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Locally isometric embeddings of quotients of the rotation group modulo finite symmetries

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ABSTRACT

The analysis of manifold-valued data using embedding based methods is linked to the problem of finding suitable embeddings. In this paper we are interested in embeddings of quotient manifolds $\mathrm{SO}(3)/\mathcal{S}$ of the rotation group modulo finite symmetry groups. Data on such quotient manifolds naturally occur in crystallography, material science and biochemistry. We provide a generic framework for the construction of such embeddings which generalizes the embeddings constructed in Arnold et al. (2018). The central advantage of our larger class of embeddings is that it includes locally isometric embeddings for all crystallographic symmetry groups.

1. Introduction

In the analysis of manifold-valued data there are two different approaches — intrinsic and extrinsic. Intrinsic methods solely rely on intrinsic properties of the manifold, e.g. the Riemannian curvature tensor, the exponential map or the Levi-Cevita connection. Those methods often work locally like moving least squares [10], multiscale methods [20] or subdivision schemes [25]. Other intrinsic approaches make use of function systems that are adapted to the geometry of the manifold, e.g. diffusion maps [5] or the eigenfunctions of the manifold Laplacian [11,12,14,15,19].

On the other hand, extrinsic methods rely on an embedding of the manifold into some higher dimensional vector space [2,7,22]. The advantage of embedding-based methods, compared to intrinsic methods, is that they often are straight forward generalizations of the corresponding linear methods. The central challenges for applying an embedding-based method to a specific manifold $\mathcal{M}$ are

1. Find a suitable embedding $\mathcal{E}\colon \mathcal{M} \to \mathbb{R}^d$ of the manifold $\mathcal{M}$ that approximately preserves distances and has moderate dimension.
2. Find an efficient algorithm for the projection $P_{\mathcal{M}}\colon U \to \mathcal{M}$ from some neighborhood $U \supset \mathcal{E}(\mathcal{M})$ back to the manifold.

In our paper we are concerned with the specific case when the manifold $\mathcal{M}$ is the quotient $\mathrm{SO}(3)/\mathcal{S} = \{[\boldsymbol{R}]_{\mathcal{S}} \colon \boldsymbol{R} \in \mathrm{SO}(3)\}$ of the rotational group $\mathrm{SO}(3)$ with respect to some finite symmetry group $\mathcal{S} < \mathrm{SO}(3)$. Here the cosets in the quotient space are defined by $[\boldsymbol{R}]_{\mathcal{S}} := \{\boldsymbol{RO} \mid \boldsymbol{O} \in \mathcal{S}\}$. As a finite subgroup of $\mathrm{SO}(3)$ the symmetry group $\mathcal{S}$ is isomorphic to one of the following: the cyclic groups C_k for $k \in \{1, 2, \ldots\}$, the dihedral groups D_k for $k \in \{2, 3, \ldots\}$, the tetrahedral group T, the

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octahedral group O and the icosahedral group Y. Since the group SO(3) is simple, the quotient $\mathrm{SO}(3)/\mathcal{S}$ is not a group for all $\mathcal{S} \neq C_1$ but forms a homogeneous space with canonical left action of the Lie group SO(3).

To give the reader an idea about the quotient $\mathrm{SO}(3)/\mathcal{S}$ we consider the representation of a rotation $\boldsymbol{R} = \boldsymbol{R}_z(\alpha)\boldsymbol{R}_y(\beta)\boldsymbol{R}_z(\gamma)$ as the composition of rotations about the axes z, y, z and Euler angles $\alpha, \gamma \in [0, 2\pi]$, $\beta \in [0, \pi]$. Let us furthermore assume that the subgroup C_k is represented by the rotations $\boldsymbol{R}_z(\ell\,\frac{2\pi}{k})$, $\ell \in \mathbb{Z}$ about the z-axis. Then C_k enforces a periodicity of $2\pi/k$ on the last Euler angle γ and the cosets in $\mathrm{SO}(3)/C_k$ are of the form

$$[\boldsymbol{R}_z(\alpha)\boldsymbol{R}_y(\beta)\boldsymbol{R}_z(\gamma)]_{C_k} = \left\{\boldsymbol{R}_z(\alpha)\boldsymbol{R}_y(\beta)\boldsymbol{R}_z(\gamma + \tfrac{2\ell\pi}{k}) \mid \ell = 0 \ldots k-1\right\}.$$

Nice geometrical visualizations of these coset spaces can be found in [16].

The analysis of data that are cosets $[\boldsymbol{R}]_{\mathcal{S}} \in \mathrm{SO}(3)/\mathcal{S}$ in the homogeneous space $\mathrm{SO}(3)/\mathcal{S}$ is of central importance in various scientific areas. For instance, they are used to describe the alignment of crystals in crystallography, material science and geology [1,4,8], the alignment of molecules and proteins in biochemistry [3] or movements in robotics [26] and motion tracking [21].

Since, locally, the quotient manifolds $\mathrm{SO}(3)/\mathcal{S}$ are isometric to the rotation group SO(3) itself all intrinsic methods for the rotation group can be easily adapted to work on the quotients as well. Unfortunately, this is not true for embedding based-methods, e.g. for the interpolation methods described in [9]. Explicit embeddings for the quotient manifolds $\mathrm{SO}(3)/\mathcal{S}$ have been investigated first by R. Arnold, P. Jupp and H. Schaeben in [2]. Our paper aims to extend their results by developing a general framework for the construction of embeddings of the quotient manifolds $\mathrm{SO}(3)/\mathcal{S}$ that include the embeddings described in [2]. Our embeddings pose several nice properties, e.g. they are all SO(3)-equivariant (see Definition 3), their images are contained in a sphere and the image measure $\mu \circ \mathcal{E}^{-1}$ induced by the rotational invariant measure μ on SO(3) is centered in $\mathbb{R}^d$, i.e., has zero mean. Furthermore, we find within our framework locally isometric embeddings of $\mathrm{SO}(3)/\mathcal{S}$ for all finite symmetry groups $\mathcal{S}$ and provide an efficient numerical method for the projection $P_{\mathcal{M}}$. The practical advantage of isometric embeddings is that locally isotropic methods in $\mathbb{R}^d$ translates into locally isotropic methods on $\mathrm{SO}(3)/\mathcal{S}$.

Our paper is organized as follows. In Section 2.1 we introduce the generic embeddings and prove in Theorem 4 and Corollary 5 that they are SO(3)-equivariant maps that map the quotient manifold into a subsphere of an Euclidean vector space. Furthermore, we provide in Table 1 the parameters such that our embeddings coincide with the embeddings found in [2]. In Section 2.2 we investigate rotational invariant subspaces of $\mathbb{R}^d$ and show in Theorem 9 that the embeddings can be centered such that their image is contained in a linear subspace of $\mathbb{R}^d$ which allows us to reduce the effective dimension of the embedding. In Section 2.3 we consider the rotational invariant Haar measure μ on SO(3) and generalize it to a left invariant measure $\mu_{\mathcal{S}}$ on $\mathrm{SO}(3)/\mathcal{S}$. Together with an embedding $\mathcal{E}\colon \mathrm{SO}(3)/\mathcal{S} \to \mathbb{R}^d$ this induces an image measure on $\mathbb{R}^d$. In Theorem 10 we show that the centered embeddings from Section 2.3 result in centered image measures. Finally, we propose in Section 2.4 an iterative algorithm for the numerical computation of the projection $P_{\mathcal{M}}$ of an arbitrary point in some neighborhood of the manifold back to the manifold. To this end, we derive in Theorem 12 the gradient of the distance functional.

In Section 3 we are interested in the discrepancy between the geodesic distance on the quotient manifold and the Euclidean distance in the embedding. A smooth embedding into $\mathbb{R}^d$, such that the pull back of the Euclidean metric tensor coincides with the metric tensor of the manifold, is called isometric. According to the Nash embedding theorem [18], there exists for every m-dimensional Riemannian manifold an isometric embedding into $\mathbb{R}^{m(3m+11)/2}$. As all our quotient manifolds are three-dimensional the result guaranties the existence of an isometric embedding into the space $\mathbb{R}^{30}$. It turns out that our embeddings are sufficiently general to include locally isometric embeddings for the quotient manifolds $\mathrm{SO}(3)/\mathcal{S}$ modulo all crystallographic symmetry groups $\mathcal{S}$. This result is proven separately for the different types of symmetry groups in Theorems 15, 18, 19, 20, 21, 22. The corresponding parameters as well as the dimension of the linear space are summarized in Table 2. The dimensions of the locally isometric embeddings vary from 8 to 32 depending on the symmetry group.

In Section 3.2 we investigate the global relationship between the geodesic distance on $\mathrm{SO}(3)/\mathcal{S}$ and the Euclidean distance in the embedding. According to [24] it is possible to construct for each smooth and compact manifold $\mathcal{M}$ an embedding $\mathcal{E}\colon \mathcal{M} \to \mathbb{R}^d$ such that the geodesic distance on the manifold and the Euclidean distance in the embedding differ only by a given $\varepsilon > 0$, i.e.,

$$(1-\varepsilon)\, d_{\mathcal{M}}(m_1, m_2) \leq d(\mathcal{E}(m_1), \mathcal{E}(m_2)) \leq (1+\varepsilon)\, d_{\mathcal{M}}(m_1, m_2). \tag{1}$$

However, the dimension d of the vector space required for such an embedding is much too large for numerical applications. In Table 3 we provide similar bounds to those in (1) for the locally isometric embeddings defined in this paper. It turns out that locally isometric embeddings do not necessarily lead to globally optimal bounds. Parameters for our embeddings optimized with respect to global preservation of distances are provided in Table 4.

2. Embeddings of the rotation group

2.1. General framework

The group of rotations SO(3) interpreted as a matrix group has a canonical embedding $\mathcal{E}\colon \mathrm{SO}(3) \to \mathbb{R}^9$ given by

$$\mathcal{E}(\boldsymbol{R}) = (\boldsymbol{R}\boldsymbol{e}_1, \boldsymbol{R}\boldsymbol{e}_2, \boldsymbol{R}\boldsymbol{e}_3) \tag{2}$$

where $\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3$ are the standard bases in $\mathbb{R}^3$. Replacing the basis vectors $\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3$ by any other list of vectors $\boldsymbol{u}_1, \boldsymbol{u}_2, \ldots, \boldsymbol{u}_n$ will always result in an embedding as long as at least two of the vectors are linearly independent. Unfortunately, this approach is not applicable to quotients $\mathrm{SO}(3)/\mathcal{S}$ since well definedness requires that $\mathcal{E}([\boldsymbol{RS}]_\mathcal{S}) = \mathcal{E}([\boldsymbol{R}]_\mathcal{S})$ for all symmetry operations $\boldsymbol{S} \in \mathcal{S}$. For that reason, we generalize the embedding (2) to tensor products of vectors $\boldsymbol{u}_1, \boldsymbol{u}_2, \ldots, \boldsymbol{u}_n$. In the next definition we will make use of the following notation. Let $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_n) \in \mathbb{N}^n$ be a multi-index. Then $\mathbb{R}^{3^{\boldsymbol{\alpha}}}$ is defined as the linear space

$$\mathbb{R}^{3^{\boldsymbol{\alpha}}} = \times_{i=1}^{n} \left(\otimes^{\alpha_i}\mathbb{R}^3\right) \cong \mathbb{R}^{\left(\sum_{i=1}^{n} 3^{\alpha_i}\right)}. \tag{3}$$

Definition 1. Let $n \in \mathbb{N}$, $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_n) \in \mathbb{N}^n$ be a multi-index and $\boldsymbol{u} = (\boldsymbol{u}_1, \ldots, \boldsymbol{u}_n) \in \mathbb{R}^{3\times n}$ be a list of n directions $\boldsymbol{u}_j \in \mathbb{R}^3$. Then we define the mapping $\mathcal{E}_{\boldsymbol{u}}^{\boldsymbol{\alpha}} \colon \mathrm{SO}(3) \to \mathbb{R}^{3^{\boldsymbol{\alpha}}}$ as

$$\mathcal{E}_{\boldsymbol{u}}^{\boldsymbol{\alpha}}(\boldsymbol{R}) = \left(\otimes^{\alpha_1}\boldsymbol{R}\boldsymbol{u}_1, \ldots, \otimes^{\alpha_n}\boldsymbol{R}\boldsymbol{u}_n\right).$$

In order to define mappings that are invariant with respect to a finite subgroup $\mathcal{S} < \mathrm{SO}(3)$ we utilize the averaging idea.

Definition 2. Let $\mathcal{S} < \mathrm{SO}(3)$ be a finite subgroup and $\mathcal{E}_{\boldsymbol{u}}^{\boldsymbol{\alpha}} \colon \mathrm{SO}(3) \to \mathbb{R}^{3^{\boldsymbol{\alpha}}}$ as defined in Definition 1. Then we denote by

$$\mathcal{E}_{\boldsymbol{u},\mathcal{S}}^{\boldsymbol{\alpha}} \colon \mathrm{SO}(3)/\mathcal{S} \to \mathbb{R}^{3^{\boldsymbol{\alpha}}}, \qquad \mathcal{E}_{\boldsymbol{u},\mathcal{S}}^{\boldsymbol{\alpha}}([\boldsymbol{O}]_\mathcal{S}) = \frac{1}{|\mathcal{S}|}\sum_{\boldsymbol{S}\in\mathcal{S}} \mathcal{E}_{\boldsymbol{u}}^{\boldsymbol{\alpha}}(\boldsymbol{OS}), \quad [\boldsymbol{O}]_\mathcal{S} = \{\boldsymbol{OR} \mid \boldsymbol{R} \in \mathcal{S}\} \in \mathrm{SO}(3)/\mathcal{S}$$

its symmetrized version.

In order to examine the properties of $\mathcal{E}_{\boldsymbol{u},\mathcal{S}}^{\boldsymbol{\alpha}}$ we consider both, the quotient $\mathrm{SO}(3)/\mathcal{S}$ and the vector space $\mathbb{R}^{3^{\boldsymbol{\alpha}}}$ of dimension $\sum_{i=1}^{n} 3^{\alpha_i}$ as $\mathrm{SO}(3)$ manifolds equipped with the left group actions

$$\boldsymbol{R} \triangleright [\boldsymbol{O}]_\mathcal{S} = [\boldsymbol{RO}]_\mathcal{S}, \qquad \boldsymbol{R} \triangleright \boldsymbol{v} = (\otimes^{\boldsymbol{\alpha}}\boldsymbol{R})\,\boldsymbol{v},$$

where $\boldsymbol{R} \in \mathrm{SO}(3)$, $[\boldsymbol{O}]_\mathcal{S} \in \mathrm{SO}(3)/\mathcal{S}$ and $\boldsymbol{v} = (\boldsymbol{v}^1, \ldots, \boldsymbol{v}^n) \in \mathbb{R}^{3^{\boldsymbol{\alpha}}}$. The multiplication of tensor product $\otimes^{\boldsymbol{\alpha}}\boldsymbol{R}$ with the tensor $\boldsymbol{v} \in \mathbb{R}^{3^{\boldsymbol{\alpha}}}$ is defined component-wise by $(\otimes^{\boldsymbol{\alpha}}\boldsymbol{R})\,\boldsymbol{v} = \left((\otimes^{\alpha_i}\boldsymbol{R})\,\boldsymbol{v}_i\right)_{i=1}^{n}$ and

$$\left[(\otimes^{\alpha_i}\boldsymbol{R})\,\boldsymbol{v}^i\right]_{k_1,\ldots,k_{\alpha_i}} = \sum_{\ell_1=1}^{3} \cdots \sum_{\ell_{\alpha_i}=1}^{3} R_{k_1\ell_1} \cdots R_{k_{\alpha_i}\ell_{\alpha_i}} v^i_{\ell_1,\ldots,\ell_{\alpha_i}}.$$

Mappings that intertwine with such group actions are called equivariant.

Definition 3. Let G be a group that acts on two sets X, Y via $g \triangleright x$ and $g \triangleright y$, $g \in G$, $x \in X$, $y \in Y$. A mapping $f \colon X \to Y$ is said to be an G-equivariant map if it intertwines with the group action, i.e.,

$$f(g \triangleright x) = g \triangleright f(x) \quad \text{for all} \quad g \in G, x \in X.$$

It turns out that the embeddings from Definitions 1 and 2 are indeed $\mathrm{SO}(3)$-equivariant maps between the quotients $\mathrm{SO}(3)/\mathcal{S}$ and Euclidean vector spaces $\mathbb{R}^{3^{\boldsymbol{\alpha}}}$.

Theorem 4. *The mapping $\mathcal{E}_{\boldsymbol{u},\mathcal{S}}^{\boldsymbol{\alpha}} \colon \mathrm{SO}(3)/\mathcal{S} \to \mathbb{R}^{3^{\boldsymbol{\alpha}}}$ is an $\mathrm{SO}(3)$-equivariant map, i.e.,*

$$\mathcal{E}_{\boldsymbol{u},\mathcal{S}}^{\boldsymbol{\alpha}}(\boldsymbol{R} \triangleright [\boldsymbol{O}]_\mathcal{S}) = \boldsymbol{R} \triangleright \mathcal{E}_{\boldsymbol{u},\mathcal{S}}^{\boldsymbol{\alpha}}([\boldsymbol{O}]_\mathcal{S})$$

for all $\boldsymbol{R} \in \mathrm{SO}(3)$ and $[\boldsymbol{O}]_\mathcal{S} \in \mathrm{SO}(3)/\mathcal{S}$.

Proof. Let $\boldsymbol{R} \in \mathrm{SO}(3)$ and $[\boldsymbol{O}]_\mathcal{S} \in \mathrm{SO}(3)/\mathcal{S}$. Then straightforward computation reveals

$$\mathcal{E}_{\boldsymbol{u},\mathcal{S}}^{\boldsymbol{\alpha}}(\boldsymbol{R} \triangleright [\boldsymbol{O}]_\mathcal{S}) = \frac{1}{|\mathcal{S}|}\sum_{\boldsymbol{S}\in\mathcal{S}} \mathcal{E}_{\boldsymbol{u}}^{\boldsymbol{\alpha}}(\boldsymbol{ROS}) = \frac{1}{|\mathcal{S}|}\sum_{\boldsymbol{S}\in\mathcal{S}} \left(\otimes^{\alpha_1}\boldsymbol{ROS}\boldsymbol{u}_1, \ldots, \otimes^{\alpha_n}\boldsymbol{ROS}\boldsymbol{u}_n\right) = \boldsymbol{R} \triangleright \mathcal{E}_{\boldsymbol{u},\mathcal{S}}^{\boldsymbol{\alpha}}([\boldsymbol{O}]_\mathcal{S}). \quad \square$$

A direct consequence of $\mathcal{E}_{\boldsymbol{u},\mathcal{S}}^{\boldsymbol{\alpha}}$ being a $\mathrm{SO}(3)$-equivariant map is that $\left\|\mathcal{E}_{\boldsymbol{u},\mathcal{S}}^{\boldsymbol{\alpha}}([\boldsymbol{R}]_\mathcal{S})\right\|$ is independent of $[\boldsymbol{R}]_\mathcal{S} \in \mathrm{SO}(3)/\mathcal{S}$.

Corollary 5. *The image $\mathcal{E}_{\boldsymbol{u},\mathcal{S}}^{\boldsymbol{\alpha}}(\mathrm{SO}(3)/\mathcal{S}) \subset \mathbb{R}^{3^{\boldsymbol{\alpha}}}$ is contained in a sphere with radius $r_\mathcal{S}$, i.e., it exists a constant $r_\mathcal{S} > 0$ such that for all $[\boldsymbol{R}]_\mathcal{S} \in \mathrm{SO}(3)/\mathcal{S}$,*

$$\left\|\mathcal{E}_{\boldsymbol{u},\mathcal{S}}^{\boldsymbol{\alpha}}([\boldsymbol{R}]_\mathcal{S})\right\| = r_\mathcal{S}.$$

Proof. Let $\boldsymbol{R} \in \mathrm{SO}(3)$ be an arbitrary rotation and $\boldsymbol{I} \in \mathrm{SO}(3)$ the identity. Then we have by Theorem 4 and the fact that the Kronecker product of orthogonal matrices is again an orthogonal matrix that

$$\begin{aligned}\left\|\mathcal{E}^{\boldsymbol{\alpha}}_{\boldsymbol{u},\mathcal{S}}([\boldsymbol{R}]_{\mathcal{S}})\right\|^2 &= \left\langle \mathcal{E}^{\boldsymbol{\alpha}}_{\boldsymbol{u},\mathcal{S}}([\boldsymbol{R}\,\boldsymbol{I}]_{\mathcal{S}}),\ \mathcal{E}^{\boldsymbol{\alpha}}_{\boldsymbol{u},\mathcal{S}}([\boldsymbol{R}\,\boldsymbol{I}]_{\mathcal{S}})\right\rangle = \left\langle \boldsymbol{R} \triangleright \mathcal{E}^{\boldsymbol{\alpha}}_{\boldsymbol{u},\mathcal{S}}([\boldsymbol{I}]_{\mathcal{S}}),\ \boldsymbol{R} \triangleright \mathcal{E}^{\boldsymbol{\alpha}}_{\boldsymbol{u},\mathcal{S}}([\boldsymbol{I}]_{\mathcal{S}})\right\rangle \\ &= \left\langle (\otimes^{\boldsymbol{\alpha}}\boldsymbol{R})\, \mathcal{E}^{\boldsymbol{\alpha}}_{\boldsymbol{u},\mathcal{S}}([\boldsymbol{I}]_{\mathcal{S}}),\ (\otimes^{\boldsymbol{\alpha}}\boldsymbol{R})\, \mathcal{E}^{\boldsymbol{\alpha}}_{\boldsymbol{u},\mathcal{S}}([\boldsymbol{I}]_{\mathcal{S}})\right\rangle = \left\|\mathcal{E}^{\boldsymbol{\alpha}}_{\boldsymbol{u},\mathcal{S}}([\boldsymbol{I}]_{\mathcal{S}})\right\|^2. \quad \square\end{aligned}$$

2.2. Rotationally invariant subspaces

In order to prove further properties of the embeddings $\mathcal{E}^{\boldsymbol{\alpha}}_{\boldsymbol{u},\mathcal{S}}$ we continue by investigating subspaces of $\mathbb{R}^{3^{\boldsymbol{\alpha}}}$ that are invariant with respect to the group action $\triangleright$. More precisely, we search for tensors $\boldsymbol{M}_\alpha \in \mathbb{R}^{3^\alpha}$, such that $\boldsymbol{R} \triangleright \boldsymbol{M}_\alpha = \boldsymbol{M}_\alpha$. For $\alpha = 1$ and $\boldsymbol{v} \in \mathbb{R}^3$ this means $\boldsymbol{R}\boldsymbol{v} = \boldsymbol{v}$ has to hold for all $\boldsymbol{R} \in \mathrm{SO}(3)$. This is only fulfilled for $\boldsymbol{v} = \boldsymbol{0}$ and, hence, the subspace of rotational invariant vectors in the $\mathbb{R}^3$ is just the trivial one. In the case $\alpha = 2$ we have for $\boldsymbol{v} = \boldsymbol{I} \in \mathbb{R}^{3^2}$ that $\otimes^2\boldsymbol{R} \triangleright \boldsymbol{I} = \boldsymbol{R}\boldsymbol{I}\boldsymbol{R}^T = \boldsymbol{I}$ and, hence, $\boldsymbol{M}_2 = \boldsymbol{I}$ spans a rotational invariant subspace of $\mathbb{R}^{3^2}$. Indeed, we find a one-dimensional rotational invariant subspace for all even α.

Lemma 6. *Let $\boldsymbol{\alpha} = (\alpha_i)_{i=1}^n$ be a multi-index. Then the tensor $\boldsymbol{M}_\alpha \in \mathbb{R}^{3^{\boldsymbol{\alpha}}}$ defined by*

$$(\boldsymbol{M}_{\alpha_i})_{j_1,\ldots,j_{\alpha_i}} = symm(\otimes^{\alpha_i/2}\boldsymbol{I}) = \frac{1}{\alpha_i!}\sum_{\sigma\in\Sigma_{\alpha_i}}\prod_{k=1}^{\alpha_i/2}\delta_{j_{\sigma(2k-1)},j_{\sigma(2k)}},$$

if α_i is even and $\boldsymbol{M}_{\alpha_i} = \boldsymbol{0} \in \otimes^{\alpha_i}\mathbb{R}^3$ if α_i is odd, is $\mathrm{SO}(3)$ invariant, i.e., $\boldsymbol{R} \triangleright \boldsymbol{M}_\alpha = \boldsymbol{M}_\alpha$, $\boldsymbol{R} \in \mathrm{SO}(3)$.

Proof. For odd α_i there is nothing to prove. For $\boldsymbol{R} = \left(R_{ij}\right)_{i,j=1}^3 \in \mathrm{SO}(3)$ and even $\alpha \in \mathbb{N}_0$ we have

$$\begin{aligned}(\boldsymbol{R} \triangleright \boldsymbol{M}_\alpha)_{i_1,\ldots,i_\alpha} &= ((\otimes^\alpha \boldsymbol{R})\boldsymbol{M}_\alpha)_{i_1,\ldots,i_\alpha} = \sum_{j_1,\ldots,j_\alpha=1}^{3} (\boldsymbol{M}_\alpha)_{j_1,\ldots,j_\alpha} R_{i_1j_1}R_{i_2j_2}\cdots R_{i_\alpha j_\alpha} \\ &= \frac{1}{\alpha!}\sum_{j_1,\ldots,j_\alpha=1}^{3}\left(\left(\sum_{\sigma\in\Sigma_\alpha}\prod_{k=1}^{\frac{\alpha}{2}}\delta_{j_{\sigma(2k-1)},j_{\sigma(2k)}}\right)R_{i_1j_1}R_{i_2j_2}\cdots R_{i_\alpha j_\alpha}\right) \\ &= \frac{1}{\alpha!}\sum_{j_1,\ldots,j_\alpha=1}^{3}\left(\sum_{\sigma\in\Sigma_\alpha}\prod_{k=1}^{\frac{\alpha}{2}}\delta_{j_{\sigma(2k-1)},j_{\sigma(2k)}}\right)\prod_{l=1}^{\alpha}R_{i_lj_l} \\ &= \frac{1}{\alpha!}\sum_{\sigma\in\Sigma_\alpha}\prod_{k=1}^{\frac{\alpha}{2}}\sum_{j_1,\ldots,j_\alpha=1}^{3}\delta_{j_{\sigma(2k-1)},j_{\sigma(2k)}}R_{i_{\sigma(2k-1)}j_{\sigma(2k-1)}}R_{i_{\sigma(2k)}j_{\sigma(2k)}} \\ &= \frac{1}{\alpha!}\sum_{\sigma\in\Sigma_\alpha}\prod_{k=1}^{\frac{\alpha}{2}}\sum_{j_1,\ldots,j_\alpha=1}^{3}R_{i_{\sigma(2k-1)}j_{\sigma(2k-1)}}R_{i_{\sigma(2k)}j_{\sigma(2k)}}.\end{aligned}$$

All the sums and products are finite, so we can interchange them. Using the orthogonality of $\boldsymbol{R}$ we obtain

$$\sum_{j_{\sigma(2k-1)}=1}^{3}\prod_{k=1}^{\frac{\alpha}{2}}R_{i_{\sigma(2k-1)}j_{\sigma(2k-1)}}R_{i_{\sigma(2k)}j_{\sigma(2k)}} = \langle R_{i_{\sigma(2k-1)}}, R_{i_{\sigma(2k)}}\rangle = \begin{cases}0, & \text{if } i_{\sigma(2k-1)} \neq i_{\sigma(2k)},\\ 1, & \text{if } i_{\sigma(2k-1)} = i_{\sigma(2k)}\end{cases}$$

and eventually,

$$(\boldsymbol{R} \triangleright \boldsymbol{M}_\alpha)_{i_1,\ldots,i_\alpha} = \frac{1}{\alpha!}\sum_{\sigma\in\Sigma_\alpha}\prod_{k=1}^{\frac{r}{2}}\delta_{i_{\sigma(2k-1)},i_{\sigma(2k)}} = (\boldsymbol{M}_\alpha)_{i_1,\ldots,i_\alpha}.$$

Applying this argument element-wise for all $\alpha \in \{\alpha_i\}_{i=1}^n$, yields the assertion. $\square$

For example in the case $\alpha = 4$, the tensor $\boldsymbol{M}_4$ can be written as

$$(\boldsymbol{M}_4)_{j_1,j_2,j_3,j_4} = \begin{cases}1, & \text{if } j_1 = j_2 = j_3 = j_4,\\ \frac{1}{3}, & \text{if pair-wise two indices are equal, but not all, i.e.} j_1 = j_2 = 1, j_3 = j_4 = 2,\\ 0, & \text{otherwise.}\end{cases}$$

Since, $\mathcal{E}^{\boldsymbol{\alpha}}_{\boldsymbol{u},\mathcal{S}}$ is an SO(3)-equivariant map, any rotationally invariant subspace is orthogonal to the image of the embedding $\mathcal{E}^{\boldsymbol{\alpha}}_{\boldsymbol{u},\mathcal{S}}(\mathrm{SO}(3))$. More precisely, we have the following result:

Lemma 7. *Let $\alpha \in \mathbb{N}$ and $\boldsymbol{R} \in \mathrm{SO}(3)$ be an arbitrary rotation. Then the inner product between $\mathcal{E}^{\alpha}_{\boldsymbol{u}}(\boldsymbol{R})$ and $\boldsymbol{M}_\alpha$ computes to*

$$\left\langle \mathcal{E}^{\alpha}_{\boldsymbol{u}}(\boldsymbol{R}), \boldsymbol{M}_\alpha \right\rangle = 1.$$

Proof. We can rewrite the definition of $\mathbf{M}_\alpha$ for even α to

$$\boldsymbol{M}_\alpha = \frac{1}{\alpha!} \sum_{\sigma \in \Sigma_\alpha} \delta_{j_{\sigma(1)},j_{\sigma(2)}} \cdot \delta_{j_{\sigma(3)},j_{\sigma(4)}} \cdots \delta_{j_{\sigma(\alpha-1)},j_{\sigma(\alpha)}} = \frac{1}{\alpha!} 2^{\frac{\alpha}{2}} \left(\frac{\alpha}{2}\right)! \underbrace{\left(\delta_{j_1,j_2} \cdot \delta_{j_3,j_4} \cdots \delta_{j_{\alpha-1},j_\alpha} + \cdots\right)}_{(\alpha-1)(\alpha-3)\cdots 1 \text{ summands}}. \tag{4}$$

The product of the δ is 1 only, if pairwise two j_i are equal. Hence, we obtain the following for the scalar product if $\boldsymbol{v} = (v_1, v_2, v_3)^\top = \boldsymbol{R}\boldsymbol{u}$

$$\left\langle \mathcal{E}^{\alpha}_{\boldsymbol{u}}(\boldsymbol{R}), \boldsymbol{M}_\alpha \right\rangle = \langle \otimes^\alpha (\boldsymbol{R}\boldsymbol{u}), \boldsymbol{M}_\alpha \rangle = \sum_{\substack{i,j,k \\ 2i+2j+2k=\alpha}} a(i,j,k) v_1^{2i} v_2^{2j} v_3^{2k}$$

with coefficients $a(i,j,k)$. These coefficients have to be determined:

$$\begin{aligned} a(i,j,k) &= \underbrace{\frac{1}{\alpha!} 2^{\frac{\alpha}{2}} \left(\frac{\alpha}{2}\right)!}_{\text{factor in (4)}} \underbrace{\binom{\alpha}{2i}\binom{\alpha-2i}{2j}\binom{\alpha-2i-2j}{2k}}_{\text{number of entries}} \\ &\quad \times \underbrace{(2i-1)(2i-3)\cdots 1 \cdot (2j-1)(2j-3)\cdots 1 \cdot (2k-1)(2k-3)\cdots 1}_{\text{number of summands unequal to 0 in (4)}} \\ &= \left(\frac{\alpha}{2}\right)! \frac{2^i(2i-1)(2i-3)\cdots 1}{(2i)!} \frac{2^j(2j-1)(2j-3)\cdots 1}{(2j)!} \frac{2^k(2k-1)(2k-3)\cdots 1}{(2k)!} = \left(\frac{\alpha}{2}\right)! \frac{1}{i!j!k!} = \binom{\frac{\alpha}{2}}{i,j,k}. \end{aligned}$$

with the multinomial theorem it follows that $\langle \otimes^\alpha \boldsymbol{v}, \boldsymbol{M}_\alpha \rangle = (v_1^2 + v_2^2 + v_3^2)^\alpha = 1$. $\square$

The previous lemma states that the embedded manifold is contained in the affine subspace of all $\boldsymbol{x} \in \mathbb{R}^{3^{\boldsymbol{\alpha}}}$ with $\langle \boldsymbol{x}, \boldsymbol{M}_\alpha \rangle = 1$. Next we want to shift the embedding into the corresponding linear subspace. To this end we need to compute the Frobenius norms $\|\boldsymbol{M}_\alpha\|_F$ of the invariant tensors $\boldsymbol{M}_\alpha$.

Lemma 8. *Let $\alpha \in 2\mathbb{N}$. Then the Frobenius norm of the tensor $\boldsymbol{M}_\alpha$ satisfies*

$$\|\boldsymbol{M}_\alpha\|_F^2 = \langle \boldsymbol{M}_\alpha, \boldsymbol{M}_\alpha \rangle = \alpha + 1.$$

Proof. We use the formulation for the tensor $\boldsymbol{M}_\alpha$ from Eq. (4). Let $i_1, i_2, i_3 \in \{0, 1, 2, \ldots, \frac{\alpha}{2}\}$ with $i_1 + i_2 + i_3 = \frac{\alpha}{2}$ such that

$$\begin{aligned} j_1, \ldots, j_{2i_1} &= 1, \\ j_{2i_1+1}, \ldots, j_{2i_1+2i_2} &= 2, \\ j_{2i_1+2i_2+1}, \ldots, j_{2i_1+2i_2+2i_3} &= 3. \end{aligned}$$

The corresponding entry in $\boldsymbol{M}_\alpha$ is

$$\begin{aligned} (\boldsymbol{M}_\alpha)_{j_1,\ldots,j_\alpha} &= \frac{1}{\alpha!} 2^{\frac{\alpha}{2}} \left(\frac{\alpha}{2}\right)! (2i_1-1)(2i_1-3)\cdots 1\,(2i_2-1)(2i_2-3)\cdots 1(2i_3-1)(2i_3-3)\cdots 1 \\ &= \frac{1}{\alpha!} \binom{\frac{\alpha}{2}}{i_1, i_2, i_3} (2i_1)!\,(2i_2)!\,(2i_3)! = \frac{(\frac{\alpha}{2})!\,(2i_1)!\,(2i_2)!\,(2i_3)!}{\alpha!\,i_1!\,i_2!\,i_3!}. \end{aligned}$$

The values in $\boldsymbol{M}_\alpha$ are equal, no matter which j_i are 1 and similarly for i_2 and i_3. Hence, there are $\binom{\alpha}{2i_1,2i_2,2i_3}$ such entries in $\boldsymbol{M}_\alpha$. Overall we obtain

$$\begin{aligned}
\|\boldsymbol{M}_\alpha\|_F^2 &= \sum_{\substack{i_1,i_2,i_3=0\\ i_1+i_2+i_3=\frac{\alpha}{2}}}^{\frac{\alpha}{2}} \binom{\alpha}{2i_1,2i_2,2i_3} \left(\frac{(\frac{\alpha}{2})!\,(2i_1)!\,(2i_2)!\,(2i_3)!}{\alpha!\,i_1!\,i_2!\,i_3!}\right)^2 \\
&= \sum_{\substack{i_1,i_2,i_3=0\\ i_1+i_2+i_3=\frac{\alpha}{2}}}^{\frac{\alpha}{2}} \frac{\alpha!}{(2i_1)!\,(2i_2)!\,(2i_3)!} \left(\frac{(\frac{\alpha}{2})!^2\,(2i_1)!^2\,(2i_2)!^2\,(2i_3)!^2}{\alpha!^2\,i_1!^2\,i_2!^2\,i_3!^2}\right) \\
&= \sum_{\substack{i_1,i_2,i_3=0\\ i_1+i_2+i_3=\frac{\alpha}{2}}}^{\frac{\alpha}{2}} \left(\frac{(\frac{\alpha}{2})!^2\,(2i_1)!\,(2i_2)!\,(2i_3)!}{\alpha!\,i_1!^2\,i_2!^2\,i_3!^2}\right) = \frac{1}{\binom{\alpha}{\frac{\alpha}{2}}} \sum_{\substack{i_1,i_2,i_3=0\\ i_1+i_2+i_3=\frac{\alpha}{2}}}^{\frac{\alpha}{2}} \binom{2i_1}{i_1}\binom{2i_2}{i_2}\binom{2i_3}{i_3}.
\end{aligned}$$

With Lemma 24 follows the assertion. □

The previous lemmata motivate to shift the embeddings for even α by a multiple of $\boldsymbol{M}_\alpha$ to reduce the dimension of the embedding space.

Theorem 9. *Let $\mathcal{E}^{\boldsymbol{\alpha}}_{\boldsymbol{u},\mathcal{S}}\colon \mathrm{SO}(3)/\mathcal{S} \to \mathbb{R}^{3^{\boldsymbol{\alpha}}}$ be the embedding defined in Definition 2. Then the image of the centered embedding*

$$\tilde{\mathcal{E}}^{\boldsymbol{\alpha}}_{\boldsymbol{u},\mathcal{S}}([\boldsymbol{O}]_\mathcal{S}) = \mathcal{E}^{\boldsymbol{\alpha}}_{\boldsymbol{u},\mathcal{S}}([\boldsymbol{O}]_\mathcal{S}) - \left(\frac{1}{\alpha_1+1}\boldsymbol{M}_{\alpha_1}, \ldots, \frac{1}{\alpha_n+1}\boldsymbol{M}_{\alpha_n}\right)$$

is contained in a linear subspace of $\mathbb{R}^{3^\alpha}$ of dimension

$$\sum_{i=1}^{n}\binom{\alpha_i+2}{\alpha_i} - \sum_{i=1}^{n}(\alpha_i + 1 \bmod 2)\,.$$

Proof. By Definition 1 all components $\boldsymbol{T}^j \in \mathbb{R}^{3^{\alpha_j}}$ of the embedding $\boldsymbol{T} = (\boldsymbol{T}^1, \ldots, T^n) = \mathcal{E}^{\boldsymbol{\alpha}}_{\boldsymbol{u}}(\boldsymbol{R})$ of an arbitrary rotation $\boldsymbol{R} \in \mathrm{SO}(3)$ are symmetric tensors, i.e., $\boldsymbol{T}^j_{i_1,\ldots,i_{\alpha_j}} = \boldsymbol{T}^j_{\sigma(i_1),\ldots,\sigma(i_{\alpha_j})}$ for any permutation σ of $\{1,\ldots,\alpha_j\}$.

The linear space $S^\alpha(\mathbb{R}^3)$ of the symmetric α-tensors has the dimension $\binom{\alpha+2}{\alpha}$, cf. [6, 3.4]. Thus the images $\mathcal{E}^{\boldsymbol{\alpha}}_{\boldsymbol{u}}(\mathrm{SO}(3))$ are contained in a subspace of $\mathbb{R}^{3^{\boldsymbol{\alpha}}}$ with dimension $\sum_{i=1}^n \binom{\alpha_i+2}{\alpha_i}$. For even α the image $\mathcal{E}^\alpha_{\boldsymbol{u}}(\mathrm{SO}(3))$ is orthogonal to $\boldsymbol{M}_\alpha$, since for $\boldsymbol{R} \in \mathrm{SO}(3)$

$$\langle \tilde{\mathcal{E}}^\alpha_{\boldsymbol{u}}(\boldsymbol{R}), \boldsymbol{M}_\alpha\rangle = \langle \mathcal{E}^\alpha_{\boldsymbol{u}}(\boldsymbol{R}) - \frac{1}{\alpha+1}\boldsymbol{M}_\alpha, \boldsymbol{M}_\alpha\rangle = \langle \mathcal{E}^\alpha_{\boldsymbol{u}}(\boldsymbol{R}), \boldsymbol{M}_\alpha\rangle - \frac{1}{\alpha+1}\langle \boldsymbol{M}_\alpha, \boldsymbol{M}_\alpha\rangle = 0.$$

Hence, the image $\tilde{\mathcal{E}}^\alpha_{\boldsymbol{u}}(\mathrm{SO}(3))$ is contained in a hyperplane of the symmetric tensors in $\mathbb{R}^{3^\alpha}$ for every even component. Thus, we can reduce the dimension of every component with even α by 1. The symmetrization with the symmetry group $\mathcal{S}$ does not change the dimensions. Hence, the images $\tilde{\mathcal{E}}^{\boldsymbol{\alpha}}_{\boldsymbol{u},\mathcal{S}}(\mathrm{SO}(3)/\mathcal{S})$ have dimension

$$\sum_{i=1}^{n}\binom{\alpha_i+2}{\alpha_i} - \sum_{i=1}^{n}(\alpha_i + 1 \bmod 2)\,. \quad \square$$

In [2] the authors were especially interested in embeddings of the rotation group modulo crystallographic point groups. These consist of the cyclic groups C_k, and the dihedral groups D_k with $k \in \{1, 2, 3, 4, 6\}$, the tetrahedral group T and the octahedral group O. For all the corresponding quotients Table 1 lists specific choices of the parameters $\boldsymbol{\alpha} \in \mathbb{R}^n$ and $\boldsymbol{u}_1, \ldots, \boldsymbol{u}_n \in \mathbb{R}^3$ such that the generic embeddings $\tilde{\mathcal{E}}^{\boldsymbol{\alpha}}_{\boldsymbol{u},\mathcal{S}}$ coincide with the embeddings reported in Table 2 of [2]. Here we assume the major rotational axis in C_k, D_k and Y to be parallel to $\boldsymbol{e}_1$. For O, T the three-fold axis is assumed to be parallel to $(1, 1, 1)^\top$.

It is important to note that at this point we have not yet proven that the mappings $\tilde{\mathcal{E}}^{\boldsymbol{\alpha}}_{\boldsymbol{u},\mathcal{S}}$ are indeed embeddings, i.e., that they are injective. This will be done in Section 3.1, where we shall prove that with some modifications they are even local isometries.

2.3. Centered measure

Since SO(3) is a Lie group it can be equipped with an unique left invariant Haar measure μ. In order to define a corresponding left invariant measure on the homogeneous space $\mathrm{SO}(3)/\mathcal{S}$ we consider the quotient mapping

$$\pi\colon \mathrm{SO}(3) \to \mathrm{SO}(3)/\mathcal{S}, \quad \pi(\boldsymbol{R}) = [\boldsymbol{R}]_\mathcal{S}$$

Table 1
Choices of the vectors $\boldsymbol{u}$ and the parameter $\boldsymbol{\alpha}$ such that the embeddings $\tilde{\mathcal{E}}^{\boldsymbol{\alpha}}_{\boldsymbol{u},\mathcal{S}}: \mathrm{SO}(3)/\mathcal{S} \to \mathbb{R}^{3^{\boldsymbol{\alpha}}}$ as defined in Theorem 9 coincides with the embeddings reported in Table 2 of [2] for all finite subgroups $\mathcal{S}$ of the rotation group SO(3).

$\mathcal{S}$	$\boldsymbol{u}$	$\boldsymbol{\alpha}$	Dimension
C_1	$(\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3)$	(1,1,1)	9
C_2	$(\boldsymbol{e}_1, \boldsymbol{e}_2)$	(1,2)	8
C_α (α even, $\alpha \geq 4$)	$(\boldsymbol{e}_1, \boldsymbol{e}_2)$	$(1, \alpha)$	$\frac{(\alpha+2)(\alpha+1)}{2} + 2$
C_α (α odd, $\alpha \geq 3$)	$(\boldsymbol{e}_1, \boldsymbol{e}_2)$	$(1, \alpha)$	$\frac{(\alpha+2)(\alpha+1)}{2} + 3$
D_2	$(\boldsymbol{e}_1, \boldsymbol{e}_2)$	(2,2)	10
D_α (α even, $\alpha \geq 4$)	$\boldsymbol{e}_1$	α	$\frac{(\alpha+2)(\alpha+1)}{2} - 1$
D_α (α odd, $\alpha \geq 3$)	$\boldsymbol{e}_1$	α	$\frac{(\alpha+2)(\alpha+1)}{2}$
O	$\boldsymbol{e}_1$	4	14
T	$\boldsymbol{e}_1$	3	10
Y	$\boldsymbol{e}_1$	10	66

that maps every rotation $\boldsymbol{R} \in \mathrm{SO}(3)$ onto its coset $[\boldsymbol{R}]_\mathcal{S} \in \mathrm{SO}(3)/\mathcal{S}$. Together with the Haar measure the quotient mapping defines a left invariant measure $\mu_\mathcal{S}$ on the quotient $\mathrm{SO}(3)/\mathcal{S}$ via

$$\mu_\mathcal{S}(A) = \mu(\pi^{-1}(A)), \quad \text{for any measurable set } A \subset \mathrm{SO}(3)/\mathcal{S}.$$

Accordingly, any embedding $\mathcal{E}: \mathrm{SO}(3)/\mathcal{S} \to \mathbb{R}^{3^{\boldsymbol{\alpha}}}$ defines a push forward measure $\mathcal{E} \circ \mu_\mathcal{S}$ on $\mathbb{R}^{3^{\boldsymbol{\alpha}}}$ via

$$\mathcal{E} \circ \mu_\mathcal{S}(B) = \mu_\mathcal{S}(\mathcal{E}^{-1}(B)), \quad \text{for any measurable set } B \subset \mathbb{R}^{3^{\boldsymbol{\alpha}}}.$$

In the following theorem we prove that for the centered embedding $\tilde{\mathcal{E}}^{\boldsymbol{\alpha}}_{\boldsymbol{u},\mathcal{S}}([\boldsymbol{O}]_\mathcal{S})$ the push forward measure $\tilde{\mathcal{E}}^{\boldsymbol{\alpha}}_{\boldsymbol{u},\mathcal{S}}([\boldsymbol{O}]_\mathcal{S}) \circ \mu_\mathcal{S}$ is centered in $\mathbb{R}^{3^{\boldsymbol{\alpha}}}$.

Theorem 10. *Let $\mathcal{E}^{\boldsymbol{\alpha}}_{\boldsymbol{u},\mathcal{S}}: \mathrm{SO}(3)/\mathcal{S} \to \mathbb{R}^{3^{\boldsymbol{\alpha}}}$ be the embedding defined in Definition 2 and let μ be the Haar measure on SO(3). Then the centered embedding $\tilde{\mathcal{E}}^{\boldsymbol{\alpha}}_{\boldsymbol{u},\mathcal{S}}([\boldsymbol{O}]_\mathcal{S})$ is an SO(3)-equivariant map with*

$$\|\tilde{\mathcal{E}}^{\boldsymbol{\alpha}}_{\boldsymbol{u},\mathcal{S}}([\boldsymbol{O}]_\mathcal{S})\| = const, \quad [\boldsymbol{O}]_\mathcal{S} \in \mathrm{SO}(3)/\mathcal{S}$$

and satisfies that the push forward measure $\tilde{\mathcal{E}}^{\alpha}_{\boldsymbol{u},\mathcal{S}} \circ \mu_\mathcal{S}$ is centered as well, i.e., its first moment satisfies

$$\mathbb{E}\mathcal{E}^{\tilde{\alpha}}_{\boldsymbol{u},\mathcal{S}} \circ \mu_\mathcal{S} = 0.$$

Proof. The SO(3)-equivariant-map-property follows from Theorem 4 together with Lemma 6. For $\boldsymbol{R} \in \mathrm{SO}(3)$ and $\boldsymbol{O} \in \mathrm{SO}(3)/\mathcal{S}$ there holds

$$\tilde{\mathcal{E}}^{\boldsymbol{\alpha}}_{\boldsymbol{u},\mathcal{S}}(\boldsymbol{R} \triangleright [\boldsymbol{O}]_\mathcal{S}) = \mathcal{E}^{\boldsymbol{\alpha}}_{\boldsymbol{u},\mathcal{S}}(\boldsymbol{R} \triangleright [\boldsymbol{O}]_\mathcal{S}) - \boldsymbol{M}_{\boldsymbol{\alpha}} = \boldsymbol{R} \triangleright \mathcal{E}^{\boldsymbol{\alpha}}_{\boldsymbol{u},\mathcal{S}}([\boldsymbol{O}]_\mathcal{S}) - \boldsymbol{R} \triangleright \boldsymbol{M}_{\boldsymbol{\alpha}} = \boldsymbol{R} \triangleright \tilde{\mathcal{E}}^{\boldsymbol{\alpha}}_{\boldsymbol{u},\mathcal{S}}([\boldsymbol{O}]_\mathcal{S}).$$

Assume $\boldsymbol{R}$ to be distributed according to the Haar measure on SO(3). Then $\boldsymbol{Ru}$ is distributed according to the spherical Borel measure σ normalized to $\sigma(\mathbb{S}^2) = 1$ for any $\boldsymbol{u} \in \mathbb{S}^2$. For the inner products with any vector $\boldsymbol{v} \in \mathbb{S}^2$ we calculate

$$\langle \mathbb{E}(\otimes^\alpha \boldsymbol{Ru}), \otimes^\alpha \boldsymbol{v}\rangle = \mathbb{E}\langle \otimes^\alpha \boldsymbol{Ru}, \otimes^\alpha \boldsymbol{v}\rangle = \mathbb{E}((\boldsymbol{Ru})^\top \boldsymbol{v})^\alpha = \int_{\mathbb{S}^2} (\boldsymbol{\xi}^\top \boldsymbol{v})^\alpha \mathrm{d}\sigma(\boldsymbol{\xi}) = \begin{cases} 0, & \text{if } \alpha \text{ odd}, \\ \frac{1}{\alpha+1}, & \text{if } \alpha \text{ even}. \end{cases}$$

If α is odd, the assertion follows directly, because $\boldsymbol{M}_\alpha = \boldsymbol{0}$ in this case. By Lemma 7 we have for even α

$$\langle \mathbb{E}\tilde{\mathcal{E}}^\alpha_{\boldsymbol{u}}(\boldsymbol{R}), \otimes^\alpha \boldsymbol{v}\rangle = \langle \mathbb{E}(\otimes^\alpha(\boldsymbol{Ru}) - \frac{1}{\alpha+1}\boldsymbol{M}_\alpha), \otimes^\alpha \boldsymbol{v}\rangle = \mathbb{E}\langle \otimes^\alpha(\boldsymbol{Ru}) - \frac{1}{\alpha+1}\boldsymbol{M}_\alpha, \otimes^\alpha \boldsymbol{v}\rangle = \mathbb{E}\left(((\boldsymbol{Ru})^\top \boldsymbol{v})^\alpha\right) - \frac{1}{\alpha+1} = 0.$$

Thanks to the rotational invariance of the tensors $\boldsymbol{M}_\alpha$ the image of centered embedding is also contained in a sphere. □

2.4. Projection onto the embedding

A central operation of embedding-based methods is projecting a point of the vector space back onto the manifold. For our embeddings $\mathcal{E}: \mathrm{SO}(3)/\mathcal{S} \to \mathbb{R}^{3^{\boldsymbol{\alpha}}}$ this means that for an arbitrary tensor $\boldsymbol{T} \in \mathbb{R}^{3^{\boldsymbol{\alpha}}}$ we ask for the rotation $[\boldsymbol{R}^*]_\mathcal{S} \in \mathrm{SO}(3)/\mathcal{S}$ with minimum distance $\left\|\mathcal{E}(\boldsymbol{R}^*) - \boldsymbol{T}\right\|$ in the embedding. This problem has a unique solution whenever $\boldsymbol{T}$ is sufficiently close to the submanifold, cf. [17].

Since, by Corollary 5, the submanifold $\mathcal{E}^{\boldsymbol{\alpha}}_{\boldsymbol{u},\mathcal{S}}(\mathrm{SO}(3)/\mathcal{S}) \subset \mathbb{R}^{3^{\boldsymbol{\alpha}}}$ is contained in a sphere, i.e., has constant norm, the above minimization problem is equivalent to the maximization problem

$$[\boldsymbol{R}^*]_\mathcal{S} = \operatorname*{argmax}_{\boldsymbol{R} \in \mathrm{SO}(3)/\mathcal{S}} J(\boldsymbol{R}), \quad J(\boldsymbol{R}) = \left\langle \mathcal{E}^{\boldsymbol{\alpha}}_{\boldsymbol{u},\mathcal{S}}(\boldsymbol{R}), \boldsymbol{T}\right\rangle. \tag{5}$$

For the symmetry group C_1, i.e. no symmetry, $\boldsymbol{u} = (\boldsymbol{u}_1, \dots, \boldsymbol{u}_n)$, $\boldsymbol{\alpha} = (1, \dots, 1) \in \mathbb{R}^n$ and $\boldsymbol{T} = (\boldsymbol{T}_1, \dots, \boldsymbol{T}_n) \in \mathbb{R}^{3\times n}$ the functional $J\colon \mathrm{SO}(3) \to \mathbb{R}$ simplifies to

$$J(\boldsymbol{R}) = \sum_{i=1}^{n} \langle \boldsymbol{R}\boldsymbol{u}_i, \boldsymbol{T}_i \rangle .$$

An explicit formula for its maximum is known as the Kabsch Algorithm [13].

Lemma 11. *Let $\boldsymbol{u}_1, \dots, \boldsymbol{u}_n, \boldsymbol{v}_1, \dots, \boldsymbol{v}_n \in \mathbb{R}^3$ be two lists of vectors. Then the solution of the maximization problem*

$$\sum_{i=1}^{n} \langle \boldsymbol{R}\boldsymbol{u}_i, \boldsymbol{v}_i \rangle \to \max, \quad \boldsymbol{R} \in \mathrm{SO}(3)$$

is given by

$$\boldsymbol{R} = \boldsymbol{V} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \det \boldsymbol{V}\boldsymbol{U}^T \end{pmatrix} \boldsymbol{U}^T,$$

where $\boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^T = \boldsymbol{H}$ is the singular value decomposition of the 3×3-matrix $\boldsymbol{H} = \sum_{i=1}^n \boldsymbol{u}_i \otimes \boldsymbol{v}_i$.

In the case of arbitrary symmetry groups and a general embedding $\mathcal{E}^{\boldsymbol{\alpha}}_{\boldsymbol{u},\mathcal{S}}$ we are not able to give such a closed form solution. For this reason, we propose to solve the maximization problem in (5) numerically using a manifold gradient method [23]. The next theorem provides an explicit formula for the required gradient of J.

Theorem 12. *Let $\boldsymbol{T} \in \mathbb{R}^{3^\alpha}$, $\boldsymbol{R} \in \mathrm{SO}(3)$, $\boldsymbol{s}$ be an arbitrary skew-symmetric matrix and hence, $\boldsymbol{s}\boldsymbol{R} \in T_{\boldsymbol{R}}\mathrm{SO}(3)$ a tangential vector at $\boldsymbol{R}$. Then the gradient of J in direction $\boldsymbol{s}\boldsymbol{R}$ is given by the inner product*

$$\nabla_{\boldsymbol{s}\boldsymbol{R}} J(\boldsymbol{R}) = \alpha \,\langle \boldsymbol{s} \rhd_1 (\boldsymbol{R} \rhd \boldsymbol{E}), \boldsymbol{T} \rangle$$

where $\boldsymbol{E} = \mathcal{E}^{\alpha}_{\boldsymbol{u}}(\boldsymbol{I}) \in \mathbb{R}^{3^\alpha}$ denotes the embedding of the identity matrix and $\rhd_1$ denotes the multiplication of the matrix $\boldsymbol{s}$ with a tensor $\boldsymbol{T} \in \mathbb{R}^{3^\alpha}$ with respect to the first dimension of $\boldsymbol{T}$, i.e.,

$$[\boldsymbol{s} \rhd_1 \boldsymbol{T}]_{k_1,\dots,k_\alpha} = \sum_{\ell_1=1}^{3} \boldsymbol{s}_{k_1\ell_1} \boldsymbol{T}_{\ell_1,k_2,\dots,k_\alpha}.$$

Proof. First of all we note that by Theorem 4 the functional J can be written as

$$J(\boldsymbol{R}) = \langle \boldsymbol{R} \rhd \boldsymbol{E}, \boldsymbol{T} \rangle, \quad \boldsymbol{R} \in \mathrm{SO}(3).$$

Considering now a tangential vector $\boldsymbol{s}\boldsymbol{R} \in T_{\boldsymbol{R}}\mathrm{SO}(3)$ the corresponding directional derivative is

$$\nabla_{\boldsymbol{s}\boldsymbol{R}} J(\boldsymbol{R}) = \lim_{h\to 0} \frac{1}{h}\Big(\langle (\boldsymbol{R} + h\boldsymbol{s}\boldsymbol{R}) \rhd \boldsymbol{E}, \boldsymbol{T} \rangle - \langle \boldsymbol{R} \rhd \boldsymbol{E}, \boldsymbol{T} \rangle \Big) = \lim_{h\to 0} \frac{1}{h}\Big\langle \big(\otimes^{\alpha}(\boldsymbol{R} + h\boldsymbol{s}\boldsymbol{R}) - \otimes^{\alpha}\boldsymbol{R}\big)\boldsymbol{E}, \boldsymbol{T} \Big\rangle.$$

In the difference of the tensor products only the terms with h^1 remain, as all terms with higher power of h converge to zero. Since the tensor $\boldsymbol{E}$ is symmetric the derivative simplifies further to

$$\nabla_{\boldsymbol{s}\boldsymbol{R}} J(\boldsymbol{R}) = \sum_{i=0}^{\alpha-1} \Big\langle \big(\otimes^{i}\boldsymbol{R} \otimes \boldsymbol{s}\boldsymbol{R} \otimes^{\alpha-1-i} \boldsymbol{R}\big)\, \boldsymbol{E}, \boldsymbol{T} \Big\rangle = \alpha \,\langle \boldsymbol{s} \rhd_1 (\boldsymbol{R} \rhd \boldsymbol{E}), \boldsymbol{T} \rangle . \quad \square$$

Remark. In the theorem above, we considered only the case $\alpha \in \mathbb{R}$, i.e. $n = 1$. For the case with multiple components, we have to sum over all components in the function

$$J(\boldsymbol{R}) = \sum_{i=1}^{n} \Big\langle \mathcal{E}^{\alpha_i}_{\boldsymbol{u}_i}(\boldsymbol{R}), \boldsymbol{T}_i \Big\rangle,$$

as well as in the gradient

$$\nabla_{\boldsymbol{s}\boldsymbol{R}} J(\boldsymbol{R}) = \sum_{i=1}^{n} \alpha_i \Big\langle \boldsymbol{s} \rhd_1 (\boldsymbol{R} \rhd \mathcal{E}^{\alpha_i}_{\boldsymbol{u}_i}(\boldsymbol{I})), \boldsymbol{T}_i \Big\rangle .$$

3. Distance preservation

In this section we are going to investigate how well the embeddings defined in Section 2.1 preserve the geodesic distance between any two rotations. While the rotation group SO(3) as a submanifold of $\mathbb{R}^{3\times 3}$ inherits a canonical Riemannian structure it differs by the factor $\sqrt{2}$ from the commonly used geodesic distance

$$d(\boldsymbol{O}_1, \boldsymbol{O}_2) = \arccos\left(\frac{1}{2}\left(-1 + \operatorname{tr}(\boldsymbol{O}_1^\top \boldsymbol{O}_2)\right)\right) \tag{6}$$

on the rotation group, which has the nice interpretation of being the angle of rotation between the two rotations $\boldsymbol{O}_1, \boldsymbol{O}_2 \in \mathrm{SO}(3)$. For cosets $[\boldsymbol{O}_1]_{\mathcal{S}}, [\boldsymbol{O}_2]_{\mathcal{S}} \in \mathrm{SO}(3)/\mathcal{S}$ the geodesic distance (6) becomes

$$d([\boldsymbol{O}_1]_{\mathcal{S}}, [\boldsymbol{O}_2]_{\mathcal{S}}) = \min_{\boldsymbol{R}\in\mathcal{S}} d(\boldsymbol{O}_1\boldsymbol{R}, \boldsymbol{O}_2), \tag{7}$$

i.e., the minimum geodesic distance between any elements of the cosets $[\boldsymbol{O}_1]_S$ and $[\boldsymbol{O}_2]_S$. We first analyze this problem locally.

3.1. Locally isometric embeddings

Let us recall that a differentiable embedding $\mathcal{E}: \mathcal{M} \to \mathbb{R}^d$ is locally isometric if its differential $d\mathcal{E}: T_m\mathcal{M} \to T_{\mathcal{E}(m)}\mathcal{E}(\mathcal{M})$ at each point $m \in \mathcal{M}$ is an isometry between vector spaces. Since in our setting in both spaces, $\mathrm{SO}(3)/\mathcal{S}$ and $\mathbb{R}^{3^\alpha}$, the metric is invariant with respect to the action $\triangleright$ of SO(3) and the embedding is an SO(3)-equivariant map, it suffices to prove isometry at the identity $[\boldsymbol{I}]_{\mathcal{S}} \in \mathrm{SO}(3)/\mathcal{S}$ only.

In order to identify locally isometric embeddings within our framework we need to generalize it slightly by multiplying the components by different weights $\boldsymbol{\beta} = (\beta_1, \dots, \beta_n) \in \mathbb{R}^n$, i.e., we define

$$\mathcal{E}_{\boldsymbol{u}}^{\boldsymbol{\alpha},\boldsymbol{\beta}}(\boldsymbol{R}) = (\beta_1 \otimes^{\alpha_1} \boldsymbol{R}\boldsymbol{u}_1, \dots, \beta_n \otimes^{\alpha_n} \boldsymbol{R}\boldsymbol{u}_n)$$

together with its symmetrization

$$\mathcal{E}_{\boldsymbol{u},\mathcal{S}}^{\boldsymbol{\alpha},\boldsymbol{\beta}}: \mathrm{SO}(3)/\mathcal{S} \to \mathbb{R}^{3^{\boldsymbol{\alpha}}}, \qquad \mathcal{E}_{\boldsymbol{u},\mathcal{S}}^{\boldsymbol{\alpha},\boldsymbol{\beta}}([\boldsymbol{O}]_{\mathcal{S}}) = \frac{1}{|\mathcal{S}|}\sum_{\boldsymbol{S}\in\mathcal{S}} \mathcal{E}_{\boldsymbol{u}}^{\boldsymbol{\alpha},\boldsymbol{\beta}}(\boldsymbol{O}\boldsymbol{S}). \tag{8}$$

Choosing the weights $\boldsymbol{\beta}$ carefully will allow us to explicitly define locally isometric embeddings for the quotients $\mathrm{SO}(3)/\mathcal{S}$ of SO(3) with respect to all crystallographic symmetry groups.

We shall analyze the derivative $d\mathcal{E}_{\boldsymbol{u},\mathcal{S}}^{\boldsymbol{\alpha},\boldsymbol{\beta}}([\boldsymbol{I}]_{\mathcal{S}})\boldsymbol{s}^{(k)}$ of the embedding with respect to the following orthogonal basis of the tangential space $T_{\boldsymbol{I}}\mathrm{SO}(3)$ given by the skew-symmetric matrices

$$\boldsymbol{s}^{(1)} = \begin{pmatrix} 0 & 0 & 0\\ 0 & 0 & -1\\ 0 & 1 & 0\end{pmatrix}, \quad \boldsymbol{s}^{(2)} = \begin{pmatrix} 0 & 0 & -1\\ 0 & 0 & 0\\ 1 & 0 & 0\end{pmatrix}, \quad \boldsymbol{s}^{(3)} = \begin{pmatrix} 0 & -1 & 0\\ 1 & 0 & 0\\ 0 & 0 & 0\end{pmatrix}.$$

The basis vectors $\boldsymbol{s}^{(1)}, \boldsymbol{s}^{(2)}, \boldsymbol{s}^{(3)}$ are normalized to $\sqrt{2}$, which is exactly the factor between the geodesic distance defined in (6) and the geodesic distance induced by the canonical embedding. Hence, we obtain the following characterization on local isometry.

Lemma 13. *The mapping $\mathcal{E}_{\boldsymbol{u},\mathcal{S}}^{\boldsymbol{\alpha},\boldsymbol{\beta}}: \mathrm{SO}(3)/\mathcal{S} \to \mathbb{R}^{3^{\boldsymbol{\alpha}}}$ as defined in (8) is locally isometric if and only if the vectors $d\mathcal{E}_{\boldsymbol{u},\mathcal{S}}^{\boldsymbol{\alpha},\boldsymbol{\beta}}([\boldsymbol{I}]_{\mathcal{S}})\boldsymbol{s}^{(k)}$ are orthonormal in $\mathbb{R}^{3^{\boldsymbol{\alpha}}}$.*

Proof. The mapping $d\mathcal{E}_{\boldsymbol{u},\mathcal{S}}^{\boldsymbol{\alpha},\boldsymbol{\beta}}([\boldsymbol{I}]_{\mathcal{S}})$ is linear and $\{\boldsymbol{s}^{(k)}\}_{k=1}^3$ is a basis in $T_{\boldsymbol{I}}\mathrm{SO}(3)$. Hence, $\mathcal{E}_{\boldsymbol{u},\mathcal{S}}^{\boldsymbol{\alpha},\boldsymbol{\beta}}$ is locally isometric if and only if the vectors $d\mathcal{E}_{\boldsymbol{u},\mathcal{S}}^{\boldsymbol{\alpha},\boldsymbol{\beta}}([\boldsymbol{I}]_{\mathcal{S}})\boldsymbol{s}^{(k)}$ are orthonormal in the tangent space $T_{\mathcal{E}(\boldsymbol{I})}\mathbb{R}^{3^{\boldsymbol{\alpha}}}$. □

For the differential of the mapping $\mathcal{E}_{\boldsymbol{u},\mathcal{S}}^{\boldsymbol{\alpha}\boldsymbol{\beta}}$ we have the following lemma.

Lemma 14. *Let $\alpha \in \mathbb{N}$, $\boldsymbol{u} \in \mathbb{S}^2$ be an arbitrary direction and $\boldsymbol{s} \in T_{\boldsymbol{I}}\mathrm{SO}(3)$ be an arbitrary skew-symmetric matrix. Then*

$$d\mathcal{E}_{\boldsymbol{u}}^{\alpha}(\boldsymbol{I})\boldsymbol{s} = \sum_{i=0}^{\alpha-1} \left(\otimes^i \boldsymbol{u}\right) \otimes \boldsymbol{s}\boldsymbol{u} \otimes \left(\otimes^{\alpha-i-1}\boldsymbol{u}\right).$$

Proof. Let $\gamma(t)$ be a curve in SO(3) such that $\dot\gamma(0) = \boldsymbol{s}$ and $\gamma(0) = \boldsymbol{I}$. The image of the map $d\mathcal{E}_{\boldsymbol{u},\mathcal{S}}^{\boldsymbol{\alpha},\boldsymbol{\beta}}([\boldsymbol{I}]_{\mathcal{S}})$ of $\boldsymbol{s}$ is given by

$$d\mathcal{E}_{\boldsymbol{u}}^{\alpha}(\boldsymbol{I})\boldsymbol{s} = \frac{\mathrm{d}}{\mathrm{d}t}\left(\otimes^{\alpha}(\gamma(t)\cdot\boldsymbol{u})\right)\Big|_{t=0}.$$

Table 2
Choices of the vectors $\boldsymbol{u}$ and the parameters $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$ for important finite subgroups $\mathcal{S}$ of the rotation group SO(3) such that the embeddings $\tilde{\mathcal{E}}^{\boldsymbol{\alpha},\boldsymbol{\beta}}_{\boldsymbol{u},\mathcal{S}}\colon \mathrm{SO}(3)/\mathcal{S} \to \mathbb{R}^{3^{\alpha}}$ as defined in (8) are locally isometric. Parameters different from the embeddings defined in Table 2 of [2] are highlighted in magenta.

$\mathcal{S}$	$\boldsymbol{u}$	$\boldsymbol{\alpha}$	$\boldsymbol{\beta}$	Dimension
C_1	$(\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3)$	$(1, 1, 1)$	$(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$	9
C_2	$(\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3)$	$(1, 2, 2)$	$\left(\frac{1}{\sqrt{2}}, \frac{1}{2}, \frac{1}{2}\right)$	13
C_3	$(\boldsymbol{e}_1, \boldsymbol{e}_2)$	$(1, 3)$	$\left(\sqrt{\frac{5}{6}}, \frac{\sqrt{4}}{3}\right)$	13
C_4	$(\boldsymbol{e}_1, \boldsymbol{e}_2)$	$(1, 4)$	$(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$	17
C_6	$(\boldsymbol{e}_1, \boldsymbol{e}_2)$	$(1, 6)$	$\left(\frac{1}{\sqrt{12}}, \frac{2\sqrt{2}}{3}\right)$	30
D_2	$(\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3)$	$(2, 2, 2)$	$\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$	15
D_3	$(\boldsymbol{e}_1, \boldsymbol{e}_2)$	$(2, 3)$	$\left(\sqrt{\frac{5}{12}}, \frac{\sqrt{4}}{3}\right)$	15
D_4	$(\boldsymbol{e}_1, \boldsymbol{e}_2)$	$(2, 4)$	$\left(\frac{1}{2}, \frac{1}{\sqrt{2}}\right)$	19
D_6	$(\boldsymbol{e}_1, \boldsymbol{e}_2)$	$(2, 6)$	$\left(\frac{1}{\sqrt{24}}, \frac{2\sqrt{2}}{3}\right)$	32
O	$\boldsymbol{e}_1$	4	$\frac{3}{2\sqrt{2}}$	14
T	$\boldsymbol{e}_1$	3	$\frac{3}{2\sqrt{2}}$	10
Y	$\boldsymbol{e}_1$	10	$\frac{75}{8\sqrt{95}}$	66

With the chain rule it follows

$$d\mathcal{E}^{\alpha}_{\boldsymbol{u}}(\boldsymbol{I})\boldsymbol{s} = \sum_{i=0}^{\alpha-1} \left(\otimes^{i}(\gamma(t)\cdot \boldsymbol{u}) \otimes \dot{\gamma}(t)\boldsymbol{u} \otimes (\otimes^{\alpha-i-1}\gamma(t)\boldsymbol{u})\right)\Big|_{t=0} = \sum_{i=0}^{\alpha-1} \left(\otimes^{i}\boldsymbol{u}\right) \otimes \boldsymbol{s}\boldsymbol{u} \otimes \left(\otimes^{\alpha-i-1}\boldsymbol{u}\right). \quad \square$$

In the following we will find locally isometric embeddings for all crystallographic symmetry groups. Therefore, we will proceed as follows. First we consider the cyclic groups C_k, $k \in \mathbb{N}$, followed by the dihedral groups D_k, $k \in \mathbb{N}$ and finally the tetrahedral group T, the octahedral group O and the icosahedral group Y. The parameters for these locally isometric embeddings are summarized in Table 2. The differences to the embeddings in [2] are marked in magenta. For the cyclic and the dihedral groups we assume the major rotational axis to be aligned in $\boldsymbol{e}_1$-direction and the two-fold axis parallel to $\boldsymbol{e}_2$.

For the symmetry group C_1 the canonical embedding (2) of SO(3) in $\mathbb{R}^{3\times 3}$ is by definition locally isometric, up to the factor $\sqrt{2}$, so multiplication of all components with $\sqrt{2}^{-1}$ leads to local isometry. The symmetry group C_2 is a special case, because in contrast to C_k for $k > 2$ the vectors $\boldsymbol{O}\boldsymbol{e}_2$ for $\boldsymbol{O} \in C_k$ do not span the plane orthogonal to $\boldsymbol{e}_1$. For this reason we need to add an additional component in contrast to the embedding in [2].

Theorem 15. *Let $\boldsymbol{u} = (\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3)$, $\boldsymbol{\alpha} = (1, 2, 2)$ and $\boldsymbol{\beta} = (\frac{1}{\sqrt{2}}, \frac{1}{2}, \frac{1}{2})$. Then $\mathcal{E}^{\boldsymbol{\alpha},\boldsymbol{\beta}}_{\boldsymbol{u},C_2}$ is a locally isometric embedding.*

Proof. There holds

$$d\mathcal{E}^{\boldsymbol{\alpha},\boldsymbol{\beta}}_{\boldsymbol{u},C_2}([\boldsymbol{I}]_{C_2})\boldsymbol{s}^{(1)} = \left(\beta_1 \begin{pmatrix}0\\0\\0\end{pmatrix}, \beta_2 \begin{pmatrix}0&0&0\\0&0&1\\0&1&0\end{pmatrix}, \beta_3 \begin{pmatrix}0&0&0\\0&0&-1\\0&-1&0\end{pmatrix}\right),$$

$$d\mathcal{E}^{\boldsymbol{\alpha},\boldsymbol{\beta}}_{\boldsymbol{u},C_2}([\boldsymbol{I}]_{C_2})\boldsymbol{s}^{(2)} = \left(\beta_1 \begin{pmatrix}0\\0\\1\end{pmatrix}, \beta_2 \begin{pmatrix}0&0&0\\0&0&0\\0&0&0\end{pmatrix}, \beta_3 \begin{pmatrix}0&0&-1\\0&0&0\\-1&0&0\end{pmatrix}\right),$$

$$d\mathcal{E}^{\boldsymbol{\alpha},\boldsymbol{\beta}}_{\boldsymbol{u},C_2}([\boldsymbol{I}]_{C_2})\boldsymbol{s}^{(3)} = \left(\beta_1 \begin{pmatrix}0\\1\\0\end{pmatrix}, \beta_2 \begin{pmatrix}0&-1&0\\-1&0&0\\0&0&0\end{pmatrix}, \beta_3 \begin{pmatrix}0&0&0\\0&0&0\\0&0&0\end{pmatrix}\right).$$

These three vectors are orthogonal. To normalize them, we have to solve

$$2\beta_2^2 + 2\beta_3^2 = \beta_1^2 + 2\beta_3^2 = \beta_1^2 + 2\beta_2^2 = 1,$$

which yields $\beta_1 = \frac{1}{\sqrt{2}}$, $\beta_2 = \beta_3 = \frac{1}{2}$. $\square$

For the symmetry groups C_k for $k > 2$ we first show the orthogonality of the tangent vectors $d\mathcal{E}^{\boldsymbol{\alpha}}_{\boldsymbol{u},C_k}([\boldsymbol{I}]_{C_k})$.

Lemma 16. *Let $k \in \mathbb{N}$ with $k > 2$, $\boldsymbol{u} = (\boldsymbol{e}_1, \boldsymbol{e}_2)$ and $\boldsymbol{\alpha} = (1, k)$. Then the vectors $d\mathcal{E}^{\boldsymbol{\alpha}}_{\boldsymbol{u},C_k}$ are orthogonal.*

Proof. For the rank one component $d\mathcal{E}^{1,\beta_1}_{\boldsymbol{e}_1,C_k}([\boldsymbol{I}]_{C_k})$ of $d\mathcal{E}^{\boldsymbol{\alpha},\boldsymbol{\beta}}_{\boldsymbol{u},C_k}([\boldsymbol{I}]_{C_k})$ orthogonality follows from

$$d\mathcal{E}^{1,\beta_1}_{\boldsymbol{e}_1,C_k}([\boldsymbol{I}]_{C_k})\boldsymbol{s}^{(1)} = \boldsymbol{0}, \quad d\mathcal{E}^{1,\beta_1}_{\boldsymbol{e}_1,C_k}([\boldsymbol{I}]_{C_k})\boldsymbol{s}^{(2)} = \beta_1\boldsymbol{e}_3, \quad d\mathcal{E}^{1,\beta_1}_{\boldsymbol{e}_1,C_k}([\boldsymbol{I}]_{C_k})\boldsymbol{s}^{(3)} = \beta_1\boldsymbol{e}_2. \tag{9}$$

For the rank k component $d\mathcal{E}^{k,\beta_2}_{\boldsymbol{e}_2,C_k}([\boldsymbol{I}]_{C_k})$ we use Lemma 14 and define for $\ell \in \{1,2,3\}$

$$\boldsymbol{B}_\ell := d\mathcal{E}^{k}_{\boldsymbol{e}_2,C_k}([\boldsymbol{I}]_{C_k})\boldsymbol{s}^{(\ell)} = \sum_{i=0}^{k-1}\frac{1}{k}\sum_{j=0}^{i-1}\left(\otimes^i \boldsymbol{v}_j\right)\otimes \boldsymbol{s}^{(\ell)}\boldsymbol{v}_j \otimes \left(\otimes^{k-i-1}\boldsymbol{v}_j\right), \tag{10}$$

where the vectors $\boldsymbol{v}_j = (0, \cos\frac{2\pi j}{k}, \sin\frac{2\pi j}{k})^\top$ result from applying all symmetries from C_k to $\boldsymbol{e}_2$. The inner products between these rank k tensors $\boldsymbol{B}_\ell$, $\ell \in \{1,2,3\}$ are

$$\left\langle \boldsymbol{B}_{\ell_1}, \boldsymbol{B}_{\ell_2}\right\rangle = \frac{k(k-1)}{k^2}\sum_{j_1=0}^{k-1}\sum_{j_2=0}^{k-1}\left\langle \boldsymbol{v}_{j_1}, \boldsymbol{v}_{j_2}\right\rangle^{k-2}\left\langle \boldsymbol{s}^{(\ell_1)}\boldsymbol{v}_{j_1}, \boldsymbol{v}_{j_2}\right\rangle\left\langle \boldsymbol{s}^{(\ell_2)}\boldsymbol{v}_{j_2}, \boldsymbol{v}_{j_1}\right\rangle + \frac{k}{k^2}\sum_{j_1=0}^{k-1}\sum_{j_2=0}^{k-1}\left\langle \boldsymbol{v}_{j_1}, \boldsymbol{v}_{j_2}\right\rangle^{k-1}\left\langle \boldsymbol{s}^{(\ell_1)}\boldsymbol{v}_{j_1}, \boldsymbol{s}^{(\ell_2)}\boldsymbol{v}_{j_2}\right\rangle. \tag{11}$$

Using

$$\boldsymbol{s}^{(1)}\boldsymbol{v}_j = \begin{pmatrix} 0 \\ -\sin\frac{2\pi j}{k} \\ \cos\frac{2\pi j}{k}\end{pmatrix}, \quad \boldsymbol{s}^{(2)}\boldsymbol{v}_j = \begin{pmatrix} -\sin\frac{2\pi j}{k} \\ 0 \\ 0\end{pmatrix}, \quad \boldsymbol{s}^{(3)}\boldsymbol{v}_j = \begin{pmatrix} -\cos\frac{2\pi j}{k} \\ 0 \\ 0\end{pmatrix},$$

we observe for all j_1, j_2 and $\ell \in \{2,3\}$ the orthogonality $\left\langle \boldsymbol{s}^{(\ell)}\boldsymbol{v}_{j_1}, \boldsymbol{v}_{j_2}\right\rangle = 0$ and hence, the first double sum in (11) is zero whenever $\ell_1 \neq \ell_2$.

In the second double sum we have $\left\langle \boldsymbol{s}^{(\ell_1)}\boldsymbol{v}_{j_1}, \boldsymbol{s}^{(\ell_2)}\boldsymbol{v}_{j_2}\right\rangle = 0$ for all $\ell_1 \neq \ell_2$ except for the pair $\ell_1, \ell_2 \in \{2,3\}$. For this specific case we use the calculation in (B.1) and get

$$\langle \boldsymbol{B}_2, \boldsymbol{B}_3\rangle = \sum_{j_1,j_2=0}^{k-1}\left\langle \boldsymbol{v}_{j_1}, \boldsymbol{v}_{j_2}\right\rangle^{k-1}\left\langle \boldsymbol{s}^{(2)}\boldsymbol{v}_{j_1}, \boldsymbol{s}^{(3)}\boldsymbol{v}_{j_2}\right\rangle = \sum_{j_1,j_2=0}^{k-1}\cos^{k-1}\tfrac{2\pi(j_1-j_2)}{k}\sin\tfrac{2\pi j_1}{k}\cos\tfrac{2\pi j_2}{k} = 0. \quad \square$$

In order to prove $\left\| d\mathcal{E}^{\boldsymbol{\alpha},\boldsymbol{\beta}}_{\boldsymbol{u},C_k}([\boldsymbol{I}]_{C_k})\boldsymbol{s}^{(k)}\right\| = 1$ we continue by calculating $\|\boldsymbol{B}_\ell\|^2 = \langle \boldsymbol{B}_\ell, \boldsymbol{B}_\ell\rangle$ for $\ell \in \{1,2,3\}$.

Lemma 17. *For the tensors $\boldsymbol{B}_\ell$ defined in Eq. (10) we have*

$$\|\boldsymbol{B}_1\|^2 = \frac{k^2}{2^{k-1}},$$

$$\|\boldsymbol{B}_2\|^2 = \|\boldsymbol{B}_3\|^2 = \begin{cases}\frac{k}{2^k}, & \text{if } k \text{ is odd},\\ \frac{k}{2^{k+1}}\left(2+\binom{k}{\frac{k}{2}}\right), & \text{if } k \text{ is even}.\end{cases}$$

Proof. By Eq. (11) and the calculations in (B.2) we obtain

$$\begin{aligned}\|\boldsymbol{B}_1\|^2 &= \frac{(k-1)}{k}\sum_{j_1=0}^{k-1}\sum_{j_2=0}^{k-1}\left\langle \boldsymbol{v}_{j_1}, \boldsymbol{v}_{j_2}\right\rangle^{k-2}\left\langle \boldsymbol{s}^{(1)}\boldsymbol{v}_{j_1}, \boldsymbol{v}_{j_2}\right\rangle\left\langle \boldsymbol{s}^{(1)}\boldsymbol{v}_{j_2}, \boldsymbol{v}_{j_1}\right\rangle\frac{1}{k}\sum_{j_1=0}^{k-1}\sum_{j_2=0}^{k-1}\left\langle \boldsymbol{v}_{j_1}, \boldsymbol{v}_{j_2}\right\rangle^{k-1}\left\langle \boldsymbol{s}^{(1)}\boldsymbol{v}_{j_1}, \boldsymbol{s}^{(1)}\boldsymbol{v}_{j_2}\right\rangle\\ &= -\frac{(k-1)}{k}\sum_{j_1=0}^{k-1}\sum_{j_2=0}^{k-1}\cos^{k-2}\left(\frac{2\pi(j_1-j_2)}{k}\right)\sin^2\left(\frac{2\pi(j_1-j_2)}{k}\right)\\ &\quad+\frac{1}{k}\sum_{j_1=0}^{k-1}\sum_{j_2=0}^{k-1}\cos^{k-1}\left(\frac{2\pi(j_1-j_2)}{k}\right)\cos\left(\frac{2\pi(j_1-j_2)}{k}\right)\\ &= \frac{k^2}{2^{k-1}}.\end{aligned}$$

Next we investigate the tensor $\boldsymbol{B}_3$. With the calculations in (B.3) in the Appendix we get the following.

$$\begin{aligned}\|\boldsymbol{B}_3\|^2 &= \frac{1}{k}\sum_{j_1=0}^{k-1}\sum_{j_2=0}^{k-1}\left\langle \boldsymbol{v}_{j_1}, \boldsymbol{v}_{j_2}\right\rangle^{k-1}\left\langle \boldsymbol{s}^{(3)}\boldsymbol{v}_{j_1}, \boldsymbol{s}^{(3)}\boldsymbol{v}_{j_2}\right\rangle = \frac{1}{k}\sum_{j_1=0}^{k-1}\sum_{j_2=0}^{k-1}\cos^{k-1}\left(\frac{2\pi(j_1-j_2)}{k}\right)\cos\left(\frac{2\pi j_1}{k}\right)\cos\left(\frac{2\pi j_2}{k}\right)\\ &= \begin{cases}\frac{k}{2^k}, & \text{if } k \text{ is odd},\\ \frac{k}{2^{k+1}}\left(2+\binom{k}{\frac{k}{2}}\right), & \text{if } k \text{ is even}.\end{cases}\end{aligned}$$

For the norm $\|\boldsymbol{B}_2\|^2$ we only have to change some signs in the previous calculation and receive in the end $\|\boldsymbol{B}_2\|^2 = \|\boldsymbol{B}_3\|^2$. □

Summarizing these lemmata we find weights $\boldsymbol{\beta}$ for all crystallographic symmetry groups $\mathcal{S}$ such that the corresponding embeddings are isometries.

Theorem 18. *Let $k \in \mathbb{N}$ with $k > 2$, $\boldsymbol{u} = (\boldsymbol{e}_1, \boldsymbol{e}_2)$ and $\boldsymbol{\alpha} = (1, k)$. Then the embeddings $\mathcal{E}^{\boldsymbol{\alpha},\boldsymbol{\beta}}_{\boldsymbol{u},C_k}$ with the factors*

$$\boldsymbol{\beta} = \left(\sqrt{1 - \frac{\|\boldsymbol{B}_2\|^2}{\|\boldsymbol{B}_1\|^2}}, \frac{1}{\|\boldsymbol{B}_1\|}\right)^\top$$

with the norms from Lemma 17 are locally isometric embeddings. The concrete factors for $k = 3, 4, 6$ are listed in Table 2.

Proof. We use Eq. (9) for the rank 1 tensor. To normalize the vectors $d\mathcal{E}^{\boldsymbol{\alpha},\boldsymbol{\beta}}_{\boldsymbol{u},C_k}([\boldsymbol{I}]_{C_k})\boldsymbol{s}^{(\ell)}$ for $\ell = 1, 2, 3$ we have to solve for every k equations of the form

$$\beta_2^2 \;\|\boldsymbol{B}_1\|^2 = \beta_1^2 + \beta_2^2 \;\|\boldsymbol{B}_2\|^2 = \beta_1^2 + \beta_2^2 \;\|\boldsymbol{B}_3\|^2 = 1,$$

which always has a solution since $\|B_2\| = \|B_3\|$. We receive the positive solution by

$$\beta_1 = \sqrt{1 - \frac{\|\boldsymbol{B}_2\|^2}{\|\boldsymbol{B}_1\|^2}}, \quad \beta_2 = \frac{1}{\|\boldsymbol{B}_1\|}. \quad \square$$

For the symmetry groups D_k the case $k = 2$ is a special case for the same reasons as C_2.

Theorem 19. *Let $\boldsymbol{u} = (\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_2)$, $\boldsymbol{\alpha} = (2, 2, 2)$ and $\boldsymbol{\beta} = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. Then $\mathcal{E}^{\boldsymbol{\alpha},\boldsymbol{\beta}}_{\boldsymbol{u},D_2}$ is an locally isometric embedding.*

Proof. The second and third components are the same as in the case C_2. Analogously to this case we have to solve

$$2\,\beta_1^2 + 2\,\beta_2^2 = 2\,\beta_2^2 + 2\,\beta_3^2 = 1,$$

which yields $\beta_1 = \beta_2 = \beta_3 = \frac{1}{2}$. □

Theorem 20. *Let $k \in \mathbb{N}$ with $k > 2$, $\boldsymbol{u} = (\boldsymbol{e}_1, \boldsymbol{e}_2)$ and $\boldsymbol{\alpha} = (2, k)$. Then there exist factors $\boldsymbol{\beta}$, such that $\mathcal{E}^{\boldsymbol{\alpha},\boldsymbol{\beta}}_{\boldsymbol{u},D_k}$ is a locally isometric embedding.*

Proof. As in the case C_k we get the same second components B_1, B_2 and B_3. Only the first component is now a 3×3-matrix and not just a vector. The three vectors $d\mathcal{E}([\boldsymbol{I}]_{D_k})\boldsymbol{s}^{(\ell)}$ are again orthogonal. For the normalization we have to solve

$$\beta_2^2 \;\|B_1\|^2 = 2\,\beta_1^2 + \beta_2^2 \;\|B_2\|^2 = 2\,\beta_1^2 + \beta_2^2 \;\|B_3\|^2 = 1,$$

which yields the same solutions for β_2 as in the case C_k, but for β_1 we have to divide the solution from C_k by $\sqrt{2}$. □

For the cubic symmetry group the locally isometric embedding requires only a single vector. More precisely, we have the following result.

Theorem 21. *Let $\boldsymbol{u} = \boldsymbol{e}_1$, $\boldsymbol{\alpha} = 4$ and $\boldsymbol{\beta} = \frac{3}{2\sqrt{2}}$. Then $\mathcal{E}^{\boldsymbol{\alpha},\boldsymbol{\beta}}_{\boldsymbol{u},O}$ is a locally isometric embedding.*

Proof. The vectors $\boldsymbol{R}\boldsymbol{e}_1$ for $\boldsymbol{R} \in O$ are in the set $\{\pm\boldsymbol{e}_1, \pm\boldsymbol{e}_2, \pm\boldsymbol{e}_3\}$. Since $\otimes^4\boldsymbol{x} = \otimes^4(-\boldsymbol{x})$, we only have to consider the three vectors $\boldsymbol{v}_i = \boldsymbol{e}_i$ for $i \in \{1, 2, 3\}$. With respect to the skew-symmetric basis $\boldsymbol{s}^{(k)}$, $k \in \{1, 2, 3\}$ we obtain

$$\begin{aligned}
&\boldsymbol{s}^{(1)}\boldsymbol{v}_1 = \boldsymbol{0}, && \boldsymbol{s}^{(1)}\boldsymbol{v}_2 = \boldsymbol{e}_3, && \boldsymbol{s}^{(1)}\boldsymbol{v}_3 = -\boldsymbol{e}_2,\\
&\boldsymbol{s}^{(2)}\boldsymbol{v}_1 = \boldsymbol{e}_3, && \boldsymbol{s}^{(2)}\boldsymbol{v}_2 = \boldsymbol{0}, && \boldsymbol{s}^{(2)}\boldsymbol{v}_3 = -\boldsymbol{e}_1,\\
&\boldsymbol{s}^{(3)}\boldsymbol{v}_1 = \boldsymbol{e}_2, && \boldsymbol{s}^{(3)}\boldsymbol{v}_2 = -\boldsymbol{e}_1, && \boldsymbol{s}^{(3)}\boldsymbol{v}_3 = \boldsymbol{0}.
\end{aligned}$$

By Lemma 14 the scalar products in the embedding are

$$\begin{aligned}
\left\langle dE^{\boldsymbol{\alpha},\boldsymbol{\beta}}_{\boldsymbol{u},O}\boldsymbol{s}^{(\ell_1)}, dE^{\boldsymbol{\alpha},\boldsymbol{\beta}}_{\boldsymbol{u},O}\boldsymbol{s}^{(\ell_2)}\right\rangle &= \frac{12}{3^2}\sum_{j_1=1}^{3}\sum_{j_2=1}^{3}\left\langle \boldsymbol{v}_{j_1}, \boldsymbol{v}_{j_2}\right\rangle^2 \left\langle \boldsymbol{s}^{(\ell_1)}\boldsymbol{v}_{j_1}, \boldsymbol{v}_{j_2}\right\rangle\left\langle \boldsymbol{s}^{(\ell_2)}\boldsymbol{v}_{j_2}, \boldsymbol{v}_{j_1}\right\rangle + \frac{4}{3^2}\sum_{j_1=1}^{3}\sum_{j_2=1}^{3}\left\langle \boldsymbol{v}_{j_1}, \boldsymbol{v}_{j_2}\right\rangle^3\left\langle \boldsymbol{s}^{(\ell_1)}\boldsymbol{v}_{j_1}, \boldsymbol{s}^{(\ell_2)}\boldsymbol{v}_{j_2}\right\rangle\\
&= \frac{1}{12}\sum_{j=1}^{3}\left\langle \boldsymbol{s}^{(\ell_1)}\boldsymbol{v}_j, \boldsymbol{v}_j\right\rangle\left\langle \boldsymbol{s}^{(\ell_2)}\boldsymbol{v}_j, \boldsymbol{v}_j\right\rangle + \frac{4}{3^2}\sum_{j=1}^{3}\left\langle \boldsymbol{s}^{(\ell_1)}\boldsymbol{v}_j, \boldsymbol{s}^{(l_2)}\boldsymbol{v}_j\right\rangle = \frac{4}{3^2}\sum_{j=1}^{3}\left\langle \boldsymbol{s}^{(\ell_1)}\boldsymbol{v}_j, \boldsymbol{s}^{(\ell_2)}\boldsymbol{v}_j\right\rangle = \frac{8}{9}\,\delta_{\ell_1,\ell_2}.
\end{aligned}$$

Hence, the tangential vectors are orthogonal and normalized for $\beta_1 = \frac{3}{2\sqrt{2}}$. $\square$

The tetrahedral symmetry T also requires only one component, so we have the following result.

Theorem 22. *Let $\boldsymbol{u} = \frac{1}{\sqrt{3}}\begin{pmatrix}1\\1\\1\end{pmatrix}$, $\boldsymbol{\alpha} = 3$ and $\boldsymbol{\beta} = \frac{3}{2\sqrt{2}}$. Then $\mathcal{E}^{\boldsymbol{\alpha},\boldsymbol{\beta}}_{\boldsymbol{u},T}$ is a locally isometric embedding.*

Proof. The vectors $\boldsymbol{R}\boldsymbol{u}_1$ for $\boldsymbol{R} \in T$ are

$$\boldsymbol{v}_1 = \frac{1}{\sqrt{3}}\begin{pmatrix}1\\1\\1\end{pmatrix}, \quad \boldsymbol{v}_2 = \frac{1}{\sqrt{3}}\begin{pmatrix}-1\\-1\\1\end{pmatrix}, \quad \boldsymbol{v}_3 = \frac{1}{\sqrt{3}}\begin{pmatrix}-1\\1\\-1\end{pmatrix}, \quad \boldsymbol{v}_4 = \frac{1}{\sqrt{3}}\begin{pmatrix}1\\-1\\-1\end{pmatrix}$$

and satisfy $\langle \boldsymbol{v}_i, \boldsymbol{v}_j\rangle = -\frac{1}{3}$ for $i \neq j$. By Lemma 14 we have

$$d\mathcal{E}^{\alpha}_{\boldsymbol{u},T}(\boldsymbol{I})\boldsymbol{s}^{(\ell)} = \sum_{j=1}^{4}\sum_{i=0}^{2}\left(\otimes^i \boldsymbol{v}_j\right) \otimes \boldsymbol{s}^{(\ell)}\boldsymbol{v}_j \otimes \left(\otimes^{2-i}\boldsymbol{v}_j\right)$$

and hence, the scalar products of the basis vectors are

$$\left\langle dE^{\boldsymbol{\alpha}}_{\boldsymbol{u},T}\boldsymbol{s}^{(\ell_1)}, dE^{\boldsymbol{\alpha}}_{\boldsymbol{u},T}\boldsymbol{s}^{(\ell_2)}\right\rangle = \frac{3\cdot 2}{4^2}\sum_{j_1=1}^{4}\sum_{j_2=1}^{4}\left\langle \boldsymbol{v}_{j_1}, \boldsymbol{v}_{j_2}\right\rangle\left\langle \boldsymbol{s}^{(\ell_1)}\boldsymbol{v}_{j_1}, \boldsymbol{v}_{j_2}\right\rangle\left\langle \boldsymbol{s}^{(\ell_2)}\boldsymbol{v}_{j_2}, \boldsymbol{v}_{j_1}\right\rangle + \frac{3}{4^2}\sum_{j_1=1}^{4}\sum_{j_2=1}^{4}\left\langle \boldsymbol{v}_{j_1}, \boldsymbol{v}_{j_2}\right\rangle^2\left\langle \boldsymbol{s}^{(\ell_1)}\boldsymbol{v}_{j_1}, \boldsymbol{s}^{(\ell_2)}\boldsymbol{v}_{j_2}\right\rangle.$$

Using the symmetry of vectors $\boldsymbol{v}_j$ and $\boldsymbol{s}^{(l)}\boldsymbol{v}_j$

$$\begin{aligned}
\boldsymbol{s}^{(1)}v_1 &= \frac{1}{\sqrt{3}}\begin{pmatrix}0\\-1\\1\end{pmatrix}, & \boldsymbol{s}^{(1)}\boldsymbol{v}_2 &= \frac{1}{\sqrt{3}}\begin{pmatrix}0\\-1\\-1\end{pmatrix}, & \boldsymbol{s}^{(1)}\boldsymbol{v}_3 &= \frac{1}{\sqrt{3}}\begin{pmatrix}0\\1\\1\end{pmatrix}, & \boldsymbol{s}^{(1)}\boldsymbol{v}_4 &= \frac{1}{\sqrt{3}}\begin{pmatrix}0\\1\\-1\end{pmatrix}\\
\boldsymbol{s}^{(2)}\boldsymbol{v}_1 &= \frac{1}{\sqrt{3}}\begin{pmatrix}-1\\0\\1\end{pmatrix}, & \boldsymbol{s}^{(2)}\boldsymbol{v}_2 &= \frac{1}{\sqrt{3}}\begin{pmatrix}-1\\0\\-1\end{pmatrix}, & \boldsymbol{s}^{(2)}\boldsymbol{v}_3 &= \frac{1}{\sqrt{3}}\begin{pmatrix}1\\0\\-1\end{pmatrix}, & \boldsymbol{s}^{(2)}\boldsymbol{v}_4 &= \frac{1}{\sqrt{3}}\begin{pmatrix}1\\0\\1\end{pmatrix}\\
\boldsymbol{s}^{(3)}\boldsymbol{v}_1 &= \frac{1}{\sqrt{3}}\begin{pmatrix}-1\\1\\0\end{pmatrix}, & \boldsymbol{s}^{(3)}\boldsymbol{v}_2 &= \frac{1}{\sqrt{3}}\begin{pmatrix}1\\-1\\0\end{pmatrix}, & \boldsymbol{s}^{(3)}\boldsymbol{v}_3 &= \frac{1}{\sqrt{3}}\begin{pmatrix}-1\\-1\\0\end{pmatrix}, & \boldsymbol{s}^{(3)}\boldsymbol{v}_4 &= \frac{1}{\sqrt{3}}\begin{pmatrix}1\\1\\0\end{pmatrix}
\end{aligned}$$

it is sufficient to consider the scalar products for $l_1 = 1, l_2 = 2$ and $l_1 = l_2 = 1$:

$$\begin{aligned}
\left\langle d\mathcal{E}^{\boldsymbol{\alpha}}_{\boldsymbol{u},T}\boldsymbol{s}^{(1)}, d\mathcal{E}^{\boldsymbol{\alpha}}_{\boldsymbol{u},T}\boldsymbol{s}^{(2)}\right\rangle &= \frac{3}{8}\sum_{\substack{j_1,j_2=1\\ j_1\neq j_2}}^{4} -\frac{1}{3}\left\langle \boldsymbol{s}^{(1)}\boldsymbol{v}_{j_1}, \boldsymbol{v}_{j_2}\right\rangle\left\langle \boldsymbol{s}^{(2)}\boldsymbol{v}_{j_2}, \boldsymbol{v}_{j_1}\right\rangle = 0,\\
\left\langle d\mathcal{E}^{\boldsymbol{\alpha}}_{\boldsymbol{u},T}\boldsymbol{s}^{(1)}, d\mathcal{E}^{\boldsymbol{\alpha}}_{\boldsymbol{u},T}\boldsymbol{s}^{(1)}\right\rangle &= \frac{3}{8}\sum_{\substack{j_1,j_2=1\\ j_1\neq j_2}}^{4} -\frac{1}{3}\left\langle \boldsymbol{s}^{(1)}\boldsymbol{v}_{j_1}, \boldsymbol{v}_{j_2}\right\rangle\left\langle \boldsymbol{s}^{(1)}\boldsymbol{v}_{j_2}, \boldsymbol{v}_{j_1}\right\rangle + \frac{3}{8}\sum_{j_1=1}^{4}\frac{2}{6} + \frac{3}{4^2}\sum_{\substack{j_1,j_2=1\\ j_1\neq j_2}}^{4}\frac{1}{9}\left\langle \boldsymbol{s}^{(1)}\boldsymbol{v}_{j_1}, \boldsymbol{s}^{(1)}\boldsymbol{v}_{j_2}\right\rangle\\
&= \frac{3}{8}\cdot\frac{1}{3}\cdot\frac{64}{18} + \frac{3}{8}\cdot\frac{4\cdot 2}{6} + \frac{3}{4^2}\cdot\frac{1}{9}\cdot\frac{-16}{6} = \frac{8}{9}.
\end{aligned}$$

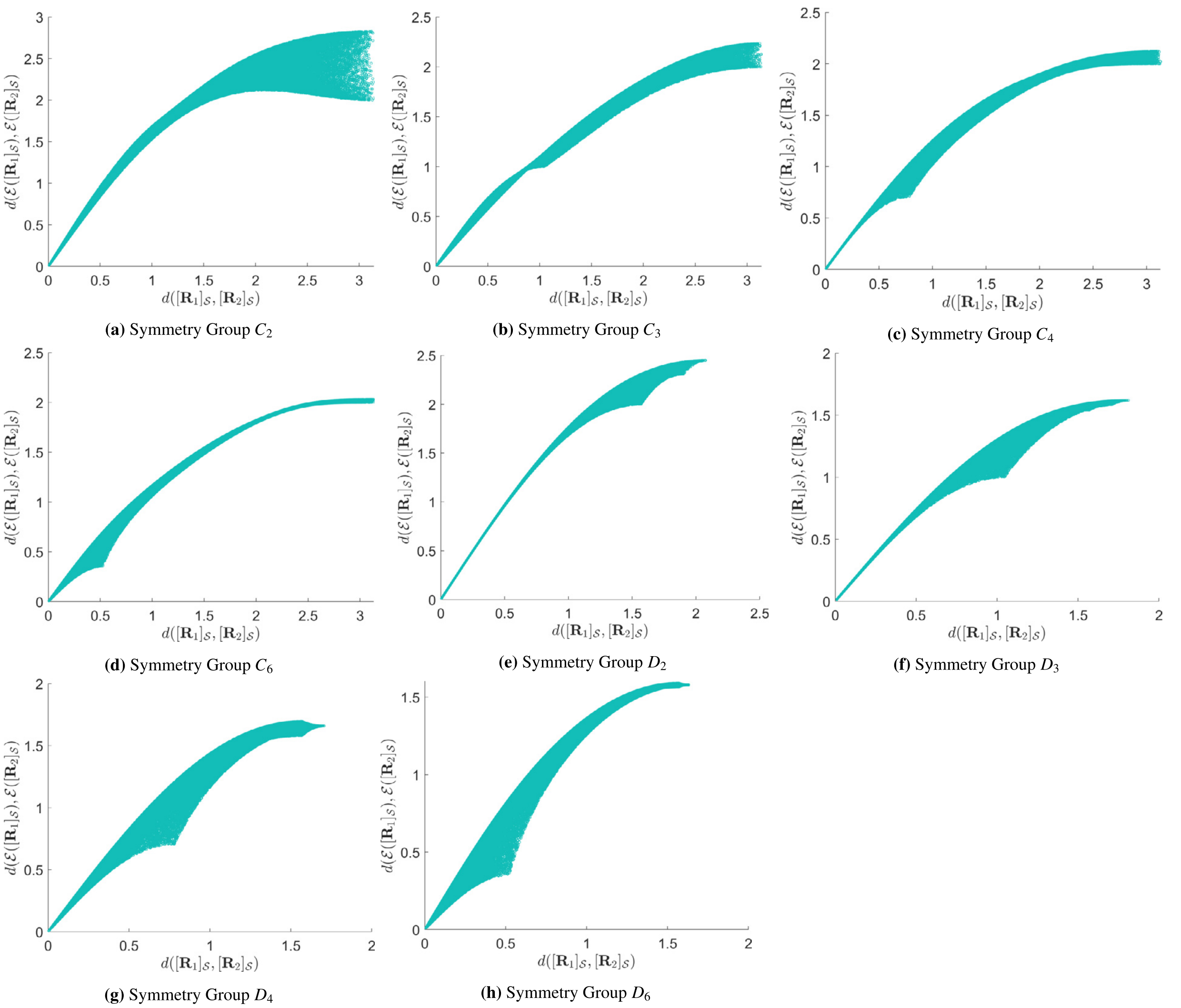
Hence, with $\beta_1 = \frac{3}{2\sqrt{2}}$ the proposed embedding is locally isometric. $\square$

Finally, we consider icosahedral symmetry Y.

Theorem 23. *Let $\boldsymbol{u} = \begin{pmatrix}0\\1\\\Phi\end{pmatrix}$, where $\Phi = \frac{1+\sqrt{5}}{2}$ is the golden ratio, $\boldsymbol{\alpha} = 10$ and $\boldsymbol{\beta} = \frac{75}{8\sqrt{95}}$. Then $\mathcal{E}^{\boldsymbol{\alpha},\boldsymbol{\beta}}_{\boldsymbol{u},Y}$ is a locally isometric embedding.*

Proof. This proof is similar to the proof of the tetrahedral symmetry T. The vectors $\boldsymbol{v}_i \in \{\boldsymbol{R}\boldsymbol{u}_1\}_{\boldsymbol{R}\in Y}$ are

$$\begin{pmatrix}0\\\pm 1\\\pm\Phi\end{pmatrix}, \quad \begin{pmatrix}\pm 1\\\pm\Phi\\0\end{pmatrix}, \quad \begin{pmatrix}\pm\Phi\\0\\\pm 1\end{pmatrix},$$



(a) Symmetry Group C_2 **(b)** Symmetry Group C_3 **(c)** Symmetry Group C_4 **(d)** Symmetry Group C_6 **(e)** Symmetry Group D_2 **(f)** Symmetry Group D_3 **(g)** Symmetry Group D_4 **(h)** Symmetry Group D_6

Fig. 1. Relation between the geodesic distance on the manifold and the Euclidean distance in the embedding for the embeddings reported in [2].

and satisfy $|\langle \boldsymbol{v}_i, \boldsymbol{v}_j\rangle| = 5^{-1/2}$ for $i \neq j$. Since α is even, we have $\otimes^\alpha(\boldsymbol{x}) = \otimes^\alpha(-\boldsymbol{x})$ and do not have to consider $-\boldsymbol{x}$, if we use $\boldsymbol{x}$. Hence, we only need six vectors $\boldsymbol{v}_i$. Again, with Lemma 14 we can calculate $\mathrm{d}\mathcal{E}^{\alpha,\beta}_{\boldsymbol{u},Y}$ and the scalar products of these. We omit these calculations here, as they are similar to the case for the tetrahedral symmetry T, but with higher-dimensional tensors. $\square$

3.2. Global inequalities

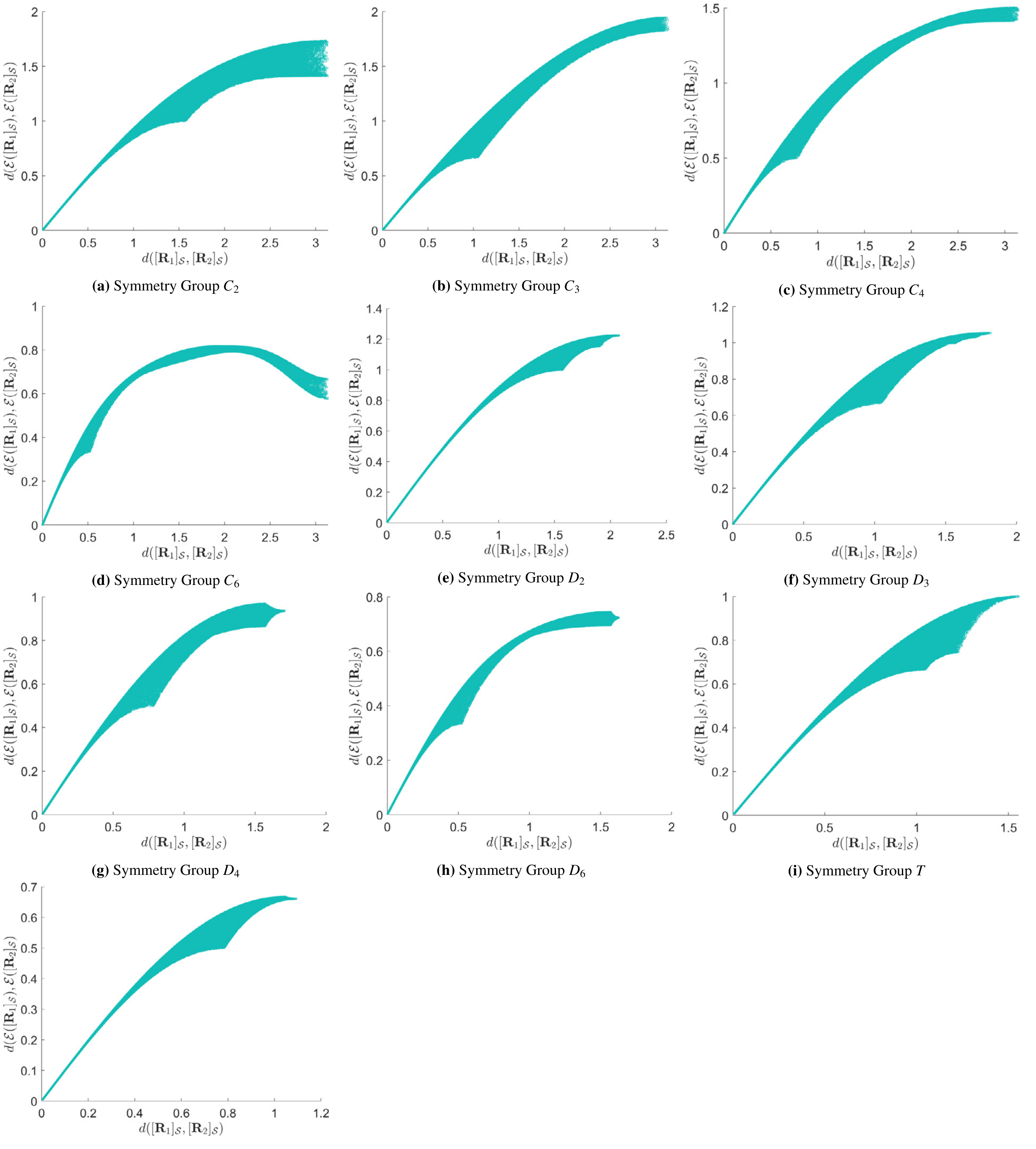
Although the embeddings found in the previous section are locally isometric they obviously do not preserve the metric globally. In this section we are interested in inequalities of the form

$$c_{\min}\, d([\boldsymbol{O}_1]_S, [\boldsymbol{O}_2]_S) \leq d(\mathcal{E}_S([\boldsymbol{O}_1]_S), \mathcal{E}_S([\boldsymbol{O}_2]_S)) \leq c_{\max}\, d([\boldsymbol{O}_1]_S, [\boldsymbol{O}_2]_S) \tag{12}$$

that relate the Euclidean distance in $\mathbb{R}^{3^\alpha}$ and the geodesic distance from Eq. (7).

The situation is easiest for $\mathcal{S} = C_1$, i.e., we just look at SO(3). In this case the Euclidean distance in the embedding is directly related to the geodesic distance on the manifold via

$$d(\mathcal{E}_{C_1}(\boldsymbol{R}_1), \mathcal{E}_{C_1}(\boldsymbol{R}_2)) = \sqrt{2}\sqrt{1 - \cos(d(\boldsymbol{R}_1, \boldsymbol{R}_2))}.$$



(a) Symmetry Group C_2 **(b)** Symmetry Group C_3 **(c)** Symmetry Group C_4

(d) Symmetry Group C_6 **(e)** Symmetry Group D_2 **(f)** Symmetry Group D_3

(g) Symmetry Group D_4 **(h)** Symmetry Group D_6 **(i)** Symmetry Group T

(j) Symmetry Group O

Fig. 2. Relation between the geodesic distance on the manifold and the Euclidean distance in the embedding for the locally isometric embeddings summarized in Table 2.

Table 3
Global lower and upper bounds $c_{\min}$, $c_{\max}$ for the distance in the embedding $d(\mathcal{E}_S([\boldsymbol{O}_1]_S), \mathcal{E}_S([\boldsymbol{O}_2]_S))$ with respect to the geodesic distance $d([\boldsymbol{O}_1]_S, [\boldsymbol{O}_2]_S)$ on $\mathrm{SO}(3)/\mathcal{S}$, cf. (12), for the locally isometric embeddings from Table 2 and all crystallographic symmetry groups $\mathcal{S}$.

$\mathcal{S}$	$c_{\min}$	$c_{\max}$	$c_{\max}/c_{\min}$
C_2	0.452	1	2.21
C_3	0.583	1	1.72
C_4	0.452	1	2.21
C_6	0.186	1	5.36
D_2	0.590	1	1.70
D_3	0.581	1	1.72
D_4	0.546	1	1.83
D_6	0.443	1	2.26
O	0.604	1	1.66
T	0.609	1	1.64

Table 4
Parameters $\boldsymbol{\beta}$ for the embeddings $\mathcal{E}_{\boldsymbol{u},\mathcal{S}}^{\boldsymbol{\alpha},\boldsymbol{\beta}}: \mathrm{SO}(3)/S \to \mathbb{R}^{3^{\alpha}}$ as defined in (8) that minimize the fraction $c_{\min}/c_{\max}$ between the upper and lower bound in (12) for some symmetry groups $\mathcal{S}$.

$\mathcal{S}$	$\boldsymbol{\beta}$	$c_{\max}/c_{\min}$
C_2	$(1, 0.5, 0.5)$	1.92
C_3	$(1, 0.67)$	1.68
C_4	$(1, 0.6)$	1.91
C_6	$(1, 0.93)$	2.15
D_3	$(1, 1.03)$	1.72
D_4	$(1, 1.11)$	1.80
D_6	$(1, 1.65)$	1.95

and we have $c_{\min} = \frac{2}{\pi}$ and $c_{\max} = 1$.

For higher symmetries there is no such one to one relationship. In order to illustrate the dependency between the geodesic distance on the manifold and the Euclidean distance in the embedding for higher symmetries we have visualized the regions of suitable combinations in Figs. 1 and 2. While Fig. 1 illustrates the embeddings from [2], Fig. 2 visualizes the locally isometric embeddings from Table 2.

In Table 3 the upper and lower bounds $c_{\min}$ and $c_{\max}$ are listed for locally isometric embeddings from Table 2. We would like to stress that non-locally-isometric embeddings might very well lead to better global bounds. Indeed, Table 4 provides alternative coefficients for the embeddings $\mathcal{E}_{\boldsymbol{u},\mathcal{S}}^{\boldsymbol{\alpha},\boldsymbol{\beta}}$ which have better upper and lower bounds.

CRediT authorship contribution statement

Ralf Hielscher: Investigation Writing. **Laura Lippert:** Investigation Writing.

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Appendix A. A binomial identity

For the calculation of $\|M_\alpha\|$ in Lemma 8 we need the following nice lemma for binomial coefficients.

Lemma 24. *Let $\alpha \in 2\mathbb{N}$ be an even integer. Then we have the equality*

$$(\alpha+1)\binom{\alpha}{\frac{\alpha}{2}} = \sum_{\substack{i_1,i_2,i_3=0 \\ i_1+i_2+i_3=\frac{\alpha}{2}}}^{\frac{\alpha}{2}} \binom{2i_1}{i_1}\binom{2i_2}{i_2}\binom{2i_3}{i_3}.$$

Proof. With the general definition of the binomial coefficient $\binom{n}{k} = \frac{n(n-1)\cdots(n-(k-1))}{k!}$ for $k > 0$ we obtain

$$\binom{2n}{n} = (-1)^n\, 4^n \binom{-\frac{1}{2}}{n}.$$

With this equation and the Chu–Vandermonde-identity it follows that

$$\begin{aligned}\sum_{\substack{i_1,i_2,i_3=0\\ i_1+i_2+i_3=\frac{\alpha}{2}}}^{\frac{\alpha}{2}} \binom{2i_1}{i_1}\binom{2i_2}{i_2}\binom{2i_3}{i_3} &= \sum_{\substack{i_1,i_2,i_3=0\\ i_1+i_2+i_3=\frac{\alpha}{2}}}^{\frac{\alpha}{2}} (-1)^{i_1+i_2+i_3}\ 4^{i_1+i_2+i_3}\binom{-\frac{1}{2}}{i_1}\binom{-\frac{1}{2}}{i_2}\binom{-\frac{1}{2}}{i_3}\\
&= (-1)^{\frac{\alpha}{2}}\ 4^{\frac{\alpha}{2}} \sum_{\substack{i_1,i_2,i_3=0\\ i_1+i_2+i_3=\frac{\alpha}{2}}}^{\frac{\alpha}{2}} \binom{-\frac{1}{2}}{i_1}\binom{-\frac{1}{2}}{i_2}\binom{-\frac{1}{2}}{i_3}\\
&= (-1)^{\frac{\alpha}{2}}\ 4^{\frac{\alpha}{2}}\binom{-\frac{3}{2}}{\frac{\alpha}{2}} = (-1)^{\frac{\alpha}{2}}\ 4^{\frac{\alpha}{2}}\left(\frac{-\frac{3}{2}\left(-\frac{3}{2}-1\right)\cdots\left(-\frac{3}{2}-\left(\frac{\alpha}{2}-1\right)\right)}{\left(\frac{\alpha}{2}\right)!}\right)\\
&= 4^{\frac{\alpha}{2}}\left(\frac{\frac{3}{2}\left(\frac{3}{2}+1\right)\cdots\left(\frac{3}{2}+\left(\frac{\alpha}{2}-1\right)\right)}{\left(\frac{\alpha}{2}\right)!}\right)\\
&= 2^{\frac{\alpha}{2}}\left(\frac{3\cdot 5\cdot 7\cdots(\alpha+1)}{\left(\frac{\alpha}{2}\right)!}\right) = (\alpha+1)\ \frac{2^{\frac{\alpha}{2}}\left(\frac{\alpha}{2}\right)!\cdot 3\cdot 5\cdot 7\cdots(\alpha-1)}{\left(\frac{\alpha}{2}\right)!^2}\\
&= (\alpha+1)\binom{\alpha}{\frac{\alpha}{2}}. \quad \square\end{aligned}$$

Appendix B. Some trigonometrical sums

Here we calculate some trigonometric sums of the proofs in Section 3. For the proof of Lemma 16 we need

$$\begin{aligned}\sum_{j_1,j_2=0}^{k-1}\cos^{k-1}\tfrac{2\pi(j_1-j_2)}{k}\sin\tfrac{2\pi j_1}{k}\cos\tfrac{2\pi j_2}{k} &= \frac{1}{2}\sum_{j_1,j_2=0}^{k-1}\cos^{k-1}\tfrac{2\pi(j_1-j_2)}{k}\left(\sin\tfrac{2\pi(j_1-j_2)}{k}+\sin\tfrac{2\pi(j_1+j_2)}{k}\right)\\
&= \frac{1}{2}\sum_{j_1,j_2=0}^{k-1}\cos^{k-1}\tfrac{2\pi j_1}{k}\left(\sin\tfrac{2\pi j_1}{k}+\sin\tfrac{2\pi j_2}{k}\right)=0.\end{aligned} \tag{B.1}$$

For the proof of Lemma 17 we need the following calculations. Using

$$\sum_{j=0}^{k-1} e^{\frac{2\pi i j n}{k}} = \begin{cases} k, & n\in\mathbb{Z},\\ 0, & \text{otherwise,}\end{cases}$$

we compute

$$\begin{aligned}\sum_{j=0}^{k-1}\cos^k\left(\frac{2\pi j}{k}\right) &= \frac{1}{2^k}\sum_{j=0}^{k-1}\left(e^{\frac{2\pi i j}{k}}+e^{\frac{-2\pi i j}{k}}\right)^k = \frac{1}{2^k}\sum_{j=0}^{k-1}\sum_{\ell=0}^{k}\binom{k}{\ell}e^{\frac{4\pi i j\ell}{k}}\\
&= \frac{1}{2^k}\sum_{\ell=0}^{k}\binom{k}{\ell}\sum_{j=0}^{k-1}e^{\frac{2\pi i j(2\ell)}{k}} = \begin{cases}\frac{k}{2^{k-1}}, & \text{if } k \text{ odd},\\ \frac{1}{2^k}\left(\binom{k}{\frac{k}{2}}\cdot k+2k\right), & \text{if } k \text{ even},\end{cases}\\
\sum_{j=0}^{k-1}\cos^{k-2}\left(\frac{2\pi j}{k}\right) &= \frac{1}{2^{k-2}}\sum_{j=0}^{k-1}\left(e^{\frac{2\pi i j}{k}}+e^{\frac{-2\pi i j}{k}}\right)^{k-2} = \frac{1}{2^{k-2}}\sum_{j=0}^{k-1}\sum_{\ell=0}^{k-2}\binom{k-2}{\ell}e^{\frac{2\pi i j(2\ell+2)}{k}}\\
&= \frac{1}{2^{k-2}}\sum_{\ell=0}^{k-2}\binom{k}{\ell}\sum_{j=0}^{k-1}e^{\frac{2\pi i j(2\ell+2)}{k}} = \begin{cases}0, & \text{if } k \text{ odd},\\ \frac{k}{2^{k-2}}\binom{k-2}{\frac{k}{2}-1}, & \text{if } k \text{ even}.\end{cases}\end{aligned}$$

We use this for the following calculations.

$$\begin{aligned}&-\frac{(k-1)}{k}\sum_{j_1=0}^{k-1}\sum_{j_2=0}^{k-1}\cos^{k-2}\left(\frac{2\pi(j_1-j_2)}{k}\right)\sin^2\left(\frac{2\pi(j_1-j_2)}{k}\right)+\frac{1}{k}\sum_{j_1=0}^{k-1}\sum_{j_2=0}^{k-1}\cos^{k-1}\left(\frac{2\pi(j_1-j_2)}{k}\right)\cos\left(\frac{2\pi(j_1-j_2)}{k}\right)\\
&= -(k-1)\sum_{j=0}^{k-1}\cos^{k-2}\left(\frac{2\pi j}{k}\right)\sin^2\left(\frac{2\pi j}{k}\right)+\sum_{j=0}^{k-1}\cos^k\left(\frac{2\pi j}{k}\right)\end{aligned}$$

$$
\begin{aligned}
&= -(k-1)\sum_{j=0}^{k-1}\cos^{k-2}\left(\frac{2\pi j}{k}\right) + k\sum_{j=0}^{k-1}\cos^{k}\left(\frac{2\pi j}{k}\right) \\
&= \begin{cases} \frac{k^2}{2^{k-1}}, & \text{if } k, \text{ odd}, \\ -\frac{k(k-1)}{2^{k-2}}\binom{k-2}{\frac{k}{2}-1} + \frac{k^2}{2^k}\left(\binom{k}{\frac{k}{2}}+2\right), & \text{if } k \text{ even}, \end{cases} = \frac{k^2}{2^{k-1}}.
\end{aligned} \tag{B.2}
$$

Also for the proof of Lemma 17 we calculate the following.

$$
\begin{aligned}
&\frac{1}{k}\sum_{j_1=0}^{k-1}\sum_{j_2=0}^{k-1}\cos^{k-1}\left(\frac{2\pi(j_1-j_2)}{k}\right)\cos\left(\frac{2\pi j_1}{k}\right)\cos\left(\frac{2\pi j_2}{k}\right) \\
&= \frac{1}{k\,2^{k+1}}\sum_{j_1=0}^{k-1}\sum_{j_2=0}^{k-1}\left(e^{\frac{2\pi i(j_1-j_2)}{k}} + e^{-\frac{2\pi i(j_1-j_2)}{k}}\right)^{k-1}\left(e^{\frac{2\pi i j_1}{k}} + e^{-\frac{2\pi i j_1}{k}}\right)\left(e^{\frac{2\pi i j_2}{k}} + e^{-\frac{2\pi i j_2}{k}}\right) \\
&= \frac{1}{k\,2^{k+1}}\sum_{j_1=0}^{k-1}\sum_{j_2=0}^{k-1}\left(e^{\frac{2\pi i(j_1+j_2)}{k}} + e^{-\frac{2\pi i(j_1+j_2)}{k}} + e^{\frac{2\pi i(j_1-j_2)}{k}} + e^{\frac{2\pi i(j_2-j_1)}{k}}\right)\sum_{l=0}^{k-1}\binom{k-1}{l}e^{\frac{2\pi i(j_1-j_2)(2l+1)}{k}} \\
&= \frac{1}{k\,2^{k+1}}\sum_{l=0}^{k-1}\binom{k-1}{l}\sum_{j_1=0}^{k-1}\sum_{j_2=0}^{k-1}\left(e^{\frac{2\pi i((j_1-j_2)(2l+1)+j_1+j_2)}{k}} + e^{\frac{2\pi i((j_1-j_2)(2l+1)-j_1-j_2)}{k}} + e^{\frac{2\pi i(j_1-j_2)(2l+2)}{k}} + e^{\frac{2\pi i(j_1-j_2)(2l)}{k}}\right) \\
&= \frac{1}{k\,2^{k+1}}\sum_{l=0}^{k-1}\binom{k-1}{l}\sum_{j_1=0}^{k-1}\sum_{j_2=0}^{k-1}\left(e^{\frac{2\pi i(j_1(2l+2)-2lj_2)}{k}} + e^{\frac{2\pi i(2lj_1-j_2(2l+2))}{k}} + e^{\frac{2\pi i(j_1-j_2)(2l+2)}{k}} + e^{\frac{2\pi i(j_1-j_2)(2l)}{k}}\right) \\
&= \frac{k}{k\,2^{k+1}}\sum_{l=0}^{k-1}\binom{k-1}{l}\sum_{j=0}^{k-1}e^{\frac{2\pi i j(2l+2)}{k}} + e^{\frac{2\pi i j(2l)}{k}} = \begin{cases} \frac{k}{2^k}, & \text{if } k \text{ is odd}, \\ \frac{k}{2^{k+1}}\left(2+\binom{k-1}{\frac{k}{2}}+\binom{k-1}{\frac{k}{2}-1}\right), & \text{if } k \text{ is even}, \end{cases} \\
&= \begin{cases} \frac{k}{2^k}, & \text{if } k \text{ is odd}, \\ \frac{k}{2^{k+1}}\left(2+\binom{k}{\frac{k}{2}}\right), & \text{if } k \text{ is even}. \end{cases}
\end{aligned} \tag{B.3}
$$

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