gamma}}$ are $L = 21$,

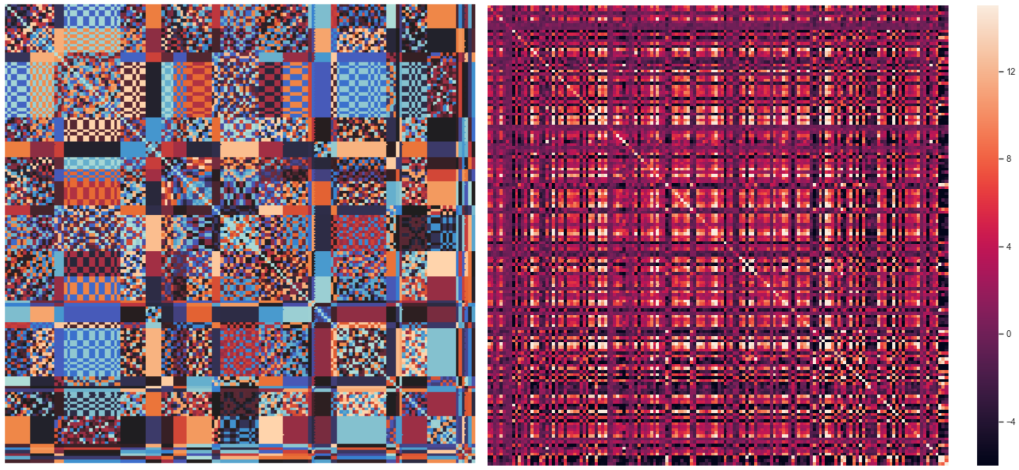
$$r = (29,1,1,1,2,8,2,1,2,2,11,1,1,6,8,1,2,1,1,2,13),$$
$$d = k = (1,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,1),$$

which imply that $\dim \mathcal{Z}_{\hat{\Gamma}} = 844$. Although the number of parameters (colors) of $\mathcal{Z}_{\hat{\Gamma}}$ is rather high, the MLE of Σ exists in this model. Indeed, in view of Corollary 12_{mf}, we have

$$n_0 = \max_{i=1,\ldots,L}\left\{\frac{r_i d_i}{k_i}\right\} = 29$$

and so $(23)_{mf}$ is satisfied.

The color pattern of the space of $p \times p$ matrices from $\mathcal{Z}_{\hat{\Gamma}}$ is depicted in Fig. 1 (a). Entries which correspond to the same color in a figure are the same. To make the picture more readable, we renumbered the variables so that the block structure is visible. For comparison, in Fig. 1 we present the heat map of data matrix U (rows and columns are permuted in the same way as in Fig. 1(a)). We can interpret this result as an indication of hidden symmetry



(a) (b)

FIG 1. *(a) The color pattern of (permuted) space $\mathcal{Z}_{\hat{\Gamma}}$. (b) The heat map of (permuted) matrix U.*

in genes and evidence that our procedure can be used as an exploratory tool for finding such symmetries.

Finally, we carry out the heuristic procedure introduced in Section 1.2_{mf} for finding an RCOP model when the true graph is not complete. We threshold the entries of the partial correlation matrix at the level $\alpha = 0.15$ and obtain a connected graph with 925 edges, see Figure 2. The largest clique consists of 12 vertices.

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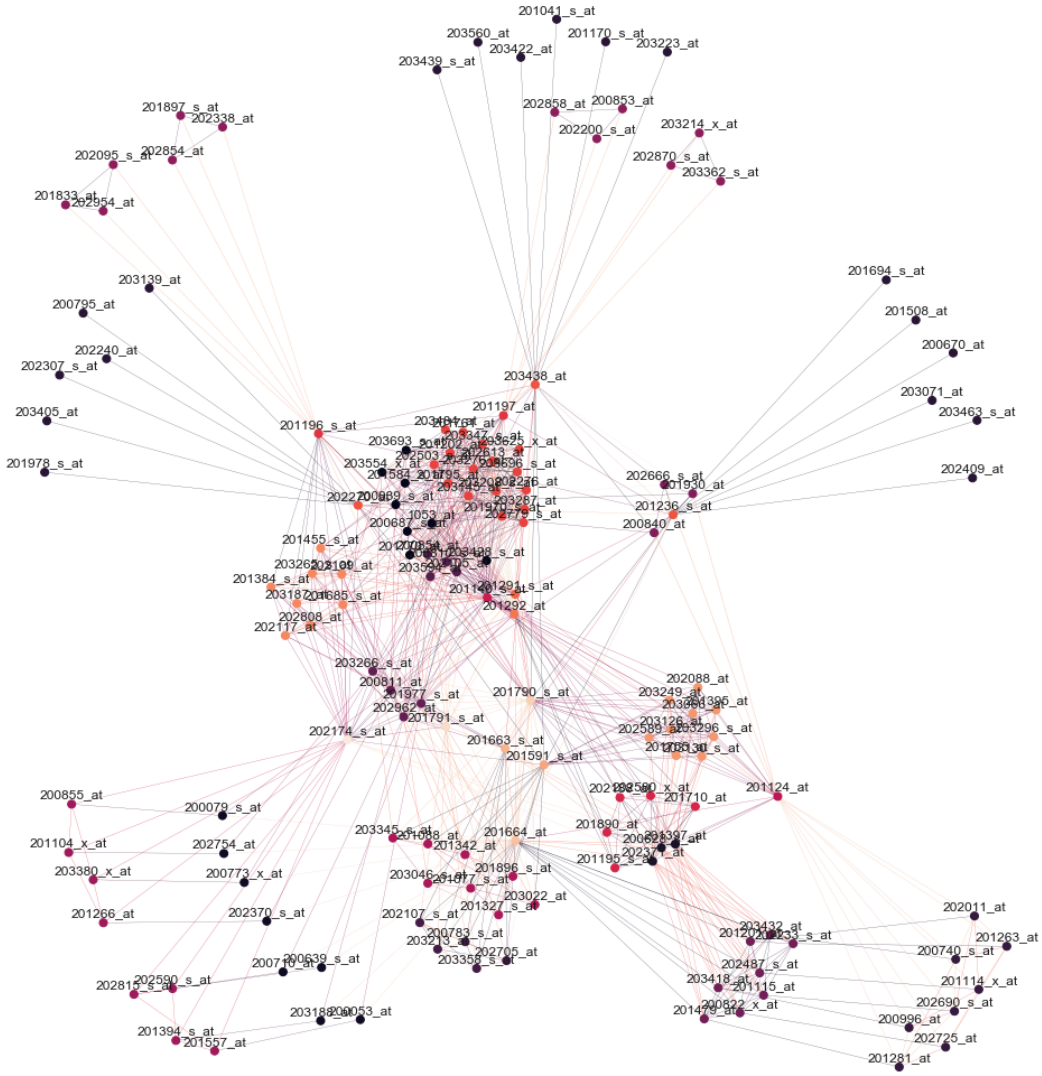

FIG 2. *Graph corresponding to thresholded ($\alpha = 0.15$) partial correlation matrix.*