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Voronoi Cells in Lie Groups and Coset Decompositions: Implications for Optimization, Integration, and Fourier Analysis

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Abstract— **The rotation group and special Euclidean group both contain discrete subgroups. In the case of the rotation group, these subgroups are the chiral point groups, and in the case of the special Euclidean group, the discrete subgroups are the chiral crystallographic space groups. Taking the quotients of either of these two Lie groups by any of their respective co-compact discrete subgroups results in coset spaces that are compact orientable manifolds. In this paper we develop methods for sampling on these manifolds by partitioning them further using double-coset decompositions. Fundamental domains associated with the aforementioned coset- and double-coset decompositions can be defined as Voronoi cells in the original groups. Division of these groups into Voronoi cells facilitates almost-uniform sampling. We explicitly compute these cells and illustrate their use in optimization, integration, and Fourier analysis on these groups. Motivating applications from the fields of protein crystallography, robotics, and control are reviewed in the context of this theory.**

I. Introduction

The group of rotations in three-dimensional space, $SO(3)$, and the groups of rigid-body motions of the plane and space, $SE(2)$ and $SE(3)$, are ubiquitous in the fields of estimation and control [2], [3], [4], [11], [12], [15], [18], [19], [33], [34], robotics [5], [23], and computer vision [20], [28]. These are Lie groups that contain discrete subgroups. In the case of $SO(3)$, which is compact, the discrete subgroups are the chiral point groups, which are finite.[1] Of these, we shall only be concerned with the groups of rotational symmetries of the Platonic solids since they fill $SO(3)$ more uniformly than other finite subgroups. In the case of $SE(2)$, the discrete subgroups of interest are the five chiral wallpaper groups consisting of lattice translations in the x-y plane and either no rotation, or rotation around the z axis by $2\pi/n$ radians where $n = 2,3,4$ or 6.

Here we develop new theory for sampling, integration, and Fourier analysis on the aforementioned Lie groups and point to literature on how this theory is applicable to a wide variety of applications ranging from kinematic state estimation of mobile robots, to robotic manipulator workspaces, to polymer statistical mechanics, and efficient searches in crystallographic computing.

This paper is structured as follows. Section II reviews definitions such as left-, right-, and double-coset spaces in general, the corresponding concept of fundamental domains in a Lie group, and reviews the concrete details regarding the groups $SE(2)$ and $SO(3)$. Section III develops an efficient sampling method in $SO(3)$ and $SE(2)$ based on coset decompositions that is directly relevant to molecular replacement searches in crystallographic computing. Section IV explains how the grids of almost-uniform points generated using this methodology are beneficial in optimization tasks over these groups, and gives concrete examples where such optimizations occur. Section V explains how the coset decompositions developed here can lead to more efficient computations of convolutions on groups and deconvolutions.

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[1] A chiral symmetry group refers to one that preserves orientation, or equivalently, the right-handedness of coordinate systems. A point group is one for which the action on Euclidean space keeps a point fixed.

II. Definitions and Terminology

If G denotes $SO(3)$ or $SE(2)$, or any finite-dimensional Lie group, and $\Gamma,\Gamma' < G$ denote discrete subgroups, then right- and left-coset-spaces are defined as [32]

$$\Gamma\backslash G \doteq \{\Gamma g \mid g \in G\} \quad \text{and} \quad G/\Gamma' \doteq \{g\Gamma' \mid g \in G\}.$$

And a double coset space is defined as

$$\Gamma\backslash G/\Gamma' \doteq \{\Gamma g\Gamma' \mid g \in G\}.$$

Associated with any (double-)coset, it is possible to define a set of distinguished (double-)coset representatives, exactly one per (double-)coset. Such a set defines a fundamental domain in G that has the same dimension as G, but lesser volume. Under the left action by Γ, the fundamental domain $F_{\Gamma\backslash G}$ is translated and the closure of the union of all translates covers G without measurable gaps[2] or overlaps. Similarly, right action by Γ' on the fundamental domain $F_{G/\Gamma'}$ and the double-sided-action of $\Gamma\times\Gamma'$ on $F_{\Gamma\backslash G/\Gamma'}$ produces translates the closure of which cover G.

One way to construct fundamental domains is as Voronoi cells within G. Since G is a Riemannian manifold, a distance function $d : G\times G \longrightarrow \mathbb{R}_{\geq 0}$ exists, and we can define

$$F_{\Gamma\backslash G} \doteq \{g \in G \mid d(e,g) < d(e,\gamma\circ g)\ ,\forall\,\gamma \in \Gamma\}$$

$$F_{G/\Gamma'} \doteq \{g \in G \mid d(e,g) < d(e,\gamma'\circ g)\ ,\forall\,\gamma' \in \Gamma'\}$$

and when $\Gamma\cap\Gamma' = \{e\}$,

$$F_{\Gamma\backslash G/\Gamma'} \doteq \{g \in G \mid d(e,g) < d(e,\gamma\circ g\circ\gamma')\ ,\forall\,(\gamma,\gamma') \in \Gamma\times\Gamma'\}. \quad (1)$$

[2] In practice, fundamental domains are often defined to be open sets, and so the union of translates themselves does not completely cover G, as it has gaps of measure zero. On the other hand, the union of the closure of fundamental domains will cover, but with a set of measure zero of duplicates. The distinction between a fundamental domain, its interior, and its closure are inconsequential for our purposes.

Explicitly, distance functions for $SO(3)$ and $SE(2)$ can be defined as

$$d^{(1)}_{SO(3)}(R_1,R_2) = \|R_1 - R_2\|$$

where $\|A\| = \sqrt{\mathrm{tr}(AA^T)}$ is the Frobenius norm, and

$$d^{(1)}_{SE(2)}(g_1,g_2) = \|g_1 - g_2\|_W \tag{2}$$

where an arbitrary element of $SE(2)$ is of the form

$$g = \begin{pmatrix} \cos\theta & -\sin\theta & x \\ \sin\theta & \cos\theta & y \\ 0 & 0 & 1 \end{pmatrix},$$

$W = W^T$ as a 3×3 positive definite weighting matrix, and $\|A\|_W = \sqrt{\mathrm{tr}(AWA^T)}$. The above distance measures are 'extrinsic' in the sense that they rely on how these matrix Lie groups are embedded in $\mathbb{R}^{3\times 3}$, but they satisfy the conditions of non-negativeness, symmetry, and the triangle inequality.

It is also possible to define 'intrinsic' measures of distance using the logarithm function. Since both $SO(3)$ and $SE(2)$ are matrix-Lie-groups, their exponential maps are the matrix exponentials. Explicitly for $SO(3)$, elements of the associated Lie algebra, $so(3)$ are skew-symmetric matrices

$$X = \begin{pmatrix} 0 & -x_3 & x_2 \\ x_3 & 0 & -x_1 \\ -x_2 & x_1 & 0 \end{pmatrix}$$

and the exponential gives

$$R(\mathbf{x}) = \exp X = \mathbb{I} + \frac{\sin\|\mathbf{x}\|}{\|\mathbf{x}\|}X + \frac{1-\cos\|\mathbf{x}\|}{\|\mathbf{x}\|^2}X^2 \tag{3}$$

where $\mathbf{x} = [x_1,x_2,x_3]^T = X^\vee$ is the vector corresponding to X. The opposite operation gives $\widehat{\mathbf{x}} = X$. And for $SE(2)$ elements of the corresponding Lie algebra, $se(2)$, are of the form

$$X = \begin{pmatrix} 0 & -\theta & v_1 \\ \theta & 0 & v_2 \\ 0 & 0 & 0 \end{pmatrix},$$

and the exponential is

$$g = \exp(X) = \begin{pmatrix} \cos\theta & -\sin\theta & x(\theta,v_1,v_2) \\ \sin\theta & \cos\theta & y(\theta,v_1,v_2) \\ 0 & 0 & 1 \end{pmatrix},$$

where the functions $x(\theta,v_1,v_2)$ and $y(\theta,v_1,v_2)$ have been computed in closed form [6], [7]. The inverse map for each is the matrix logarithm. This degenerates when $\|\mathbf{x}\|$ or θ is π. By restricting the discussion to the case when $\|\mathbf{x}\|,\theta < \pi$, log is uniquely defined on a subset of $SO(3)$ depleted by a set of measure zero. This depletion will have no effect on our formulation. For example, it becomes possible to define

$$d^{(2)}_{SO(3)}(R_1,R_2) = \|\log(R_1^T R_2)\|$$

when $R_1^T R_2$ is not a rotation by π, and otherwise $d^{(2)}_{SO(3)}(R_1,R_2) = \pi$ and similarly

$$d^{(2)}_{SE(2)}(g_1,g_2) = \|\log(g_1^{-1}\circ g_2)\|_{W'}$$

where W' could be different than W. As in the $SO(3)$ case, a map from $se(2)$ to $\mathbb{R}^3$ can be defined as $X^\vee = [v_1,v_2,\theta]^T$.

It is interesting to note that regardless of whether the intrinsic or extrinsic measures are used, the above distance functions for $SO(3)$ are bi-invariant:

$$d_{SO(3)}(R_1,R_2) = d_{SO(3)}(QR_1,QR_2) = d_{SO(3)}(R_1Q,R_2Q)$$

for arbitrary $Q \in SO(3)$, whereas no such bi-invariant metric for $SE(2)$ is possible.

III. Applications to Almost-Uniform Sampling in Structural Biology Problems

Structural biology is concerned with understanding the 3D arrangement of atoms in large biomolecules such as proteins, nucleic acids, carbohydrates, and fats, and the multi-molecule complexes that they form. Various experimental modalities such as crystallography, nuclear magnetic resonance, fluorescence spectroscopy, and and cryo-electron-microscopy provide different information about 3D biomolecular structures, and how these structures change shape as they undergo their function. In each of these experimental modalities it is often the case that prior knowledge about the composition and shape of particular fragments of a biomolecule are known in advance. In fact, as of this writing, the protein data bank (PDB) contains more than 80,000 protein structures that can be used as prior models when doing new experiments.

X-ray crystallography has been responsible for the vast majority of entries in the PDB. In order to interpret the information contained in an x-ray diffraction pattern when the shape of fragments of the proteins in crystal are known in advance, it is critical to find unknown rigid-body motions that relate the fragments to each other. The computational problem of finding these rigid-body motions is known as 'molecular replacement' and algorithms for solving the problem have been investigated for half a century [27], [29]. Similar rotational correlation problems are necessary in the context of cryo-EM [14]. We note that deterministic sampling of rotations in an almost-uniform way also has application in robot motion planning [35].

Obviously, when performing a search over rotations, one desires the samples to be generated as 'uniformly' as possible, since having samples clumped in some areas and sparse in others will be a waste of computational resources. In [8], [9], [36], [37] we devised new strategies for sampling based on coset decompositions. These are particularly natural in the context of molecular replacement problems because a crystal has space group symmetry and the functions of rigid-body motion that need to be minimized have the property $f(\gamma\circ g) = f(g)$ for all $\gamma \in \Gamma$, a crystallographic space group. That is, $f : G \longrightarrow \mathbb{R}$ is invariant on all cosets Γg, and is therefore a 'right-coset function'. Hence in sampling problems in molecular replacement, the only samples that need to be generated are in the space $\Gamma\backslash G$, or equivalently, $F_{\Gamma\backslash G}$.

Here we establish for the first time what these fundamental regions look like when $G = SE(2)$ and Γ is one of the five chiral wallpaper groups. $SE(2)$ is mapped to $\mathbb{R}^3$ with x-y

axes representing translations in the x and y directions and z axis representing the rotation angle θ. The Voronoi cells are generated using the metric (2). Fig. 1 illustrates the lattice structure for wallpaper group $p1$ and the corresponding Voronoi cells of $SE(2)$. The Voronoi cells centered at the identity for all the five wallpaper groups $p1$, $p2$, $p4$, $p3$ and $p6$ are shown in Fig. 2. The group $p1$ consists only of translations, in a parallelogrammatic lattice. Its center Voronoi cell looks like a hexagonal box with the height from $-\pi$ to π. We note that when the lattice is square, the center Voronoi cell becomes a square box. The group $p2$ differs only from $p1$ in that it contains 180° rotations, or rotations of order 2, so its center Voronoi cell has the same hexagonal shape in $x-y$ cross section, but the height is from $-\pi/2$ to $\pi/2$, reduced by half along the θ-axis. $p4$ is the group with a 90° rotation, in a square lattice, so it has square-shaped center Voronoi cell, with the height from $-\pi/4$ to $\pi/4$, further cut by half from $p2$. $p3$ and $p6$ are the symmetry groups for a hexagonal lattice, with a 120° rotation and a 60° rotation, respectively. So they have regular hexagonal-shaped center Voronoi cells, with the height from $-\pi/3$ to $\pi/3$ and from $-\pi/6$ to $\pi/6$, respectively.

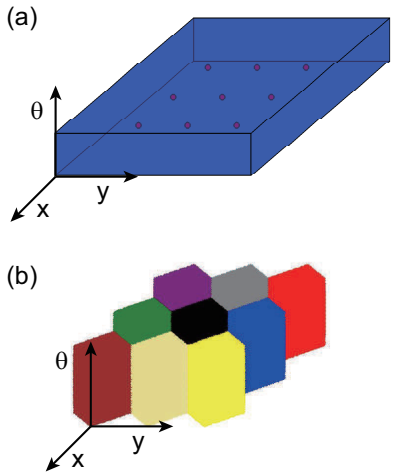

Fig. 1. (a) $SE(2)$ illustrated in $\mathbb{R}^3$ and the parallelogrammatic lattice for $p1$; (b) the Voronoi cells for $SE(2)$ based on $p1$.

This discussion of the 2D case is instructive. As can be seen, the cells can be viewed as having the same cross section for different values of θ. The spatial generalization of this is that if $G = \mathbb{R}^3 \rtimes SO(3)$ and $\Gamma = \mathbb{Z}^3 \rtimes \mathbb{P}$ where $\mathbb{P} < SO(3)$ is the crystallographic point group and $\mathbb{Z}^3 < \mathbb{R}^3$ is the lattice translation group, then

$$F_{\Gamma\backslash G} \cong F_{\mathbb{Z}^3\backslash\mathbb{R}^3} \times F_{\mathbb{P}\backslash SO(3)}.$$

It has been known for more than a century that of the 230 space groups, 65 are chiral ones, and only these occur in protein crystallography. Of these, 24 can be written as semi-direct products, as above. These are called symmorphic, and the other 41 are called nonsymmorphic. In the planar case discussed above, all five chiral wallpaper groups are

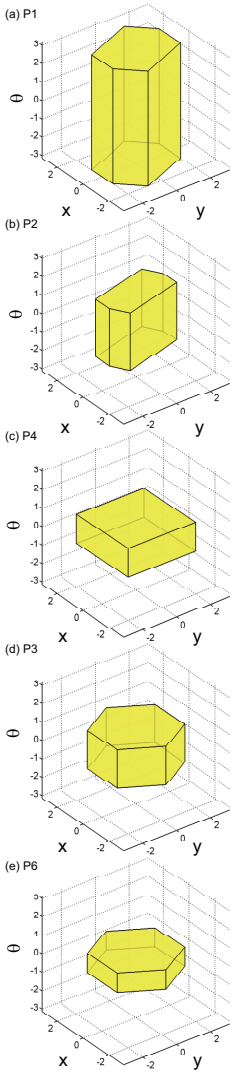

Fig. 2. $F_{\Gamma_i\backslash SE(2)}$ for chiral wallpaper groups $p1$ (a), $p2$ (b), $p4$ (c), $p3$ (d) and $p6$ (e).

symmorphic. Though motivated by the symmorphic case, in general $F_{\Gamma\backslash G}$ can be decomposed into a product of something akin to $F_{\mathbb{P}\backslash SO(3)}$ with a sample space of translations (though in the nonsymmorphic case it will not be as simple as $F_{\mathbb{Z}^3\backslash\mathbb{R}^3}$). For this reason we investigate almost-uniform sampling on $F_{\mathbb{P}\backslash SO(3)}$ by further subdividing it using double-coset decompositions.

IV. Applications to Optimization

In many problems (including the structural biology one), but also in attitude estimation, medical image registration, and in maximum likelihood computations in robot localization, one seeks to minimize a function on a Lie group (typically either $SO(n)$ or $SE(n)$ or their products). Such minimizations can be performed either using gradient descent, or using a grid-based search strategy [1]. Grid-based strategies are often favored when the terrain of the function is rugged with many local minima. Here we establish a group-theory based method for establishing grids with points that are spaced well, in contrast to a uniform grid in Euler

angles. In so doing, computational resources are not wasted on poorly constructed grid searches.

Given two finite subgroups $H,\ K < G$ where $G = SO(3)$, and the condition $|H \cap K| = 1$, then $F_{H\backslash G/K}$ can be defined as in (1) and the resulting nonoverlapping tiles generated by the action of $H \times K$ on $F_{H\backslash G/K}$ satisfy

$$G = \bigcup_{h\in H}\bigcup_{k\in K} h\overline{F_{H\backslash G/K}}k^{-1}.$$

Some examples of double-coset spaces are given in Fig. 3 with K taken as the icosahedral group for all cases and H taken as the conjugated tetrahedral group (a), the conjugated octahedral group (b) and the conjugated icosahedral group (c), respectively, where the conjugated group H with respect to the original group H_0 is defined as $H = gH_0g^{-1}$ for $g \in G$. In all cases conjugation is taken with respect to an element of G that is not in H_0 or K. In all of these figures, the shaded region is the fundamental domain for the double-coset space, the yellow dodecahedron is the fundamental domain for the single-coset space of $SO(3)$ modulo the icosahedral group computed in [36], and the plot is in terms of exponential coordinates, with $SO(3)$ itself being represented as a solid ball of radius π with antipodal points glued (not shown).

A great advantage to use the double-coset space to sample $SO(3)$ is that it can result in less metric distortion. A measure of distortion is how different the metric tensor $J^T(\mathbf{x})J(\mathbf{x})$ is from the identity matrix:

$$C(\mathbf{x}) = \frac{1}{\sqrt{3}}\|J^T(\mathbf{x})J(\mathbf{x}) - \mathbb{I}\|.$$

Explicit expressions for the Jacobians for the $SO(3)$ exponential map are known (see e.g. [6] and references therein). Here the vector of Cartesian coordinates, $\mathbf{x}$, corresponds to the exponential coordinates for $SO(3)$ in (3). Since the exponential parametrization behaves like Cartesian coordinates near the identity, i.e., $\exp\hat{\mathbf{x}} \approx \mathbb{I} + \hat{\mathbf{x}}$ when $\|\mathbf{x}\| << 1$, the metric tensor becomes $J^T(\mathbf{x})J(\mathbf{x}) \approx \mathbb{I}$, and the distortion measure $C(\mathbf{x})$ of the samples on $SO(3)$ parametrized by Cartesian grids on the center Voronoi cell is close to zero. Therefore, as $|H| \cdot |K|$ increases and the size of the center Voronoi cells shrinks, the smaller the overall distortion will be. $C(\mathbf{x})$ is the same distortion measure used in [36] to calculate the distortions in different single and double-coset spaces. In Fig. 4, we can see the maximum distortion is only 0.0074 using the double-coset space with H as the icosahedral group and K as a conjugated icosahedral group, which is only 21% of the smallest maximum distortion from the single-coset space, i.e., when one copy of the icosahedral group is used.

When $H = K$, it is possible to construct $F_{H\backslash G/H}$, but not in the way described above. In this scenario, the way to interpret $F_{H\backslash G/H}$ is as a barycentric subdivision of $F_{H\backslash G}$ such that the original coset space can be reconstructed (up to a missing set of measure zero) by the following combination of adjoint action and union

$$\overline{F_{H\backslash G}} = \bigcup_{h\in H} h\overline{F_{H\backslash G/H}}h^{-1}$$

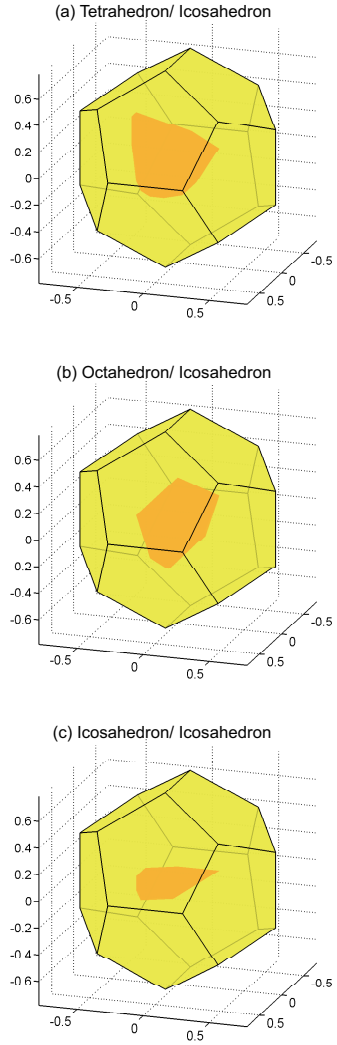

Fig. 3. The center Voronoi cell in a single-coset-space decomposition ($F_{K\backslash SO(3)} = F_{SO(3)/K}$ = yellow-shaded region) with K as the icosahedral group, and the center Voronoi cells in double-coset-space decompositions (red-shaded regions) with K as the icosahedral group for all cases and H as the conjugated tetrahedral group (a), the conjugated octahedral group (b) and the conjugated icosahedral group (c), respectively.

For example, if H is the group of rotational symmetry operations of the icosahedron, and $G = SO(3)$, then $|H| = 60$ and $\log(F_{H\backslash G})$ can be viewed as a dodecahedral cell (see Fig. 5) centered at the origin of the Lie algebra, $\mathcal{G} = so(3)$, and each $F_{H\backslash G/H}$ can be viewed as an irregular tetrahedron (the red-shaded region in Fig. 5).

Similarly, if $K < H$, then a $|K|$-fold division of $F_{H\backslash G}$ can be computed to represent $F_{H\backslash G/K}$ and these pieces can be reconstructed by adjoint action, which has the effect of rotation in $so(3)$ since $(RXR^T)^\vee = R\mathbf{x}$.

This means that when using two copies of the icosahedral group, we can divide $SO(3)$ into 3600 tetrahedral pieces of equal size and shape. A reasonably uniform and fine sampling can be obtained by choosing the point at the barycenter of each of these tetrahedra (and at their vertices if desired). If even finer samples are required, then sampling from an arbitrarily fine Cartesian grid in the Lie algebra can

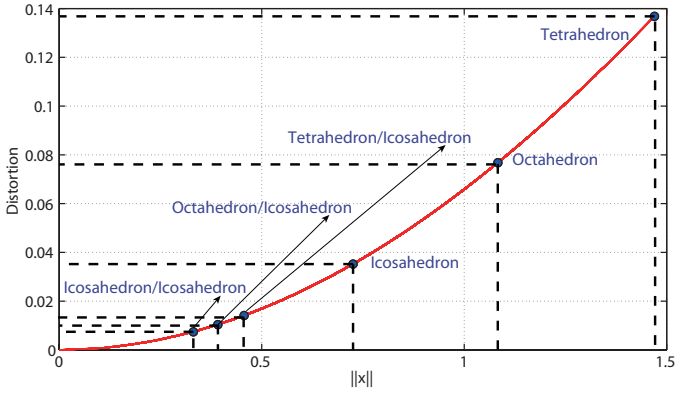

Fig. 4. The maximum distortions from different double and single coset spaces.

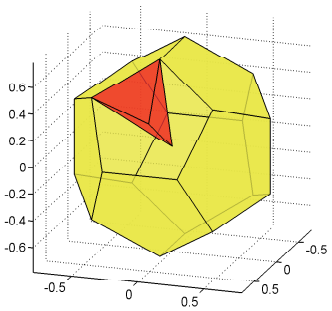

Fig. 5. The dodecahedral cell (yellow-shaded region) and the tetrahedral wedge (red-shaded region). The dodecahedral cell can be decomposed into 60 identical tetrahedral wedges like this, with 5 packed to form a pyramid with pentagonal base corresponding to a face of the dodecahedron.

be imposed within each tetrahedron.

V. FFTs and Fast Convolutions Based on Coset Decompositions

In a wide variety of problems in engineering and the physical sciences, convolutions of the form

$$(f_1 * f_2)(g) = \int_G f_1(h) f_2(h^{-1} \circ g) dh \tag{4}$$

arise [6]. Here dh is the natural integration measure for G, which can be any unimodular Lie group such as $SO(3)$, $SE(2)$, or $SE(3)$. Efficient algorithms for computing convolutions on rotation and motion groups have been developed previously using "group FFTs" [6], [13], [16], [21], [22]. In this context, usually Euler angle decompositions are used for $SO(3)$. Classical FFTs are used for the α and γ Euler angles, and various fast "Wigner-d-function transforms" in the β variable. Both Wigner-d-functions and IUR (irreducible unitary representation) matrices as developed in [30], [31].

Here we introduce two potential alternatives to this approach: (1) computing convolutions directly using the double-coset decompositions described earlier, without converting to the Fourier domain; (2) by rapidly computing Fourier transforms on groups using double-coset decompositions of the sort derived earlier.

A. Fast Convolutions by Direct Evaluation

Any integral over G can be decomposed as [32]

$$\int_G f(g) dg = \sum_{(h,k) \in H \times K} \int_{F_{H \backslash G / K}} f(h \circ g' \circ k) dg' \tag{5}$$

where dg' is the same volume volume element as for G, but restricted to $F_{H \backslash G / K} < G$.

In analogy with the FFT, which predicates speed only under the restriction that $f(g)$ is a band-limited function, we can assume that $f(g)$ can be approximated to any desired precision on $F_{H \backslash G / K}$ as a polynomial in exponential coordinates. Then, if we seek to compute (5) we can compute each $\int_{F_{H \backslash G / K}} f(h \circ g' \circ k) dg'$ rapidly via a combination of the divergence theorem and closed-form quadrature rules. The effect of this is that instead of evaluating an integral such as (5) at B sample points in each coordinate direction, which would normally take $\mathcal{O}(B^{\dim(G)})$ computations, it will take $\mathcal{O}(B^{\dim(G)-1})$ (and some constant factor that depends on the quadrature). Since a convolution involves an integral for each value of the argument, when doing by brute force, it requires $\mathcal{O}(B^{2 \cdot \dim(G)})$. However, since the values of a polynomial function can be reconstructed on the interior of the cells $F_{H \backslash G / K}$ from values on their faces, this means that effectively convolutions can be computed in $\mathcal{O}(B^{2 \cdot \dim(G)-2})$. For example, for $SO(3)$ and $SE(2)$, this is $\mathcal{O}(B^4)$ which is much more manageable than $\mathcal{O}(B^6)$

The next section reviews Fast Fourier methods on groups, which have theoretical estimates of speed that can be faster than this, but can have numerical stability problems. We then introduce a new FFT method that builds on the double-coset decompositions of G with respect to discrete subgroups.

B. Euler-Angle-Based Sampling and FFTs for $SO(3)$

The need for FFTs on the rotation group has been articulated in the context of many different applications ranging from x-ray crystallography [10], [14], [17], [26], [27], [29] to satellite attitude estimation [18], [33], [34]. Here we review the most well-known FFTs on the rotation group. In the next section we introduce our own.

Sampling and fast Fourier transforms for the rotation group were developed in [13], [21], [22]. Essentially, the double coset decomposition of $SO(3)$ as $SO(2) \backslash SO(3) / SO(2)$ corresponding to ZXZ Euler angles

$$R(\alpha, \beta, \gamma) = \exp(\alpha \widehat{\mathbf{e}}_3) \exp(\beta \widehat{\mathbf{e}}_1) \exp(\gamma \widehat{\mathbf{e}}_3)$$

yields matrix elements of the IUR matrices that lend themselves to fast transforms in each coordinate (Euler angle). In some instances, speed is sacrificed for stability when computing d-function transforms, as in [14], [24], [25].

The concept of a Fourier transform of functions with group-valued argument is well established, and the details for $SO(3)$, $SE(2)$, and $SE(3)$ have all been worked out [6], [16]. Here we focus on an alternative formulation for the $SO(3)$ case. In this context, the group Fourier transform is computed as

$$\hat{f}(l) = \int_{SO(3)} f(R) U^*(R, l) dR$$

where $U(g,l)$ is a $(2l+1)\times(2l+1)$ IUR matrix and $*$ denotes the Hermitian conjugate. IURs satisfy certain conditions such as $U(R_1R_2,l)=U(R_1,l)U(R_2,l)$, $U^*(R,l)=U(R^T,l)$ and $U(\mathbb{I}_3,l)=\mathbb{I}_{2l+1}$. By the famous Peter-Weyl theorem (which holds for any compact Lie group), the entries in these matrices form a complete orthonormal basis with which to reconstruct any $f\in L^2(SO(3))$. Any such function on $SO(3)$ can be reconstructed from its 'spectrum' $\{\hat{f}(l)\,|\,l=0,1,2,...\}$ using the Fourier inversion formula

$$f(R)=\sum_{l\in\mathbb{Z}}(2l+1)\text{trace}(\hat{f}(l)U(R,l)).$$

One reason why Fourier analysis on groups is a valuable tool is that it provides a way to compute convolutions efficiently as

$$\widehat{(f_1*f_2)}(l)=\hat{f}_2(l)\,\hat{f}_1(l).$$

Even without a 'fast' Fourier transform, this provides a speed-up over brute-force evaluation of the convolution integral at all values of its argument.

Using the notational simplification

$$f(R(\alpha,\beta,\gamma))=f(\alpha,\beta,\gamma),$$

it is possible to expand a function on the rotation group into harmonics, similar to what is done on the circle or sphere:

$$f(\alpha,\beta,\gamma)=\sum_{l=0,1,2...<B}(2l+1)\sum_{m=-l}^{l}\sum_{n=-l}^{l}\hat{f}^l_{mn}D^l_{nm}(\alpha,\beta,\gamma) \tag{6}$$

where

$$U_{mn}(R,l)=D^l_{mn}(\alpha,\beta,\gamma)=e^{-im\alpha}d^l_{mn}(\cos\beta)e^{-in\gamma} \tag{7}$$

where $-l\le m,n\le l$. $D^l_{mn}(\alpha,\beta,\gamma)$ and $d^l_{mn}(\cos\beta)$ are referred to as Wigner-D (or Wigner-d) functions, and they play a central role in quantum mechanics, where these functions serve as a complete orthonormal basis for the set of square-integrable functions on the rotation group, $L^2(SO(3))$. Essentially (6) is a Fourier series, and the coefficients can be obtained by the computation

$$\hat{f}^l_{mn}=\frac{1}{8\pi^2}\int_{\beta=0}^{\pi}\int_{\gamma=0}^{2\pi}\int_{\alpha=0}^{2\pi}f(\alpha,\beta,\gamma)\overline{D^l_{nm}(\alpha,\beta,\gamma)}\sin\beta\,d\alpha\,d\beta\,d\gamma \tag{8}$$

which is shorthand for $\hat{f}_{mn}(l)$. The whole spectrum[3] can be calculated fast in principle by using the classical FFT over α and γ and fast transforms over β. By using a quadrature rule, (8) can be sampled in each coordinate at $\mathcal{O}(B)$ values to exactly compute the integral because of the structure of U in (7). In this context the three-dimensional group manifold $SO(3)$ is then sampled at $N=\mathcal{O}(B^3)$ points.

The $\mathcal{O}(B(\log B)^2)$ required for the fast transform in the variable β is the limiting calculation, making the whole procedure is $\mathcal{O}(N(\log N)^2)$ for all values of m,n,l up to the band-limit. If the expansion in β is done directly (i.e., using $\mathcal{O}(B^2)$ operations instead of using an $\mathcal{O}(B(\log B)^2)$ fast polynomial transform), then the number of arithmetic operations to compute the $SO(3)$ Fourier transforms for all m,m,l up to the band-limit would be $\mathcal{O}(B^4)=\mathcal{O}(N^{4/3})$.

[3]Collection of Fourier transform matrix elements in (8).

Reconstructing a function on $SO(3)$ from its spectrum is a dual problem and has the same cost.

Since convolution of functions on $SO(3)$ with band-limit B requires the multiplication of matrices of dimensions $(2l+1)\times(2l+1)$ for $l=0,...,B$, the cost of convolution will be

$$\mathcal{O}\left(\sum_{l=0}^{B}(2l+1)^\gamma\right)=\mathcal{O}(B^{\gamma+1}).$$

Hence, when Gaussian elimination is used ($\gamma=3$), the order of computation of the Fourier transforms will be no greater than the cost of convolution (even when the $\mathcal{O}(B^4)$ version is used). In principle, matrix multiplication can be computed with lower exponent than $\gamma=3$, but in practice these methods can be unstable.

There are several problems with current algorithms for FFTs on $SO(3)$. First, sampling Euler angles on a grid does not result in rotational samples that are equally spaced, even when β is sampled with a $\cos^{-1}$ distribution, as in [21]. This requires over sampling of β to ensure sufficient coverage around $\beta=\pi/2$. Second, the recurrence relations used for fast Wigner-d function transforms in the β variable are notoriously unstable for large values of l. The essential reason for this is that Euler angles have singularities at $\beta=0$ and π. In the next section we show how FFTs based on coset decompositions allow for potentially fast (yet stable) approximate FFTs on the rotation group and on $SE(2)$.

C. Double-Coset Decompositions and Fast Approximate FFTs on $SO(3)$ and $SE(2)$

Euler angles are by no means the only way to parameterize $SO(3)$. And one can imagine different FFT algorithms based on different parameterizations and coset decompositions with respect to subgroups other than $SO(2)$.

The specific property of IURs that will be used in this section is that [7]

$$U(\exp X,l)=\exp(W(X,l)) \tag{9}$$

where $W(X,l)=\sum_{i=1}^{3}x_iW_i(l)$ with

$$(W_1(l))_{mn}=-\frac{i}{2}c^l_{-n}\delta_{m+1,n}-\frac{i}{2}c^l_n\delta_{m-1,n}$$

$$(W_2(l))_{mn}=+\frac{i}{2}c^l_{-n}\delta_{m+1,n}-\frac{i}{2}c^l_n\delta_{m-1,n}$$

$$(W_3(l))_{mn}=-in\delta_{m,n}$$

where $\delta_{m,n}$ is the Kronecker delta, and $c^l_n=\sqrt{(l-n)(l+n+1)}$ for $|n|\le l$. We use the property in (9) together with the double-coset decomposition. Explicitly,

$$\hat{f}(l)=\sum_{(P,Q)\in\mathbb{P}\times\mathbb{Q}}\int_{F_{\mathbb{P}\backslash SO(3)/\mathbb{Q}}}f(PRQ)U((PRQ)^T,l)dR,$$

which can be rewritten as

$$\sum_{(P,Q)\in\mathbb{P}\times\mathbb{Q}}U(Q^T,l)\left[\int_{F_{\mathbb{P}\backslash SO(3)/\mathbb{Q}}}f(PRQ)U(R^T,l)dR\right]U(P^T,l).$$

where $\mathbb{P},\mathbb{Q}<SO(3)$ are finite. We can think of $f(PRQ)$ as the function $f(R)$ being moved under left and right action so

that the point initially at R is now in the vicinity of $\mathbb{I}$. The fact that on the fundamental domain centered on the identity $U(\exp X, l)$ can be expressed as a truncated Taylor series in X is then very useful because $W(X,l)$ will have polynomial entries, each of which can be computed by evaluation on their boundary. And hence the computation of the integral over $F_{\mathbb{P}\backslash SO(3)/\mathbb{Q}}$ is efficient.

The number of terms needed in the truncation of $U(\exp X, l)$ is related to how fine the subdivision of $SO(3)$ into cells is; The finer the subdivision, the fewer terms needed in the Taylor series.

Regarding the Fourier inversion formula, the double-coset decompositions of the sort used throughout this paper have the benefit that they can use the tri-diagonal nature of the W_i matrices (when each PRQ is close to the identity, which is the case by our choice of fundamental domain for double cosets). This is in place of the recurrence relations that are usually used for matrix elements of $D(R,l)$, which can be unstable.

VI. Conclusions

We make a connection between Voronoi cells in the groups $SO(3)$ and $SE(2)$ centered on elements of discrete subgroups, and coset- and double-coset-spaces. We show that sampling within these Voronoi cells can be made almost uniform by exponentiating a Cartesian grid in a region of the corresponding Lie algebra, which is the pre-image of these cells under the exponential map. We show how the resulting cells, and the samples therein, can be used for searches, optimization, and Fourier analysis on certain Lie groups of interest in robotics and control.

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