Estimation under group actions: recovering orbits from invariants

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Abstract

Motivated by geometric problems in signal processing, computer vision, and structural biology, we study a class of orbit recovery problems where we observe noisy copies of an unknown signal, each acted upon by a random element of some group (such as \( \mathbb{Z}/p \) or \( \text{SO}(3) \)). The goal is to recover the orbit of the signal under the group action. This generalizes problems of interest such as multi-reference alignment (MRA) and the reconstruction problem in cryo-electron microscopy (cryo-EM). We obtain matching lower and upper bounds on the sample complexity of these problems in high generality, showing that the statistical difficulty is intricately determined by the invariant theory of the underlying symmetry group.

In particular, we determine that for cryo-EM with noise variance \( \sigma^2 \) and uniform viewing directions, the number of samples required scales as \( \sigma^6 \). We match this bound with a novel algorithm for ab initio reconstruction in cryo-EM, based on invariant features of degree at most 3. We further discuss how to recover multiple molecular structures from heterogeneous cryo-EM samples.

1 Introduction

Many computational problems throughout the sciences exhibit rich symmetry and geometry, especially in fields such as signal and image processing, computer vision, and microscopy. This is exemplified in cryo-electron microscopy (cryo-EM) [ADLM84, SS11, Nog16], an imaging technique in structural biology that was recently awarded the 2017 Nobel Prize in Chemistry. This technique seeks to estimate the structure of a large biological molecule, such as a protein, from many noisy tomographic projections (2-dimensional images) of the molecule from random unknown directions in 3-dimensional space.

In cryo-EM, our signal of interest is the density \( \theta \) of the molecule, considered as an element of the vector space of functions on \( \mathbb{R}^3 \). We have access to observations of the following form: our microscopy sample contains many rotated copies \( R_i \theta \) of the molecule, where \( R_i \in \text{SO}(3) \) are random, unknown 3D
rotations, and we observe the noisy projections \( \Pi(R_i \theta) + \xi_i \), where \( \Pi \) denotes tomographic projection (in a fixed direction) and \( \xi_i \) is a large noise contribution, perhaps Gaussian. This specific problem motivates the following abstraction.

Fix a compact group \( G \) acting (by orthogonal transformations) on a vector space \( V \). Throughout, the vector space will be taken to be \( \mathbb{R}^p \) and the group can be thought of as a subgroup of \( O(p) \), the orthogonal group \( O(p) \). Let \( \theta \in V \) be the signal we want to estimate. We receive noisy measurements of its orbit as follows: for \( i = 1, \ldots, n \) we observe a sample of the form

\[
y_i = g_i \cdot \theta + \xi_i
\]

where \( g_i \) is drawn randomly (in Haar measure) from \( G \) and \( \xi_i \sim N(0, \sigma^2 I) \) is noise. The goal is to recover the orbit of \( \theta \) under the action of \( G \). We refer to this task as the orbit recovery problem.

This abstraction, already a rich object of study, neglects the tomographic projection in cryo-EM; we will also study a generalization of the problem which allows such a projection. We will also consider the additional extension of heterogeneity \[ Jon16 \] \[ LS16 \] \[ LS17 \] \[ BBL17 \], where mixtures of signals are allowed: we have \( K \) signals \( \theta_1, \ldots, \theta_K \), and each sample \( y_i = g_i \cdot \theta_k_i + \xi_i \) comes from a random choice \( 1 \leq k_i \leq K \) of which signal is observed. This extension is of paramount importance for cryo-EM in practice, since the laboratory samples often contain one protein in multiple conformations, and understanding the range of conformations is key to understanding the function of the protein.

### 1.1 Prior work

Several special cases of the orbit recovery problem have been studied for their theoretical and practical interest. Besides cryo-EM, another such problem is multi-reference alignment (MRA) \[ BCSZ14 \] \[ BRW17 \] \[ PWB17 \], a problem from signal processing \[ ZvdHGC03 \] \[ PZAF05 \] with further relevance to structural biology \[ Dia92 \] \[ TS12 \]. In this problem, one observes noisy copies of a signal \( \theta \in \mathbb{R}^p \), each with its coordinates permuted by a random cyclic shift. This is an example of the orbit recovery problem where \( G \) is taken to be the cyclic group \( \mathbb{Z}/p \) acting by cyclic permutations of the coordinates. Since the cyclic group \( \mathbb{Z}/p \) is simpler than \( SO(3) \), understanding MRA has been seen as a useful stepping stone towards a full statistical analysis of cryo-EM.

Many prior methods for orbit recovery problems employ the so-called synchronization approach where the unknown group elements \( g_i \) are estimated based on pairwise comparison of the samples \( y_i \). If the samples were noiseless, one would have \( g_i g_j^{-1} y_j = y_i \); thus noisy samples still give some weak information about \( g_i g_j^{-1} \). Synchronization is the problem of using such pairwise information to recover all the group elements \( g_i \) (up to a global right-multiplication by some group element). Once the group elements \( g_i \) are known, the underlying signal can often be easily recovered.

The synchronization approach to cryo-EM can be summarized as follows \[ VG86 \] \[ VHS7 \] \[ SS11 \]. By the Fourier projection-slice theorem, the Fourier transforms of the tomographic projections are 2D slices of the Fourier transform of the molecule density. Given a hypothesis as to the angles of two slices, we can predict a 1D line of intersection along which those slices should agree. By measuring correlation along that common line, we obtain some weak information by which to confirm or refute our hypothesized angles. Indeed, this test only depends on the relative angle of the slices, thus providing weak information about the value of \( g_i g_j^{-1} \). We then use a synchronization algorithm to recover the \( g_i \) using this information.

Methods to solve the synchronization problem over various groups include spectral methods \[ Sin11 \] \[ SS11 \], semidefinite programming \[ Sin11 \] \[ SS11 \] \[ BCSZ14 \] \[ BCS15 \] \[ Ban15 \] \[ BZS15 \], and approximate message passing (AMP) \[ PWB16a \]. A general Gaussian model for synchronization problems over any compact group is studied in \[ PWB16b \] \[ PWB16a \]; ideas from statistical physics suggest that for this model, AMP is

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1. We alert the reader to the fact that we will use \( O(p) \) to refer to the group of orthogonal matrices in dimension \( p \) and \( O(r(n)) \) as the standard big-O notation: \( f(n) = O(g(n)) \) if and only if there exists a constant \( C \) such that \( f(n) \leq C g(n) \) for all \( n \) sufficiently large. It will be clear from context which one is meant.

2. We note that any distribution of \( g_i \) can be reduced to Haar by left multiplying \( y_i \) by a Haar-distributed group element. However, as illustrated in \[ ABL+17 \], it is sometimes possible to exploit deviations from Haar measure.
optimal among all efficient algorithms \[PWBM16a\]. However, the model does not capture the underlying signal \(\theta\) and instead assumes that for every pair \(i, j\) of samples, independent noisy measurements of the relative group elements \(g_i g_j^{-1}\) are observed. This independence does not correctly capture problems like MRA and cryo-EM, which have independent noise on each sample, rather than on each pairwise comparison of samples.

The synchronization approach has proven to be effective both in theory and practice when the noise is sufficiently small. However, once the noise level is large, no consistent estimation of the group elements \(g_i\) is possible \[ADBS16\]. Moreover, it is the high-noise regime that is the practically relevant one for many applications, including cryo-EM, where the presence of large noise is a primary obstruction to current techniques \[Sig16\]. As a result, recent work has focused on approaches to cryo-EM and MRA which provably succeed even in the large-noise limit. One striking finding of this line of work is that the sample complexity of the statistical estimation problem increases drastically as the noise level increases. For instance, for the multi-reference alignment problem with noise variance \(\sigma^2\), consistent estimation of typical signals requires \(\Omega(\sigma^6)\) samples \[BRW17\, APS17\], with significantly worse rates for atypical signals. By contrast, when \(\sigma^2\) is smaller than some threshold, only \(O(\sigma^2)\) samples are required. Moreover, in contrast with the \(O(\sigma^2)\) rate—which would hold even in the absence of a group action—the \(\Omega(\sigma^6)\) bound obtained in previous works depends on particular properties of the cyclic group. In this work, we significantly extend this prior work by determining the sample complexity of the estimation problem in the high-noise regime for general groups.

The leading theoretical framework for the high-noise regime is the invariant features approach \[BRW17, BBM+17, PWB+17, BLB+17\]. This approach has a long history in the signal processing literature \[Kam80, Sad89, SG92\] and is analogous to the well known “method of moments” in statistics \[vdV98\]. In brief, the invariant features approach bypasses entirely the problem of estimating the group elements and focuses instead on estimating features of the signal which are preserved by the action of the group. So long as these invariant features uniquely specify the orbit of the original signal, the invariants are sufficient statistics for the problem of recovering the orbit of the original signal. This simple approach yields optimal dependence of the sample complexity on the noise level for the multi-reference alignment problem \[BRW17, PWB+17\].

The application of invariant features to cryo-EM dates back to 1980 with the work of Kam \[Kam80\], who partially solved cryo-EM by means of degree-2 invariant features, reducing the unknown molecule structure to a collection of unknown orthogonal matrices. Subsequent work has explored methods to estimate these orthogonal matrices \[BZS15\], including recent work showing how two noiseless tomographic projections suffice to recover these orthogonal matrices \[LBB+17\]. Our work can be viewed as a degree-3 extension of Kam’s method that fully solves cryo-EM while circumventing the orthogonal retrieval issue, and without requiring any noiseless projections. Our approach is \textit{ab initio}, i.e. it does not require an initial guess of what the molecule looks like and thus cannot suffer from \textit{model bias}, which is a documented phenomenon \[Coh13\] where the initial guess can have a significant effect on the result. Ab initio estimates are particularly useful to serve as a model-free starting point for popular iterative refinement algorithms such as RELION \[Sch12\].

Throughout, we focus on the case where the group elements are Haar-distributed. In the basic orbit recovery problem (projection), any distribution of \(g_i\) can be reduced to Haar by left-multiplying each sample \(y_i\) by a Haar-distributed group element. However, as illustrated in \[ABL+17\], it is sometimes possible to exploit deviations from Haar measure. The situation is different when we add projection to the problem setup, as is the case with Cryo-EM; if the viewing direction is not distributed uniformly then there may exist parts of the molecule that are systematically imaged less than others, which can cause serious difficulties in reconstruction.

The present paper connects the orbit recovery problem to the invariant theory of groups, a classical and well-developed branch of algebra (see for example \[Kac94, Dol03, Stu08, DK15\]). Invariant theory’s traditional goal is to describe the ring of all polynomial functions on a vector space that are invariant under the action of a group – the \textit{invariant algebra}. Since the 19th century, culminating in the pioneering work of David Hilbert \[Hil90, Hil93\], it has been known that the invariant algebra is finitely generated in many cases of interest, and so a fundamental problem has been to bound the degrees of the generators. In 2002, Derksen and Kemper \[DK15\] introduced the notion of a \textit{separating algebra} – a subring of the invariant algebra that separates all orbits of the group action which are separated by the full invariant algebra. Our connection
to orbit recovery motivates the question of bounding the degree required to generate a separating algebra (see Section 4.3), a problem which has been recently studied [KK10 Dom16]. Our work also motivates the question of bounding the degree at which the field of invariant rational functions is generated as a field (see Section 4.3), which does not appear to have been the focus of research attention before.

1.2 Our contributions

In this paper we extend the results of [BRW17] and show that the method of moments yields optimal sample complexity for orbit recovery problems over any compact group. Specifically, we show that optimal sample complexity is achieved by an algorithm that estimates the moments from the samples and then solves a polynomial system of equations in order to find a signal \( \theta \) that would produce such moments. As the sample complexity depends on the number of moments used, this gives rise to the algebraic question of how many moments suffice to determine the orbit of \( \theta \). Using tools from invariant theory and algebraic geometry, we investigate this question for various success criteria and obtain sharp results in a number of settings. Our main focus is on the case where the signal is assumed to be generic and the goal is to output a finite list of signals, one of which is the truth. In this case we give a simple efficient algorithm for determining the number of moments required for any given orbit recovery problem. The main step of the algorithm is to compute the rank of a particular Jacobian matrix.

We note that ours is an information-theoretic result rather than a computational one because even with knowledge of the number of moments required, estimating the original signal still requires solving a particular polynomial system of equations and we do not attempt to give a computationally-efficient method for this. There are fast non-convex heuristic methods to solve these systems in practice [BBLST17] but we leave for future work the question of analyzing such methods rigorously and exploring whether or not they reach the information-theoretic limits determined in this paper. For the case of finite groups, another efficient method for solving the polynomial system is via tensor decomposition, which has been analyzed for MRA [PWB+17].

Concrete results for problems such as MRA and cryo-EM are in Section 5.

1.3 Motivating examples

In addition to the examples of MRA and cryo-EM, it is helpful to have the following motivating examples in mind:

1. Learning a “bag of numbers”: let \( G \) be the symmetric group \( S_p \), acting on \( V = \mathbb{R}^p \) by permutation matrices. Thus we observe random rearrangements of the entries of a vector, plus noise.

2. Learning a rigid body: let \( G \) be the rotation group \( SO(p) \), acting on the matrix space \( V = \mathbb{R}^{p \times m} \) by left-multiplication. We imagine the columns of our matrix as vertices defining a rigid body; thus we observe random rotations of this rigid body (with vertices labeled) plus noise.

3. \( S^2 \) registration: Let \( S^2 \subseteq \mathbb{R}^3 \) be the unit sphere. Let \( V \) be the finite-dimensional vector space of functions on \( S^2 \to \mathbb{R} \) that are band-limited, i.e. linear combinations of spherical harmonics up to some fixed degree (spherical harmonics are the appropriate “Fourier basis” for functions on the sphere); let \( \theta \in V \) be such a function \( S^2 \to \mathbb{R} \). Let \( G = SO(3) \), acting on the sphere by 3-dimensional rotation; this induces an action on \( V \) via \((g \cdot \theta)(x) = \theta(g^{-1} \cdot x)\). Thus we observe many noisy copies of a fixed function on the sphere, each rotated randomly.

1.4 Problem statement

Throughout, we consider a compact (topological) group \( G \) acting linearly, continuously, and orthogonally on a finite-dimensional real vector space \( V = \mathbb{R}^p \). In other words, \( G \) acts on \( V \) via a linear representation \( \rho : G \to O(V) \), and \( \rho \) itself is a continuous function. Here \( O(V) \) denotes the space of real orthogonal \( p \times p \) matrices. Let \( Haar(G) \) denote Haar measure (i.e., the “uniform distribution”) on \( G \). We define the orbit recovery problem as follows.
Problem 1.1 (orbit recovery). Let \( V = \mathbb{R}^p \) and let \( \theta \in V \) be the unknown signal. Let \( G \) be a compact group that acts linearly, continuously, and orthogonally on \( V \). For \( i \in \{1, 2, \ldots, n\} \) we observe

\[
y_i = g_i \cdot \theta + \xi_i
\]

where \( g_i \sim \text{Haar}(G) \) and \( \xi_i \sim \mathcal{N}(0, \sigma^2 I_{p \times p}) \), all independently. The goal is to estimate \( \theta \). Note that we can only hope to recover \( \theta \) up to action by \( G \); thus we aim to recover the orbit \( \{ g \cdot \theta : g \in G \} \) of \( \theta \).

In practical applications, \( \sigma \) is often known in advance and, when it is not, it can generally be estimated accurately on the basis of the samples. We therefore assume throughout that \( \sigma \) is known and do not pursue the question of its estimation in this work.

Our primary goal is to study the sample complexity of the problem: how must the number of samples \( n \) scale with the noise level \( \sigma \) (as \( \sigma \to \infty \) with \( G \) and \( V \) fixed) in order for orbit recovery to be statistically possible? All of our results will furthermore apply to a generalized orbit recovery problem (Problem 2.3) allowing for projection and heterogeneity (see Section 1.6).

Our work reveals that it is natural to consider several different settings in which to state the orbit recovery problem. We consider the following two decisions:

1. Do we assume that \( \theta \) is a *generic* signal, or do we allow for a *worst-case* signal? (Here *generic* means that there is a measure-zero set of disallowed signals.)

2. Do we want to output a \( \theta' \) such that \( \theta' \) (approximately) lies in the orbit of \( \theta \) (*unique recovery*), or simply a finite list \( \theta_1, \ldots, \theta_s \) of candidates such that one of them (approximately) lies in the orbit of \( \theta \) (*list recovery*)?

The terminology “list recovery” is borrowed from the idea of *list decoding* in the theory of error-correcting codes [El57]. By taking all combinations of the two options above, there are four different recovery criteria. Strikingly, these different recovery criteria can be very different in terms of sample complexity, as the following examples show (see Section 5 for more details):

1. **Multi-reference alignment (MRA):** Recall that this is the case \( G = \mathbb{Z}/p \) acting on \( V = \mathbb{R}^p \) by cyclic shifts. It is known [PWB+17] that if \( \theta \) is generic then unique recovery is possible with \( O(\sigma^6) \) samples. However, for a worst-case \( \theta \), many more samples are required (even for list recovery); as shown in [BRW17], there are some very particular infinite families of signals that cannot be distinguished without \( \Omega(\sigma^{2p}) \) samples. This illustrates a large gap in difficulty between the generic and worst-case problems.

2. **Learning a rigid body:** Let \( G \) be the rotation group \( \text{SO}(p) \) acting on the matrix space \( \mathbb{R}^{p \times m} \) by left multiplication. We imagine the columns of our matrix as vertices defining a rigid body; thus we observe random rotations of this rigid body (with vertices labeled) plus noise. With \( O(\sigma^4) \) samples it is possible to recover the rigid body up to reflection, so that list recovery (with a list of size 2) is possible. However, unique recovery (even for a generic signal) requires drastically more samples: \( \Omega(\sigma^{2p}) \).

We will address all four recovery criteria but our main focus will be on the case of *generic list recovery*, as it is algebraically the most tractable to analyze. For the following reasons we also argue that it is perhaps the most practically relevant case. Clearly real-world signals are generic. Also, unique recovery is actually impossible in some practical applications; for instance, in cryo-EM it is impossible to determine the chirality of the molecule. Furthermore, one could hope to use application-specific clues to pick the true signal out from a finite list; for instance, in cryo-EM we might hope that the spurious solutions in our finite list do not look like “reasonable” molecules and can be thrown out.

1.5 Method of moments

Our techniques rely on estimation of the following moments:

**Definition 1.2** (moment tensor). The *order-\( d \) moment tensor* is \( T_d(\theta) := \mathbb{E}_g[(g \cdot \theta)^{\otimes d}] \) where \( g \sim \text{Haar}(G) \).
Theorem 1.4. error probability

Consider for now the simple problem of distinguishing between two fixed hypotheses \( \theta = \tau_1 \) and \( \theta = \tau_2 \), where \( \tau_1 \) and \( \tau_2 \) are two fixed vectors in \( V \). One method is to find an invariant polynomial \( f \) for which \( f(\tau_1) \neq f(\tau_2) \) and to estimate \( f(\theta) \) using the samples. The sample complexity of this procedure depends on the degree of \( f \) because if \( f \) has degree \( d \), we need \( O(\sigma^{2d}) \) samples to accurately estimate \( f(\theta) \). We will prove the following (see Section 3).

**Theorem 1.4** (distinguishing upper bound). Fix \( \tau_1, \tau_2 \in V \). If there exists a degree-\( d \) invariant polynomial \( f \in \mathbb{R}[x]^G \) with \( f(\tau_1) \neq f(\tau_2) \) then, using \( O(\sigma^{2d}) \) samples, it is possible to distinguish between \( \theta = \tau_1 \) and \( \theta = \tau_2 \) with type-I and type-II error probabilities each at most \( 1/3 \).

Here, \( O(\cdots) \) hides factors that depend on \( G \) (and its action on \( V \)), \( \tau_1 \), and \( \tau_2 \), but not \( \sigma \); we are most interested in how the sample complexity scales as \( \sigma \) becomes large (with everything else held fixed). The error probability \( 1/3 \) is arbitrary and can be boosted by taking more samples (see Theorem 1.4).

Furthermore, we have a matching lower bound to show that the method of moments is optimal: the sample complexity is driven by the minimum degree of an invariant polynomial that separates \( \tau_1 \) and \( \tau_2 \).

**Theorem 1.5** (distinguishing lower bound). Fix \( \tau_1, \tau_2 \in V \). Let \( d^* \) be the smallest positive integer \( d \) for which \( T_d(\tau_1) \neq T_d(\tau_2) \). Then \( \Omega(\sigma^{2d^*}) \) samples are required to distinguish between \( \theta = \tau_1 \) and \( \theta = \tau_2 \) with type-I and type-II error probabilities each at most \( 1/3 \).

See Section 3 for more details.

1.5.2 Recovery

We now address the problem of recovering the signal \( \theta \) from the samples. Our goal is to recover the orbit of \( \theta \), defined as follows.

**Definition 1.6.** For \( \theta_1, \theta_2 \in V \), define an equivalence relation \( \sim \) by letting \( \theta_1 \sim \theta_2 \) if there exists \( g \in G \) such that \( g \cdot \theta_1 = \theta_2 \). The orbit of \( \theta \) (under the action of \( G \)) is the equivalence class of \( \theta \) under \( \sim \), i.e. the set \( \{ g \cdot \theta \mid g \in G \} \). Denote by \( V/G \) the set of orbits of \( V \), that is, the equivalence classes of \( V \) modulo the relation \( \sim \).

We need the following definitions to capture the notion of approximately recovering the orbit of \( \theta \).
Definition 1.7. For \( \theta_1, \theta_2 \in V \), let
\[
d_G(\theta_1, \theta_2) = \min_{g \in G} \| \theta_1 - g \cdot \theta_2 \|_2.
\]
This pseudometric induces a metric on the quotient space \( V/G \) in the obvious way, so we can write \( d_G(\sigma_1, \sigma_2) \) for \( \sigma_1, \sigma_2 \in V/G \). By slight abuse of notation, we write \( d_G(\theta_1, \sigma_2) \) for \( d_G(\sigma_1, \sigma_2) \), where \( \sigma_1 \) is the orbit of \( \theta_1 \).

Theorem 1.5 already shows that if the orbit of \( \theta \) is not determined by knowledge of the first \( d-1 \) moment tensors, then at least \( \Omega(\sigma^{2d}) \) samples are required to recover the orbit of \( \theta \). We are now ready to (informally) state our main result on recovery (see Section 3 for more details), which provides a matching upper bound.

**Theorem 1.8** (recovery upper bound, informal). Fix \( \theta \in V \). If the moments \( T_1(\theta), \ldots, T_d(\theta) \) uniquely determine the orbit of \( \theta \), then using \( O(\sigma^{2d}) \) samples, we can produce an estimator \( \hat{\theta} \) such that \( d_G(\theta, \hat{\theta}) \leq \varepsilon \) with high probability.

The analogous result holds for list recovery (see Section 3): if the moments determine a finite number of possibilities for the orbit of \( \theta \) then we can output a finite list of estimators, one of which is close to the orbit of \( \theta \).

Thus, we have reduced to the algebraic question of determining how many moments are necessary to determine the orbit of \( \theta \) (either uniquely or in the sense of list recovery). In Section 4 we will use tools from invariant theory and algebraic geometry in order to address these questions.

1.6 Extensions: projection and heterogeneity

We now consider some extensions to the basic orbit recovery problem (Problem 1.1), motivated by the application of cryo-EM:

1. **Projection**: In cryo-EM, we do not observe a noisy 3-dimensional model of the rotated molecule; we only observe a 2-dimensional projection of it. We will model this projection by a linear map \( \Pi : \mathbb{R}^p \rightarrow \mathbb{R}^q \) that maps a 3-dimensional model to its 2-dimensional projection (from a fixed viewing direction). The samples are then given by \( y_i = \Pi(g_i \cdot \theta) + \xi_i \) where \( \xi_i \sim N(0, \sigma^2 I) \).

2. **Heterogeneity**: In cryo-EM we observe images of many different copies of the same molecule, each rotated differently. However, if our sample is not pure, we may have a mixture of different molecules and want to recover the structure of all of them. We will model this by taking \( K \) different unknown signals \( \theta_1, \ldots, \theta_K \) along with positive mixing weights \( w_1, \ldots, w_K \) which sum to 1. Each sample takes the form \( y_i = g_i \cdot \theta_{k_i} + \xi_i \) where \( k_i \) is chosen at random according to the mixing weights.

In Section 2 we will formally define a generalization of the orbit recovery problem that allows for either (or both) of the above extensions. All of our methods will apply to this general case.

1.7 Organization of the remainder of the paper

In Section 2 we define a generalization of Problem 1.1 which encompasses projection and heterogeneity, and specify the basic algebraic objects which relate to our generalized problem. In Section 3 we formally state statistical upper and lower bounds for the generalized orbit recovery problem in terms of invariants. In Section 4 we establish our basic algebraic results and specify the algebraic criteria that correspond to the different recovery criteria defined in Section 1.4. We also give an efficient algorithm to decide the algebraic criterion corresponding to generic list recovery. Finally, in Section 5 we apply our work to several examples of the orbit recovery problem, including MRA and cryo-EM. We conclude in Section 6 with questions for future work.

Sections 7–9 contain proofs of results from preceding sections. Appendix A contains an account of the invariant theory of \( \text{SO}(3) \), and Appendix B contains a proof (using Galois theory) of generic unique recovery in a particular special case of the orbit recovery problem (the regular representation of a finite Abelian group).
2 General problem statement

Our results will apply not only to the basic orbit recovery problem (Problem 1.1) but to a generalization (Problem 2.3 below) that captures the projection and heterogeneity extensions discussed in Section 1.6. We first define mixing weights for heterogeneous problems.

**Definition 2.1** (mixing weights). Let \( w = (w_1, \ldots, w_K) \in \Delta_K := \{ \{z_1, \ldots, z_K\} : z_k \geq 0 \ \forall k, \sum_{k=1}^K z_k = 1 \} \). Let \( k \overset{\text{rand}}{\sim} [K] \) indicate that \( k \) is sampled from \([K] = \{1, \ldots, K\}\) such that \( k = \ell \) with probability \( w_\ell \). We will sometimes instead parametrize the mixing weights by \( \pi_k = w_k - 1/K \) so that \( \pi \) lies in the vector space \( \Delta := \{ \{z_1, \ldots, z_K\} : \sum_{k=1}^K z_k = 0 \} \).

In a heterogeneous problem with \( K \) different signals, we can only hope to recover the signals up to permutation. To formalize this, our compound signal will lie in a larger vector space \( V \) and we will seek to recover its orbit under a larger group \( \hat{G} \).

**Definition 2.2** (setup for heterogeneity). Let \( \hat{G} \) be a compact group acting linearly, continuously, and orthogonally on \( \hat{V} = \mathbb{R}^p \). Let \( V = \hat{V} \rtimes K \), so that \( \theta \in V \) encodes \( K \) different signals along with mixing weights: \( \theta = (\theta_1, \ldots, \theta_K, \pi) \). We let an element \((g_1, \ldots, g_K, \pi)\) of the Cartesian product set \( \hat{G}^K \times S_K \) act on \( V \) as follows: first, each \( g_k \) acts on the corresponding \( \theta_k \), and then \( \pi \) permutes the \( \theta_k \) and the coordinates of \( \pi \). Note that this action is linear and orthogonal (where \( \Delta \) uses the usual inner product inherited from \( \mathbb{R}^K \)).

There is a natural group structure on the set \( \hat{G}^K \times S_K \) such that the action just described is actually a group action by \( G \); the semidirect product \( G = \hat{G}^K \rtimes_{\phi} S_K \), where \( \phi \) denotes the action of \( S_K \) on \( \hat{G}^K \) by permutations of the factors. This is also called the wreath product of \( \hat{G} \) by \( S_K \) and written \( \hat{G} \wr S_K \). The product topology on \( \hat{G}^K \times S_K \) makes \( G \) a topological group; it is compact with respect to this topology since all the factors are compact, and the action described above is continuous.

Of course, by taking \( K = 1 \) we recover the basic setup (without heterogeneity) as a special case. We are now ready to give the general problem statement.

**Problem 2.3** (generalized orbit recovery). Let \( \hat{V} = \mathbb{R}^p \) and \( W = \mathbb{R}^q \). Let \( \hat{G} \) be a compact group acting linearly, continuously, and orthogonally on \( \hat{V} \). Let \( \hat{V} = \hat{V} \rtimes K \), so that \( \theta \in \hat{V} \) encodes \( K \) different signals with mixing weights \( \theta = (\theta_1, \ldots, \theta_K, \pi) \). We let an element \((g_1, \ldots, g_K, \pi)\) of the Cartesian product set \( \hat{G}^K \times S_K \) act on \( V \) as follows: first, each \( g_k \) acts on the corresponding \( \theta_k \), and then \( \pi \) permutes the \( \theta_k \) and the coordinates of \( \pi \). Note that this action is linear and orthogonal (where \( \Delta \) uses the usual inner product inherited from \( \mathbb{R}^K \)). There is a natural group structure on the set \( \hat{G}^K \times S_K \) such that the action just described is actually a group action by \( G \); the semidirect product \( G = \hat{G}^K \rtimes_{\phi} S_K \), where \( \phi \) denotes the action of \( S_K \) on \( \hat{G}^K \) by permutations of the factors. This is also called the wreath product of \( \hat{G} \) by \( S_K \) and written \( \hat{G} \wr S_K \). The product topology on \( \hat{G}^K \times S_K \) makes \( G \) a topological group; it is compact with respect to this topology since all the factors are compact, and the action described above is continuous.

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Of course, by taking \( K = 1 \) we recover the basic setup (without heterogeneity) as a special case. We are now ready to give the general problem statement.
Theorem establishes that we can approximately learn the order-
and \( n^\hat{\epsilon} \) exists an estimator \( \phi \)
of polynomials (one for each entry of \( T_d(\theta) \)) that map \( \theta \) to \( T_d(\theta) \).

We will be interested in whether the subspace \( U_{\leq d}^T \) contains enough information to uniquely determine the orbit of \( \theta \) (or determine a finite list of possible orbits) in the following sense.

**Definition 2.7.** A subspace \( U \subseteq \mathbb{R}[x]^G \) resolves \( \theta \in V \) if there exists a unique \( \phi \in V/G \) such that \( f(\theta) = f(\phi) \) for all \( f \in U \). Similarly, \( U \) list-resolves \( \theta \) if there are only finitely many orbits \( \phi_1, \ldots, \phi_\ell \) such that \( f(\theta) = f(\phi_i) \) for all \( f \in U \).

Here we have abused notation by writing \( f(\phi) \) to denote the (constant) value that \( f \) takes on every \( \theta \in \phi \). The following question is of central importance.

**Question 2.8.** Fix \( \theta \in V \). How large must \( d \) be in order for \( U_{\leq d}^T \) to uniquely resolve \( \theta \)? How large must \( d \) be in order for \( U_{\leq d}^T \) to list-resolve \( \theta \)?

The answer depends on \( G \) and \( V \) but also on whether \( \theta \) is a generic or worst-case signal, and whether we ask for unique recovery or list recovery. Our statistical results in Section 3 will show that the sample complexity of the generalized orbit recovery problem is \( \Theta(\sigma^{2d}) \) where \( d \) is the minimal \( d \) from Question 2.8. More specifically, the recovery procedure that obtains this bound is based on estimating the moments \( T_1(\theta), \ldots, T_d(\theta) \) and solving a system of polynomial equations to (approximately) recover \( \theta \). Our algebraic results in Section 4 will give general methods to answer Question 2.8 for any \( G \) and \( V \).

## 3 Statistical results

In this section, we state upper and lower bounds on the performance of optimal estimators for the orbit recovery problem. Proofs are deferred to Section 7. Our approach will be the method of moments introduced in Section 1.3. We assume for normalization purposes that there exists a constant \( c \geq 1 \) such that \( c^{-1} \leq ||\theta|| \leq c \), so that \( \sigma \) captures entirely the signal-to-noise ratio of the problem. We denote by \( \Theta \) the subset of \( V \) consisting of vectors satisfying this requirement.

Denote by \( P_\theta \) the distribution of a sample arising from the generalized orbit recovery problem (Problem 2.4) with parameter \( \theta \).

**Definition 3.1.** Given \( \theta \in \Theta \), the order-\( d \) matching set for \( \theta \), \( \mathcal{M}_{\theta,d} \), is the set consisting of all \( \tau \in V \) such that \( f(\tau) = f(\theta) \) for all \( f \in U_{\leq d}^T \).

We note that \( U_{\leq d}^T \) resolves \( \theta \) exactly when \( \mathcal{M}_{\theta,d} \) contains a single orbit, and \( U_{\leq d}^T \) list-resolves \( \theta \) when \( \mathcal{M}_{\theta,d} \) is the union of a finite number of orbits.

We are now ready to state a formal theorem justifying Theorems 1.4 and 1.8 above. The following theorem establishes that we can approximately learn the order-\( d \) matching setting for \( \theta \) with probability at least \( 1-\delta \) on the basis of \( O(\sigma^{2d}\log(1/\delta)) \) samples. Denote by \( \mathcal{M}_{\theta,d}^\epsilon \) the \( \epsilon \)-fattening of \( \mathcal{M}_{\theta,d} \), i.e., the set of all \( \phi \in \Theta \) such that \( \min_{\tau \in \mathcal{M}_{\theta,d}^\epsilon} ||\phi - \tau|| \leq \epsilon \).

**Theorem 3.2.** For any positive integer \( n \), noise level \( \sigma \geq \max_{\theta \in \Theta} ||\theta|| \), and accuracy parameter \( \delta > 0 \), there exists an estimator \( \hat{\mathcal{M}}_n = \hat{\mathcal{M}}_n(y_1, \ldots, y_n) \subseteq V \) such that, for any positive constant \( \epsilon \), if \( y_1, \ldots, y_n \sim P_\theta \) i.i.d. and \( n \geq c_{\theta,\epsilon,d}\log(1/\delta)\sigma^{2d} \), then with probability at least \( 1-\delta \),

\[
\mathcal{M}_{\theta,d} \subseteq \hat{\mathcal{M}}_n \subseteq \mathcal{M}_{\theta,d}^\epsilon.
\]

The constant \( c_{\theta,\epsilon,d} \) in Theorem 3.2 can be replaced by \( c_{\theta,d}\epsilon^{-2} \) in the unique recovery setting if \( \theta \) is suitably generic, but the dependence on \( \epsilon \) can be worse in general. What is key is that \( c_{\theta,\epsilon,d} \) does not depend on \( \sigma \), so that Theorem 3.2 captures the behavior of the sample complexity in the large \( \sigma \) limit.
Theorem 3.2 essentially follows from the observation that, since the variance of \( y_i \) is \( O(\sigma^2) \), a degree-\( d \) polynomial in the entries of \( y_i \) has variance \( O(\sigma^{2d}) \). This implies that for any \( f \in U_{\leq d}^T \), the evaluation \( f(\theta) \) can be accurately estimated on the basis of \( O(\sigma^{2d}) \) samples. By inverting a suitable polynomial system, we can thereby identify \( M_{\theta,d} \), at least approximately. A full proof of Theorem 3.2 appears in Section 7.

Theorem 3.2 captures the behavior described in both Theorem 1.4 and Theorem 1.8. Indeed, if \( \tau_1 \) and \( \tau_2 \) differ on some \( f \in U_{\geq d}^T \), then \( M_{\tau_1,d} \) is separated from \( M_{\tau_2,d} \), and Theorem 3.2 implies that we can therefore distinguish between the two distributions when \( \varepsilon \) is sufficiently small. Moreover, as the following corollary shows, Theorem 3.2 implies that the confidence set \( \hat{M}_n \) allows us to recover or list-recover the orbit of \( \theta \).

**Corollary 3.3.** Suppose that \( M_{\theta,d} \) is the union of \( M \) orbits \( o_1, \ldots, o_M \), where \( M \) is finite. There exists an \( \varepsilon_\theta \) such that, for \( \varepsilon < \varepsilon_\theta \), if \( n \geq c_{\theta,\varepsilon,d} \log(1/\delta)\sigma^{2d} \), then on the basis of \( n \) i.i.d. samples from \( P_\theta \) we can produce \( M \) estimators \( \hat{\theta}_1, \ldots, \hat{\theta}_M \) such that, with probability at least \( 1 - \delta \), there exists a permutation \( \pi : [M] \to [M] \) satisfying

\[
d_G(\hat{\theta}_i, o_{\pi(i)}) \leq \varepsilon
\]

for all \( i \in [N] \).

**Proof.** Since \( G \) is a compact group acting continuously on \( V \), the orbits are compact. By assumption \( M_{\theta,d} \) is a union of a finite number of orbits, so there exists an \( \varepsilon_\theta \) such that \( d_G(o_i, o_j) \geq 4\varepsilon_\theta \) for any \( i \neq j \). For any \( \varepsilon < \varepsilon_\theta \), let \( N' \) be an \( \varepsilon/2 \)-net of \( V/G \), and construct \( \hat{M}_n \) as in Theorem 3.2. Theorem 3.2 implies the existence of a constant \( c_{\theta,\varepsilon,d} \) such that as long as \( n \geq c_{\theta,\varepsilon,d} \log(1/\delta)\sigma^{2d} \), with probability at least \( 1 - \delta \), \( M_{\theta,d} \subseteq \hat{M}_n \subseteq M_{\theta,d}^{1/2} \).

Consider the set \( C \) consisting of \( o \in N \) such that \( d_G(o, \hat{M}_n) \leq \varepsilon/2 \). With probability \( 1 - \delta \), any element of \( C \) is within \( \varepsilon \) of \( o_i \) for some \( i \in [M] \), and for each \( o_i \), there exists an \( o \in C \) that is at most \( \varepsilon \) away. By assumption, distinct orbits in \( M_{\theta,d} \) are separated by more than \( 4\varepsilon \), so if any two elements of \( C \) are separated by at most \( 2\varepsilon \), then they are close to the same element of \( M_{\theta,d} \). As a result, it is possible to partition \( C \) into \( M \) sets \( C_1, \ldots, C_M \) such that \( d_G(o, o') \leq 2\varepsilon \) if \( o, o' \) are in the same set, and \( d_G(o, o') > 2\varepsilon \) if \( o \) and \( o' \) are in different sets. For \( i \in [M] \), let \( \hat{\theta}_i \) be any element of \( V \) such that the orbit of \( \hat{\theta}_i \) lies in \( \hat{C}_i \). The claim follows.

The constant \( \varepsilon_\theta \) in the statement of Corollary 3.3 will not be known in general. However, a weaker statement still holds when \( \varepsilon \geq \varepsilon_\theta \). Indeed, consider the image of the set \( \hat{M}_n \) under the projection \( V \to V/G \). There exists a finite partition of the resulting set such that any two orbits in the same cluster are closer than any two orbits in different clusters. (Note that the clustering into a single set always satisfies this requirement.) If we are able to choose this partition such that the diameter of each set is at most \( \varepsilon' \), then by choosing a representative from each cluster, we obtain a finite set of estimators, at least one of which is guaranteed to be \( \varepsilon' \)-close to \( \theta \) with high probability. Corollary 3.3 implies that this partition can be taken to consist of at most \( M \) clusters for \( \varepsilon' \) arbitrarily small, as long as \( n \geq C_{\varepsilon'}\sigma^{2d} \).

We now prove a lower bound showing that the dependence on \( \sigma \) in Theorem 3.2 is tight. We show that if \( U_{\leq d-1}^T \) fails to resolve (or list-resolve) \( \theta \), then \( \Omega(\sigma^{2d}) \) samples are necessary to recover (or list-recover) the orbit of \( \theta \). Together with Theorem 3.2 this lower bound implies that if \( d^* \) is the smallest positive integer for which \( U_{\geq d}^T \) resolves (or list-resolve) \( \theta \), then \( \Omega(\sigma^{2d^*}) \) samples are required to recover (or list-recover) the orbit of \( \theta \). We make this lower bound precise in Theorem 3.4.

**Theorem 3.4.** For any positive integer \( d \), there exists a constant \( c_d \) such that if \( \tau_1 \) and \( \tau_2 \) are elements in \( M_{\theta,d-1} \) lying in different orbits, then no procedure can distinguish between \( P_{\tau_1} \) and \( P_{\tau_2} \) with probability greater than \( 2/3 \) if \( n \leq c_d\sigma^{2d} \).

Note that via Le Cam’s method [LeC73], Theorem 3.4 translates into lower bounds for the problem of recovering \( \theta \). The proof of Theorem 3.2 relies on a tight bound for the Kullback-Leibler divergence between the distributions \( P_{\theta_1} \) and \( P_{\theta_2} \) established in [BRW17]. More details appear in Section 7.
4 Algebraic results

In this section, we will consider the four recovery criteria defined in Section 1.3 and give algebraic characterizations of each case. The results of Section 3 imply that it suffices to focus our attention on deciding when a subspace $U$ resolves (or list-resolves) a parameter $\theta$. We show below how to answer this question by purely algebraic means. Moreover, for generic list recovery, we show how this question can be answered algorithmically in polynomial time. For generic and worst-case unique recovery, we also give algorithms to decide the corresponding algebraic condition; however, these algorithms are not efficient.

Throughout, we assume the setup defined in Section 2 for the generalized orbit recovery problem. In particular, $G$ is a compact group acting linearly and continuously on a finite-dimensional real vector space $V$ (although we do not require in this section that the action be orthogonal). We have the invariant ring $\mathbb{R}[x]^G$ corresponding to the action of $G$ on $V$, and a subspace $U \subseteq \mathbb{R}[x]^G$ (e.g. $U_{\leq d}^T$) of invariants that we have access to. We are interested in whether the values $f(\theta)$ for $f \in U$ determine the orbit of $\theta \in V$ under $G$. The specific structure of $G$ and $U_{\leq d}^T$ (as defined in Section 2) will be largely unimportant and can be abstracted away.

4.1 Invariant theory basics

We will often need the following basic operator that averages a polynomial over the group $G$.

**Definition 4.1** (Reynolds operator). The Reynolds operator $\mathcal{R}: \mathbb{R}[x] \to \mathbb{R}[x]^G$ is defined by

$$\mathcal{R}(f) = \mathbb{E}_{g \sim \text{Haar}(G)} [g \cdot f].$$

Note that the Reynolds operator is a linear projection from $\mathbb{R}[x]$ to $\mathbb{R}[x]^G$ that preserves the degree of homogeneous polynomials (i.e. a homogeneous polynomial of degree $d$ gets mapped either to a homogeneous polynomial of degree $d$ or to zero).

**Observation 4.2.** Let $\mathbb{R}[x]^G_d$ denote the vector space consisting of homogeneous invariants of degree $d$. We can obtain a basis for $\mathbb{R}[x]^G_d$ by applying $\mathcal{R}$ to each monomial in $\mathbb{R}[x]$ of degree $d$. (This yields a spanning set which can be pruned to a basis if desired.)

In our setting, we have the following basic fact from invariant theory.

**Theorem 4.3** (e.g. [Kac94] Theorem 4.1-3). The invariant ring $\mathbb{R}[x]^G$ is finitely generated as an $\mathbb{R}$-algebra. In other words, there exist generators $f_1, \ldots, f_m \in \mathbb{R}[x]^G$ such that $\mathbb{R}[f_1, \ldots, f_m] = \mathbb{R}[x]^G$.

Furthermore, there is an algorithm to find a generating set; see Section 8. Another basic fact from invariant theory implies that the entire invariant ring is sufficient to determine the orbit of $\theta$. (This is not always true for non-compact groups; see Example 2.3.1 in [DK15].)

**Theorem 4.4** ([Kac94] Theorem 6-2.2). The full invariant ring $\mathbb{R}[x]^G$ resolves every $\theta \in V$.

**Proof.** Let $o_1, o_2 \in V/G$ be distinct (and therefore disjoint) orbits. Since $G$ is compact and acts continuously, $o_1$ and $o_2$ are compact subsets of $V$. Thus by Urysohn’s lemma there exists a continuous function $\bar{f} : V \to \mathbb{R}$ such that $\bar{f}(\tau) = 0$ $\forall \tau \in o_1$ and $\bar{f}(\tau) = 1$ $\forall \tau \in o_2$. The Stone–Weierstrass theorem states that a continuous function on a compact domain can be uniformly approximated to arbitrary accuracy by a polynomial. This means there is a polynomial $f \in \mathbb{R}[x]$ with $f(\tau) \leq 1/3$ $\forall \tau \in o_1$ and $f(\tau) \geq 2/3$ $\forall \tau \in o_2$. It follows that $h = \mathcal{R}(f)$ is an invariant polynomial that separates the two orbits: $h(o_1) \leq 1/3$ and $h(o_2) \geq 2/3$.

Thus, in order to determine the orbit of $\theta$ it is sufficient to determine the values of all invariant polynomials. (This condition is clearly also necessary in the sense that if the orbit is uniquely determined then so are the values of all invariants.)
Remark 4.5. In what follows we will be discussing algorithms that take the problem setup as input (including $G$ and its action on $\tilde{V}$, along with $\Pi$, $K$) and decide whether or not $U_{\leq d}^T$ (for some given $d$) is capable of a particular recovery task (e.g. list recovery of a generic $\theta \in V$). We will always assume that these algorithms have a procedure to compute a basis for $U_{\leq d}^T$ (for any $d$) in exact symbolic arithmetic. This is non-trivial in some cases because $T_d(x)$ (and thus $U_{T_d}^T$) involves integration over the group (and may involve irrational values), but we will not worry about these details here. For the important case of SO(3), it is possible to write down a basis for the invariants in closed form (see Appendix A).

Remark 4.6. We will draw from various references for algorithmic aspects of invariant theory. The case of finite groups is treated by [Stu08]. Although the invariant ring is sometimes taken to be $\mathbb{C}[x]^G$ instead of $\mathbb{R}[x]^G$, this is unimportant in our setting because the two are essentially the same: since our group action is real, a basis for $\mathbb{R}[x]^G$ (over $\mathbb{R}$) is a basis for $\mathbb{C}[x]^G$ (over $\mathbb{C}$). The case of infinite groups is covered by [DK15]. Here the group is assumed to be a reductive group over $\mathbb{C}$ (or another algebraically-closed field). This means in particular that the group is a subset of complex-valued matrices that is defined by polynomial constraints. Although compact groups such as SO(3) do not satisfy this, the key property of a reductive group is the existence of a Reynolds operator satisfying certain properties; since this exists for compact groups (Definition 4.1), some (but not all) results still hold in our setting.

4.2 Generic list recovery

We will see that the case of list recovery of a generic signal is governed by the notion of algebraic independence.

Definition 4.7. Polynomials $f_1, \ldots, f_m \in \mathbb{R}[x]$ are algebraically dependent if there exists a nonzero polynomial $P \in \mathbb{R}[y_1, \ldots, y_m]$ such that $P(f_1, \ldots, f_m) = 0$ (i.e. $P(f_1(x), \ldots, f_m(x))$ is equal to the zero polynomial). Otherwise, they are algebraically independent.

Definition 4.8. The transcendence degree of a subspace $U \subseteq \mathbb{R}[x]$, denoted trdeg($U$) is the maximum value of $m$ for which there exist algebraically independent $f_1, \ldots, f_m \in U$. A set of trdeg($U$) such polynomials is called a transcendence basis of $U$.

We now present our algebraic characterization of the generic list recovery problem.

Theorem 4.9 (generic list recovery). Let $U \subseteq \mathbb{R}[x]^G$ be a finite-dimensional subspace. If trdeg($U$) = trdeg($\mathbb{R}[x]^G$) then there exists a set $S \subseteq V$ of full measure such that if $\theta \in S$ then $U$ list-resolves $\theta$. Conversely, if trdeg($U$) < trdeg($\mathbb{R}[x]^G$) then there exists a set $S \subseteq V$ of full measure such that if $\theta \in S$ then $U$ does not list-resolve $\theta$.

The proof is deferred to Sections 8.2 and 8.3. A set has full measure if its complement has measure zero. The intuition behind Theorem 4.9 is that trdeg($\mathbb{R}[x]^G$) is the number of degrees of freedom that need to be pinned down in order to learn the orbit of $\theta$, and so we need this many algebraically independent constraints (invariant polynomials). Note that we have not yet given any bound on how large the finite list might be; we will address this in Section 4.3.

In order for Theorem 4.9 to be useful, we need a way to compute the transcendence degree of both $\mathbb{R}[x]^G$ and $U$. In what follows, we will discuss methods for both of these: in Section 4.2.1 we show how to compute trdeg($\mathbb{R}[x]^G$) analytically, and in Section 12.2 we give an efficient algorithm to compute trdeg($U$) for a subspace $U$. By taking $U = U_{T_d}^T$ this yields an efficient algorithm to determine the smallest degree $d$ at which $U_{\leq d}^T$ list-resolves a generic $\theta$ (thereby answering Question 2.8 for the case of generic list recovery).

4.2.1 Computing the transcendence degree of $\mathbb{R}[x]^G$.

Intuitively, the transcendence degree of $\mathbb{R}[x]^G$ is the number of parameters required to describe an orbit of $G$. For finite groups, this is simply the dimension of $V$:

Proposition 4.10 ([Stu08] Proposition 2.1.1). If $G$ is a finite group, trdeg($\mathbb{R}[x]^G$) = dim($V$).
For infinite groups, the situation may be slightly different. For instance, if SO(3) acts on $V = \mathbb{R}^3$ in the standard way (rotations in 3 dimensions), then a generic orbit is a sphere, with dimension two. This means there is only one parameter to learn, namely the 2-norm, and we expect $\mathbb{R}[x]^G$ to have transcendence degree 1 accordingly. On the other hand, if SO(3) acts on a rich class of functions $S^2 \to \mathbb{R}$ (as in the $S^2$ registration problem; see Section 5.4) then each orbit resembles a copy of SO(3) which has dimension 3. This is formalized in the following.

**Proposition 4.11** ([DK15] Corollary 6.2). If $G$ is an algebraic group, then
\[
\text{trdeg}(\mathbb{R}[x]^G) = \dim(V) - \dim(G) + \min_{v \in V} \dim(G_v),
\]
where $G_v$ is the stabilizer at $v$ of the action of $G$ (that is, the subgroup of all $g \in G$ fixing $v$).

An alternate approach to the transcendence degree of $\mathbb{R}[x]^G$ uses a central object in invariant theory: the Hilbert series (see e.g. [DK15]).

**Definition 4.12.** Let $\mathbb{R}[x]^G$ be the subspace (over $\mathbb{R}$) of $\mathbb{R}[x]^G$ consisting of homogeneous invariants of degree $d$. The Hilbert series of $\mathbb{R}[x]^G$ is the formal power series
\[
H(t) := \sum_{d=0}^{\infty} \dim(\mathbb{R}[x]^G_d) t^d.
\]

For a given $G$ acting on $V$, there is an explicit formula (Molien’s formula) for the Hilbert series:

**Proposition 4.13** ([Kac94] Remark 3.1.8). Let $\rho : G \to \text{GL}(V)$ be the representation by which $G$ acts on $V$. Then for $|t| < 1$, $H(t)$ converges and we have
\[
H(t) = \prod_{g \sim \text{Haar}(G)} \det(I - t \rho(g))^{-1}.
\]

This formula is tractable to compute, even for complicated groups; see Section 5.4 for details in the case of SO(3). Once we have the Hilbert series, it is easy to extract $\text{trdeg}(\mathbb{R}[x]^G)$ as follows.

**Proposition 4.14.** The order of the pole at $t = 1$ of $H(t)$ is equal to $\text{trdeg}(\mathbb{R}[x]^G)$.

The proof comes from [DK15]; see Section 5.4 for more details.

For heterogeneous problems ($K > 1$), the transcendence degree can be computed easily from the transcendence degree of the corresponding homogeneous ($K = 1$) problem.

**Proposition 4.15.** Let $\tilde{G}$ be a compact group acting linearly and continuously on $\tilde{V}$, and let $G = \tilde{G}^K \times S_K$ act on $V = \tilde{V} \oplus K \oplus \sum K$ as in Definition 2.2. Let $\mathbb{R}[x]^\tilde{G}$ be the invariant ring corresponding to the action of $G$ on $V$, and let $\mathbb{R}[\tilde{x}]^{\tilde{G}}$ be the invariant ring corresponding to the action of $\tilde{G}$ on $\tilde{V}$ (i.e. the $K = 1$ problem). Then $\text{trdeg}(\mathbb{R}[x]^G) = K \cdot \text{trdeg}(\mathbb{R}[\tilde{x}]^{\tilde{G}}) + K - 1$.

The proof can be found in Section 5.5. Note, however, that the result is intuitively reasonable by counting parameters. We know $\text{trdeg}(\mathbb{R}[\tilde{x}]^{\tilde{G}})$ is the number of parameters required to describe an orbit of $\tilde{G}$ acting on $\tilde{V}$. Thus, in the heterogeneity problem we have $\text{trdeg}(\mathbb{R}[\tilde{x}]^{\tilde{G}})$ parameters for each of the $K$ signals, plus an additional $K - 1$ parameters for the $K$ mixing weights (since they sum to 1).

### 4.2.2 Algorithm for transcendence basis of $U$

In this section we prove the following.

**Theorem 4.16.** There is an efficient algorithm to perform the following task. Given a basis $\{u_1, \ldots, u_s\}$ for a finite-dimensional subspace $U \subseteq \mathbb{R}[x]$, output a transcendence basis for $U$.
Our first ingredient is the following simple classical test for algebraic independence (see, e.g., \cite{ER93, BMS13} for a proof).

**Definition 4.17 (Jacobian).** Given polynomials \( f_1, \ldots, f_m \in \mathbb{R}[x] = \mathbb{R}[x_1, \ldots, x_p] \), we define the Jacobian matrix \( J_x(f_1, \ldots, f_m) \in (\mathbb{R}[x])^{m \times p} \) by \( (J_x(f_1, \ldots, f_m))_{ij} = \frac{\partial f_i}{\partial x_j} \), where \( \frac{\partial}{\partial x_j} \) denotes formal partial derivative with respect to \( x_j \).

**Proposition 4.18 (Jacobian criterion for algebraic independence).** Polynomials \( f = (f_1, \ldots, f_m) \) are algebraically independent if and only if the Jacobian matrix \( J_x(f) \) has full row rank (over the field \( \mathbb{R}(x) \)).

It suffices to test the rank of the Jacobian at a generic point \( x \).

**Corollary 4.19.** Fix \( f = (f_1, \ldots, f_m) \). Let \( z \sim \mathcal{N}(0, I_{p \times p}) \). If \( f \) is algebraically dependent then \( J_x(f)|_{x=z} \) does not have full row rank. If \( f \) is algebraically independent then \( J_x(f)|_{x=z} \) has full row rank with probability 1.

**Proof.** An \( m \times p \) matrix has deficient row rank if and only if either \( m > p \) or every maximal square submatrix has determinant zero. Every such determinant of \( J_x(f) \) is a polynomial in \( x \); if this polynomial is not identically zero then plugging in generic values for \( x \) will not cause it to vanish.

**Remark 4.20.** In practice we may choose to plug in random rational values for \( x \) so that the rank computation can be done in exact symbolic arithmetic. The Jacobian test will still succeed with overwhelming probability (provided we use a fine enough mesh of rational numbers). Also note that if we find any value of \( x \) for which the Jacobian has full row rank, this constitutes a proof of algebraic independence.

**Remark 4.21.** In some cases (e.g. if the polynomials involve irrational values) it may be slow to compute the Jacobian rank in exact symbolic arithmetic. We can alternatively compute the singular values numerically and count how many are reasonably far from zero. This method works reliably in practice (i.e., it is extremely clear how to separate the zero and nonzero singular values) but does not constitute a rigorous proof of algebraic independence.

Curiously, although the Jacobian criterion gives an efficient test for algebraic dependence, it is much harder (\#P-hard) to actually find the algebraic dependence (i.e., the polynomial relation) when one exists \cite{Kay09}.

The Jacobian criterion implies the well-known fact that the collection of algebraically independent subsets of \( \mathbb{R}[x] \) form a matroid; this is called an algebraic matroid (see e.g. \cite{Sch03}). In particular, we have the following exchange property:

**Proposition 4.22.** Let \( I, J \) be finite subsets of \( \mathbb{R}[x] \), each algebraically independent. If \( |I| < |J| \) then there exists \( f \in J \setminus I \) such that \( I \cup \{f\} \) is algebraically independent.

We next note that in the task from Theorem 4.16 a transcendence basis can always be taken from the basis \( \{u_1, \ldots, u_s\} \) itself.

**Lemma 4.23.** Let \( U \) be a finite-dimensional subspace of \( \mathbb{R}[x] \) with basis \( B = \{u_1, \ldots, u_s\} \). If \( U \) contains \( r \) algebraically independent elements, then so does \( B \).

**Proof.** Let \( B' \subseteq B \) be a maximal set of algebraically independent elements of \( B \). If \( |B| < r \) then by the exchange property (Proposition 4.22) there exists \( v \in U \setminus B' \) such that \( B' \cup \{v\} \) is algebraically independent. Write \( v = \sum_{i=1}^{s} \alpha_i u_i \). Since \( B' \) is maximal, we have from the Jacobian criterion (Proposition 4.18) that for all \( 1 \leq i \leq s \), the row vector \( J_x(u_i) \) lies in the \( \mathbb{R}(x) \)-span of \( B := \{ J_x(b) \}_{b \in B'} \). But this means that \( J_x(v) = \sum_{i=1}^{s} \alpha_i J_x(u_i) \) lies in the \( \mathbb{R}(x) \)-span of \( B \). By the Jacobian criterion this contradicts the fact that \( B' \cup \{v\} \) is algebraically independent.

**Proof of Theorem 4.16**
Let \( \{u_1, \ldots, u_s\} \) be a basis (or spanning set) for \( U \). From above we have that the transcendence degree of \( U \)
is the row rank of the Jacobian $J(u_1, \ldots, u_s)$ evaluated at a generic point $x$. A transcendence basis for $U$ is the set of $u_i$ corresponding to a maximal linearly independent set of rows.

We proceed by induction. The claim is vacuously true when $a$ maximal independent subset of $\{u_1, \ldots, u_s\}$. Initialize $I = \emptyset$. For $i = 1, \ldots, s$, add $\{u_i\}$ to $I$ if $I \cup \{u_i\}$ is algebraically independent, and do nothing otherwise. (Note that this condition can be efficiently tested by Corollary 4.19.)

Output the resulting set $I$.

We now show correctness. Let $I_i$ be the set after item $u_i$ has been considered (and possibly added), and set $I_0 = \emptyset$. It suffices to show that for each $i \in \{0, \ldots, s\}$, $I_i$ is a maximal independent subset of $\{u_1, \ldots, u_i\}$. We proceed by induction. The claim is vacuously true when $i = 0$. Assume it holds for $i - 1$. If $I_i$ is not a maximal independent subset of $\{u_1, \ldots, u_i\}$, then there exists an independent set $J \subseteq \{u_1, \ldots, u_i\}$ with $|J| > |I_i|$, so by the exchange property (Proposition 4.12), there exists a $u_j$ with $j \leq i$ such that $u_j \notin I_i$ and $I_i \cup \{u_j\}$ is independent. In particular, the subset $I_{j-1} \cup \{u_j\}$ of $I_i \cup \{u_j\}$ is independent. But the fact that $u_j$ was not added at the $(j-1)$th step implies that $I_{j-1} \cup \{u_j\}$ is not independent, a contradiction. So $I_i$ is indeed maximal.

We obtain that $I = I_s$ is a maximal independent subset of $\{u_1, \ldots, u_s\}$, and hence by Lemma 4.22 a transcendence basis of $U$.

4.3 Generic unique recovery

For list recovery problems, the following gives an explicit upper bound on the size of the list.

**Theorem 4.24.** Let $U$ be a subspace of the invariant ring $\mathbb{R}[x]^G$. Let $F_G$ be the field of fractions of $\mathbb{R}[x]^G$. If $[F_G : \mathbb{R}(U)] = D < \infty$ then there exists a set $S \subseteq V$ of full measure such that for any $\theta \in S$, $U$ list-resolves $\theta$ with a list of size $\leq D$.

The proof is deferred to Section 8.2. Here $\mathbb{R}(U)$ is the smallest subfield of $F_G$ containing both $\mathbb{R}$ and $U$, and $[F_G : \mathbb{R}(U)]$ denotes the degree of a field extension; see Section 8.2 for more details. Since $[F_G : \mathbb{R}(U)] = 1$ is equivalent to $\mathbb{R}(U) = F_G$, we have the following criterion for unique recovery.

**Corollary 4.25** (generic unique recovery). If $\mathbb{R}(U) = F_G$ then there exists a set $S \subseteq V$ of full measure such that if $\theta \in S$ then $U$ resolves $\theta$.

The intuition here is that we want to be able to learn every invariant polynomial by adding, multiplying, and dividing polynomials from $U$ (and scalars from $\mathbb{R}$). We need $\theta$ to be generic so that we never divide by zero in the process.

**Theorem 4.26.** For a finite-dimensional subspace $U \subseteq \mathbb{R}[x]^G$, there is an algorithm to compute the degree of the field extension from Theorem 4.24. As input, the algorithm requires a basis for $U$ and the ability to compute the Reynolds operator (Definition 4.1).

We give the algorithm and the proof in Section 8.6. The algorithm uses Gröbner bases and is unfortunately inefficient to run in practice.

Additionally, in Appendix 14 we present a method for proving field generation using Galois theory. There we use it to show generic unique recovery in the case where $G$ is a finite Abelian group and $V$ is its regular representation (over $\mathbb{R}$). These ideas may be helpful for proving generic unique recovery in other settings.

4.4 Worst-case unique recovery

We give a sufficient algebraic condition for worst-case unique recovery:

**Theorem 4.27** (worst-case unique recovery). Let $U \subseteq \mathbb{R}[x]^G$ be a finite-dimensional subspace with basis $\{f_1, \ldots, f_m\}$. If $U$ generates $\mathbb{R}[x]^G$ as an $\mathbb{R}$-algebra (i.e. $\mathbb{R}[f_1, \ldots, f_m] = \mathbb{R}[x]^G$) then $U$ resolves every $\theta \in V$.

**Proof.** Every element of $\mathbb{R}[x]^G$ can be written as a polynomial in the $f_i$ (with coefficients in $\mathbb{R}$). This means the values $f_1(\theta), \ldots, f_m(\theta)$ uniquely determine all the values $f(\theta)$ for $f \in \mathbb{R}[x]^G$ and so the result follows because $\mathbb{R}[x]^G$ resolves every $\theta \in V$ (Theorem 4.4).
Theorem 4.28. There is an algorithm to test whether or not $U$ generates $\mathbb{R}[x]^G$ as an $\mathbb{R}$-algebra. As input, the algorithm requires a basis for $U$ and the ability to compute the Reynolds operator (Definition 4.1).

We give the algorithm and the proof in Section 8.6. The algorithm uses Gröbner bases and is unfortunately inefficient to run in practice.

If $G$ is a finite group, it is known that $\mathbb{R}[x]^G$ has a generating set for which all elements have degree at most $|G|$ (this is Noether’s degree bound; see Theorem 2.1.4 in [Stu08]). It follows that $\mathbb{R}[x]^G$ resolves every $\theta \in V$. Recall (from Section 1.4) that this is tight for MRA: degree $|G|$ is necessary for worst-case signals.

A precise characterization of when $U$ resolves every $\theta \in V$ is (by definition) that $U$ should be a separating set or (equivalently) should generate a separating algebra (see [DK15] Section 2.4). The notions of generating and separating sets do not always coincide, as illustrated by Example 2.4.2 in [DK15]. Furthermore, generating sets may require strictly higher maximum degree [Dom10].

4.5 Worst-case list recovery

We give a sufficient algebraic condition for worst-case list recovery:

Theorem 4.29 (worst-case list recovery). Let $U \subseteq \mathbb{R}[x]^G$ be a subspace with finite basis $\{f_1, \ldots, f_m\}$. If $\mathbb{R}[x]^G$ is finitely generated as a $\mathbb{R}[f_1, \ldots, f_m]$-module, then $U$ list-resolves every $\theta \in V$.

In other words, this condition says that there exists a basis $g_1, \ldots, g_s \in \mathbb{R}[x]^G$ such that every element of $\mathbb{R}[x]^G$ can be written as a linear combination of $g_1, \ldots, g_s$ with coefficients from $\mathbb{R}[f_1, \ldots, f_m]$. It is sufficient to take $U$ to be a set of primary invariants from a Hironaka decomposition (see Section 5.3).

Proof. Since $\mathbb{R}[x]^G$ finitely generated as an $\mathbb{R}$-algebra (Theorem 4.3), if $\mathbb{R}[x]^G$ is finitely generated as a $\mathbb{R}[f_1, \ldots, f_m]$-module then it follows that (see [Stu08] Section 5.3) every $h \in \mathbb{R}[x]^G$ satisfies a monic polynomial

$$h^k + c_{k-1}h^{k-1} + \cdots + c_1h + c_0 = 0$$

with $c_i \in \mathbb{R}[f_1, \ldots, f_m]$. Letting $h_1, \ldots, h_s$ be generators for $\mathbb{R}[x]^G$ (as an $\mathbb{R}$-algebra), we have that the values $f_1(\theta), \ldots, f_m(\theta)$ determine a finite set of possible values for $h_1(\theta), \ldots, h_s(\theta)$, each of which determines (at most) one orbit for $\theta$. \hfill \Box

5 Examples

In this section we work out some specific examples, determining the degree at which generic list recovery is possible using the methods of Section 4.2 (We focus on generic list recovery because our algorithms for the other recovery criteria are unfortunately too slow even for quite small examples.) We obtain several recovery theorems for problems such as MRA and cryo-EM within finite ranges of parameters where we have verified the Jacobian criterion using a computer, and beyond these parameter ranges, we state conjectural patterns.

The following themes emerge in the examples studied in this section. First, we see that many problems are possible at degree 3, which is promising from a practical standpoint. Second, we do not encounter any unexpected algebraic dependencies, and so we are able to show that heuristic parameter-counting arguments are correct. In particular, we see that if there are enough linearly independent invariants, there are also enough algebraically independent invariants.

5.1 Learning a bag of numbers

Let $G$ be the symmetric group $S_p$ acting on $V = \mathbb{R}^p$ by permutation matrices. The invariant ring consists of the symmetric polynomials, which are generated by the elementary symmetric polynomials $e_1, \ldots, e_p$ where $e_i$ has degree $i$. Worst-case unique recovery is possible at degree $p$ since $\mathbb{R}[x]^{G_p}$ generates the full invariant ring. Furthermore, degree $p$ is actually required, even for generic list recovery. This is because any invariant

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of degree \( \leq p - 1 \) can be expressed as a polynomial in \( e_1, \ldots, e_{p-1} \) and thus \( \text{trdeg}(\mathbb{R}[x]_{\leq p-1}^G) = p - 1 \). So this problem has a steep sample complexity of order \( \sigma^{2p} \).

5.2 Learning a rigid body

Let \( G \) be the rotation group \( \text{SO}(p) \) acting on the matrix space \( \mathbb{R}^{p \times m} \) by left multiplication. We imagine the columns of our matrix as vertices defining a rigid body; thus we observe random rotations of this rigid body (with vertices labeled) plus noise. Let \( U \in \mathbb{R}^{p \times m} \) be such a matrix signal. With \( O(\sigma^4) \) samples, we can estimate the degree-2 Gram matrix \( U^\top U \); taking a Cholesky factorization, we recover \( U \) up to left action by an element of the larger group \( \text{O}(p) \). Thus we recover the rigid body up to a reflection ambiguity, demonstrating list recovery (with a list of size 2). Surprisingly, assuming \( p \) action by an element of the larger group \( \text{O}(p) \), we can estimate a \( p \times p \) minor of \( U \), which is a degree-\( p \) invariant that changes sign under reflection.

The impossibility of unique recovery until degree \( p \) is a consequence of the “first fundamental theorem” for the special orthogonal group \( \text{SO}(p) \), which asserts that the invariant ring is generated by the entries of the Gram matrix \( U^\top U \) together with the \( p \times p \) minors of \( U \) (see for instance \cite{Kac94}); thus the invariants of degree 3, \ldots, \( p - 1 \) carry no information in addition to the degree-2 invariants.

5.3 Multi-reference alignment (MRA)

Recall that this is the case of \( G = \mathbb{Z}/p \) acting on \( V = \mathbb{R}^p \) by cyclic shifts. It is already known that for the basic MRA problem (without projection or heterogeneity), generic unique recovery is possible at degree 3 for any \( p \) \cite{BRW17}. The methods of Section 5.2 confirm the weaker result that generic list recovery is possible at degree 3 (at least for the values of \( p \) that we tested). Note the stark contrast in difficulty from the case of the full symmetric group \( G = S_p \) above.

Remark 5.1. This result for MRA is actually a special case of a more general phenomenon. Let \( G \) be any finite group and let \( V \) be the regular representation i.e. the space of functions \( f : G \to \mathbb{R} \) with the action \((g \cdot f)(h) = f(g^{-1} h)\). (Note that for \( G = \mathbb{Z}/p \) this is precisely the MRA problem.) It is known \cite{Kac09} that for this setup, the triple correlation (a collection of degree-3 invariants) is sufficient to resolve a generic signal, and thus generic unique recovery is possible at degree 3. In Appendix E we give a short proof for the special case where the group is Abelian; our proof illustrates a method based on Galois theory which may be useful to prove generic unique recovery in other settings.

We can also verify that for MRA with \( p \geq 3 \), generic list recovery is impossible at degree 2. This follows from Theorem 4.9 because \( \text{trdeg}(\mathbb{R}[x]^G) = p \) (since \( G \) is finite) but the number of algebraically independent invariants of degree \( \leq 2 \) is at most \( \lfloor p/2 \rfloor + 1 \). We can see this as follows. A basis for the invariants of degree \( \leq 2 \) is \( \{ \mathcal{R}(x_1), \mathcal{R}(x_1^2), \mathcal{R}(x_1 x_2), \mathcal{R}(x_1 x_3), \ldots, \mathcal{R}(x_1 x_m) \} \) with \( s = \lfloor p/2 \rfloor + 1 \). Here \( \mathcal{R} \) denotes the Reynolds operator, which averages over cyclic shifts of the variables. For instance, \( \mathcal{R}(x_1 x_2) = \frac{1}{p} (x_1 x_2 + x_2 x_3 + x_3 x_4 + \cdots + x_p x_1) \). Note that the basis above has size \( \lfloor p/2 \rfloor + 2 \) but there is an algebraic dependence within it because \( \mathcal{R}(x_1^2) \) can be written in terms of the other basis elements. The claim now follows.

Generic list recovery is possible at degree 1 for \( p = 1 \) and at degree 2 for \( p = 2 \). (This is true even for worst-case unique recovery; recall from Section 4.4 that degree \( |G| \) is always sufficient for this.)

We now move on to variants of the MRA problem.

5.3.1 MRA with projection

We now consider MRA with a projection step. We imagine that the coordinates of the signal are arranged in a circle so that \( G \) acts by rotating the signal around the circle. We then observe a projection of the circle onto a line so that each observation is the sum of the two entries lying “above” it on the circle. This is intended to resemble the tomographic projection in cryo-EM. We formally define the setup as follows.
We call the associated generalized orbit recovery problem (Problem 2.3) the homogeneous case $K$ odd-$q$ shifts. Let impossible in the even-$p$ case rather than the seemingly more elegant even-$p$ case is because generic list recovery is actually impossible from the samples, even if there is no noise.

We now consider heterogeneous MRA, i.e. the generalized orbit recovery problem (Problem 2.3) with heterogeneous MRA can only make it harder for $U^{T_d}$ to list-resolve $\theta$.

5.3.2 Heterogeneous MRA

We now consider heterogeneous MRA, i.e. the generalized orbit recovery problem (Problem 2.3) with $G = \mathbb{Z}/p$ acting on $\mathbb{R}^p$ by cyclic shifts, $K \geq 2$ heterogeneous components, and no projection (i.e., $\Pi$ is the identity).

We will see that generic list recovery is possible at degree 3 provided that $p$ is large enough compared to $K$. First note that the number of degrees of freedom to be recovered is $\operatorname{trdeg}(\mathbb{R}[x]/\mathcal{G}) = Kp + K - 1$ (see Propositions 4.11 and 4.12). Let us now count the number of distinct entries of $T_d(x)$ for $d \leq 3$. Note that $T_d(x)$ is symmetric (under permutations of indices) but we also have additional symmetries given by cyclic shifts, e.g. $(T_3(x))_{i,j,k} = (T_3(x))_{i+c,j+c,k+c}$ where $c$ is an integer and the sums $i+c,j+c,k+c$ are computed modulo $p$. One can compute that $T_1(x)$ has 1 distinct entry, $T_2(x)$ has $|p/2|$ + 1 distinct entries, and $T_3(x)$ has $p + \lceil (p-1)(p-2)/6 \rceil$ distinct entries. The total number of distinct entries is

$$U := p + 2 + |p/2| + \lceil (p-1)(p-2)/6 \rceil.$$

By Theorem 4.9 list recovery is impossible when $U < Kp + K - 1$. By testing the Jacobian condition, we observe that the converse also appears to hold. We tested this up to $K = 15$ and up to the corresponding critical $p$ value.

Conjecture 5.4. For heterogeneous $(K \geq 2)$ MRA, generic list recovery is possible at degree 3 precisely if $U \geq Kp + K - 1$. This condition on $U$ can be stated more explicitly as follows:

- $K = 2$ requires $p \geq 1$.
- $K = 3$ requires $p \geq 12$.
- $K = 4$ requires $p \geq 18$.
- Each $K \geq 5$ requires $p \geq 6K - 5$. 

Note that generic list recovery is possible at degree 3 provided that
Recent work \[BBLS17\] also studies the heterogeneous MRA problem. Similarly to the present work, they apply the method of moments and solve a polynomial system of equations in order to recover the signals. To solve the system they use an efficient heuristic method that has no provable guarantees but appears to work well in practice. Their experiments suggest that if the signals have i.i.d. Gaussian entries, this method succeeds only when (roughly) \( K \leq \sqrt{p} \) instead of the condition (roughly) \( K \leq p/6 \) that we see above (and that \[BBLS17\] also identified based on parameter-counting). Exploring this discrepancy is an interesting direction for future work.

One question of particular interest is whether this example evinces a statistical-computational gap, whereby all polynomial-time methods fail to succeed once \( K \) exceeds \( \sqrt{p} \). Some evidence for why we might expect this is as follows. Recent work on tensor decomposition \[MSS16\] gives a polynomial-time algorithm to decompose a third order tensor of the form \( \sum_{i=1}^{N} a_i^{\otimes 3} + E \) where \( a_i \in \mathbb{R}^p \) are i.i.d. from the unit sphere and \( E \) is noise, provided \( N \leq p^{1.5} \) (up to factors of \( \log p \)). The heterogeneous MRA problem can be cast as such a tensor decomposition problem with \( N = Kp \) components \( a_i \); the components are the \( p \) cyclic shifts of each of the \( K \) signals. Although these \( a_i \) are not independent, we expect that if the signals are random then the \( a_i \) are “random enough” for the same tensor decomposition result to hold, which exactly yields the condition \( K \leq \sqrt{p} \) (up to factors of \( \log p \)).

### 5.4 \( S^2 \) registration

Recall that this is the case where the signal \( \theta \) is a real-valued function defined on the unit sphere \( S^2 \) in \( \mathbb{R}^3 \).

The formal setup is as follows.

Let \( G = \text{SO}(3) \). For each \( \ell = 0, 1, 2, \ldots \) there is an irreducible representation \( V_\ell \) of \( \text{SO}(3) \) of dimension \( 2\ell + 1 \). These representations are of real type, i.e. they can be defined over the real numbers so that \( V_\ell = \mathbb{R}^{2\ell+1} \). Let \( F \) be a finite subset of \( \{0,1,2,\ldots\} \) and consider the orbit recovery problem in which \( G \) acts on \( V = \bigoplus_{\ell \in F} V_\ell \).

As intuition for the above setup, \( V_\ell \) is a basis for the degree-\( \ell \) spherical harmonic functions \( S^2 \to \mathbb{R} \) defined on the surface of the unit sphere \( S^2 \subseteq \mathbb{R}^3 \). The spherical harmonics are a complete set of orthogonal functions on the sphere and can be used (like a “Fourier series”) to represent a function \( S^2 \to \mathbb{R} \). Thus the signal \( \theta \in V \) can be thought of as a function on the sphere, with \( \text{SO}(3) \) acting on it by rotating the sphere. See Appendix \[A\] for details on spherical harmonics.

The primary case of interest is \( F = \{1, \ldots, F\} \) for some \( F \) (the number of “frequencies”). We will see that generic list recovery is possible at degree 3 so long as \( F \geq 10 \). We will see that it is convenient to not include 0 \( \in F \), but we now justify why this is without loss of generality. \( V_0 \) is the trivial representation, i.e. the 1-dimensional representation on which every group element acts as the identity. In the interpretation of spherical harmonics, the \( V_0 \)-component is the mean value of the function over the sphere. We claim that the \( S^2 \) registration problem with \( 0 \in F \) can be easily reduced to the problem with \( F' = F \setminus \{0\} \). This is because the \( V_0 \)-component is itself a degree-1 invariant; given the value of this invariant, one can subtract it off and reduce to the case without a \( V_0 \)-component (i.e. the case where the function on the sphere is zero-mean).

Thus we have that e.g. generic list recovery is possible (at a given degree) for \( F \) if and only if it is possible for \( F' \).

Using Proposition \[4.11\] we compute that \( \text{trdeg}(\mathbb{R}[X]^G) = p - p' \), where

\[
p = \dim(V) = \sum_{\ell \in F} (2\ell + 1)
\]

and

\[
p' = \begin{cases} 0 & \ell_{\text{max}} = 0 \\ 2 & \ell_{\text{max}} = 1 \\ 3 & \ell_{\text{max}} \geq 2 \end{cases} \quad \text{where } \ell_{\text{max}} = \max_{\ell \in F} \ell.
\]

After all, \( V_0 \) is the trivial representation on the 1-dimensional vector space, with 3-dimensional stabilizer \( \text{SO}(3) \), and \( V_1 \) is the standard 3-dimension representation of \( \text{SO}(3) \) on \( \mathbb{R}^3 \) by rotations, which yields a one-dimensional \( \text{SO}(2) \) stabilizer at each nonzero point. When \( \ell_{\text{max}} \geq 2 \), the representation \( V \) is known to have zero-dimensional stabilizer at some points (see e.g. \[Ete96\]).
In the following we restrict to the case $0 \notin \mathcal{F}$ for simplicity (but recall that this is without loss of generality). There are therefore no degree-1 invariants, i.e. $\mathbb{R}[x]_{G}^{G}$ is empty. By Theorem 4.9 if $\dim(\mathbb{R}[x]_{G}^{G}) + \dim(\mathbb{R}[x]_{G}^{G}) < \text{trdeg}(\mathbb{R}[x]^{G})$ then generic list recovery is impossible at degree 3; this rules out generic list recovery for $\mathcal{F} = \{1, 2, \ldots, F\}$ when $F \leq 9$. (We will see below how to compute $\dim(\mathbb{R}[x]_{d}^{G})$.) Beyond this threshold, the situation is more hopeful:

**Theorem 5.5.** If $\mathcal{F} = \{1, 2, \ldots, F\}$ and $10 \leq F \leq 16$ then the degree-3 method of moments achieves generic list recovery.

This theorem is based on computer verification of the Jacobian criterion for $10 \leq F \leq 16$ using exact arithmetic in a finite extension of $\mathbb{Q}$. This result lends credence to the following conjecture.

**Conjecture 5.6.** Consider the $S^2$ registration problem with $0 \notin \mathcal{F}$. We conjecture the following.

1. Generic list recovery is possible at degree 3 if and only if $\dim(\mathbb{R}[x]_{G}^{G}) + \dim(\mathbb{R}[x]_{G}^{G}) \geq \text{trdeg}(\mathbb{R}[x]^{G})$ (where $\text{trdeg}(\mathbb{R}[x]^{G})$ is computed above and $\dim(\mathbb{R}[x]_{G}^{G})$ can be computed from Proposition 5.7 below).

2. In particular, if $\mathcal{F} = \{1, 2, \ldots, F\}$ then generic list recovery is possible at degree 3 if and only if $F \geq 10$.

The reason it is convenient to exclude the trivial representation is because it simplifies the parameter-counting: if we use the trivial representation then we have a degree-1 invariant $f$ and so there is an algebraic relation between the degree-2 invariant $f^2$ and the degree-3 invariant $f^3$.

We now discuss how to compute $\dim(\mathbb{R}[x]_{G}^{G})$. Using the methods in Section 4.6 of [DK15], we can give a formula for the Hilbert series of $\mathbb{R}[x]^{G}$; see Section 9.1. However, if one wants to extract a specific coefficient $\dim(\mathbb{R}[x]_{d}^{G})$ of the Hilbert series, we give an alternative (and somewhat simpler) formula:

**Proposition 5.7.** Consider $S^2$ registration with frequencies $\mathcal{F}$. Let $\chi_0(\phi) : \mathbb{R} \to \mathbb{R}$ be defined recursively by

$$\chi_0(\phi) = 1,$$

$$\chi_1(\phi) = \sum_{\ell \in \mathcal{F}} \left[ 1 + 2 \sum_{m=1}^{\ell} \cos(m \phi) \right],$$

and

$$\chi_d(\phi) = \frac{1}{d} \sum_{i=1}^{d} \chi_1(i \phi) \chi_{d-i}(\phi).$$

Then we have

$$\dim(\mathbb{R}[x]_{d}^{G}) = \frac{1}{\pi} \int_{0}^{\pi} (1 - \cos \phi) \chi_d(\phi) \, d\phi.$$  

We give the proof in Section 9.2. Additionally, in Appendix A.6 we give explicit formulas for the invariants (up to degree 3), which yields a combinatorial analogue of Proposition 5.7 (up to degree 3).

### 5.5 Cryo-EM

We adapt the following simple model for the cryo-EM reconstruction problem. We will use properties of the 3-dimensional Fourier transform, including the projection-slice theorem; see e.g. [Osg07] for a reference.

The signal is a 3-dimensional molecule, which we can think of as encoded by a density function $f : \mathbb{R}^3 \to \mathbb{R}$. The 3-dimensional Fourier transform of $f$ is $\hat{f} : \mathbb{R}^3 \to \mathbb{C}$ given by

$$\hat{f}(k_x, k_y, k_z) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-2\pi i (xk_x + yk_y + zk_z)} f(x, y, z) \, dx \, dy \, dz. \quad (1)$$

It is sufficient to learn $\hat{f}$ because we can then recover $f$ using the inverse Fourier transform. $\text{SO}(3)$ acts on the molecule by rotating it in 3-dimensional space (keeping the origin fixed). When $f$ is rotated in
There are various other choices one could make for the basis in which to represent the Remark 5.8. common basis is the Fourier–Bessel basis (used in e.g. [LBB + ] a radial delta function (i.e. a delta function applied to the radius, resulting in a spherical shell). Another (Fourier transform of the) molecule. Each of our basis functions is the product of a spherical harmonic and harmonics with any set of radial basis function. It turns out that the choice of radial basis is unimportant because the resulting problem will be isomorphic to our case (spherical shells) and so the same results hold.

Theorem 5.9. There are various other choices one could make for the basis in which to represent the (Fourier transform of the) molecule. Each of our basis functions is the product of a spherical harmonic and a radial delta function (i.e. a delta function applied to the radius, resulting in a spherical shell). Another common basis is the Fourier–Bessel basis (used in e.g. [LBB + ] where each basis function is the product of a spherical harmonic and a radial Bessel function. More generally we can take the product of spherical harmonics with any set of radial basis function. It turns out that the choice of radial basis is unimportant because the resulting problem will be isomorphic to our case (spherical shells) and so the same results hold.

By the projection-slice theorem, the 2-dimensional Fourier transform of $f_{\text{proj}}$ is equal to the slice $\hat{f}_{\text{slice}} : \mathbb{R}^2 \to \mathbb{C}$ given by

$$
\hat{f}_{\text{slice}}(k_x, k_y) = \hat{f}(k_x, k_y, 0).
$$

Thus we think of $\hat{f}$ as our unknown signal with $\text{SO}(3)$ acting by rotation, and with post-projection which reveals only the slice of $\hat{f}$ lying in the plane $k_z = 0$.

This does not yet conform to our definition of a (generalized) orbit recovery problem because the signal needs to lie in a finite-dimensional real vector space. Instead of thinking of $\hat{f}$ as a function on $\mathbb{R}^3$, we fix a finite number $S$ of nested spherical shells in $\mathbb{R}^3$, each of different radius and all centered at the origin. We consider only the restriction of $\hat{f}$ to these shells. We fix a finite number $F$ of frequencies and on each shell we expand $\hat{f}$ (restricted to that shell) in the basis of spherical harmonics, truncated to $1 \leq \ell \leq F$. (As in $S^2$ registration, we can discard the trivial representation $\ell = 0$ without loss of generality, and it is convenient to do so.) Being the Fourier transform of a real-valued function, $\hat{f}$ satisfies

$$
\hat{f}(-k_x, -k_y, -k_z) = \hat{f}(k_x, k_y, k_z)
$$

(see (2)) and so we can use a particular basis $H_{\ell m}$ of spherical harmonics for which the expansion coefficients are real; see Appendix A. We have now parametrized our signal by a finite number of real values $\theta_{\ell m}$ with $1 \leq s \leq S$, $1 \leq \ell \leq F$, and $-\ell \leq m \leq \ell$. In particular, the restriction of $\hat{f}$ to shell $s$ has expansion

$$
\sum_{1 \leq \ell \leq F} \sum_{-\ell \leq m \leq \ell} \theta_{\ell m} H_{\ell m}.
$$

SO(3) acts on each shell by 3-dimensional rotation; see Section A.4 for the details of how SO(3) acts on spherical harmonics. The projection $\Pi$ reveals only the values on the equator $z = 0$ (or in spherical coordinates, $\theta = \pi/2$) of each shell. Using again the property (2), the output of $\Pi$ on each shell has an expansion with real coefficients in a particular finite basis $h_m$; see Section A.4.

**Remark 5.8.** We now present our results on the above cryo-EM model. We focus on identifying the regime of parameters for which generic list recovery is possible at degree 3. Again using Proposition 4.11 we have for $F \geq 2$:

$$
\text{trdeg}(\mathbb{R}[x]^G) = \dim(V) - 3 = S \sum_{\ell=1}^{F} (2\ell + 1) - 3 = S(F^2 + 2F) - 3
$$

where again we have a zero-dimensional stabilizer.

In Appendix A we give an explicit construction of the invariant polynomials in $U_{\leq 3}$. By testing the Jacobian criterion in exact arithmetic on small examples, we arrive at the following theorem:

**Theorem 5.9.** Consider the homogeneous ($K = 1$) cryo-EM problem with $S$ shells and $F$ frequencies.
• If $S = 1$ then for any $F \geq 2$, generic list recovery is impossible at degree 3.

• If $2 \leq S \leq 4$ and $2 \leq F \leq 6$, the degree-3 method of moments achieves generic list recovery.

The first assertion results from a simple counting argument: there are fewer invariants at degree $\leq 3$ than degrees of freedom. The second part is by confirming that the Jacobian of the invariants has rank equal to $\text{trdeg}(\mathbb{R}[x]^G)$, through computer-assisted exact arithmetic over an appropriate finite extension of $\mathbb{Q}$.

In floating-point arithmetic, we have further verified that the Jacobian appears to have appropriate rank for $2 \leq S \leq 10$ and $2 \leq F \leq 10$, leading us to conjecture the following:

**Conjecture 5.10.** If $S \geq 2$ then the degree-3 method of moments achieves generic list recovery (regardless of $F$).

Intuitively, when there is a single shell ($S = 1$) there are simply not enough invariants in $U^T_{\leq 3}$. However, when $S \geq 2$, the number of invariants increases dramatically due to cross-terms that involve multiple shells.

### 5.5.1 Heterogeneous cryo-EM

We now consider heterogeneous cryo-EM ($K \geq 2$). By combining (3) with Proposition 4.15 we can compute $\text{trdeg}(\mathbb{R}[x]^G)$. Based on testing the Jacobian criterion on small examples, we conjecture that the degree-3 method of moments achieves generic list recovery if and only if $\dim(U^T_2) + \dim(U^T_3) \geq \text{trdeg}(\mathbb{R}[x]^G)$. In other words, we expect no unexpected algebraic dependencies among $U^T_{\leq 3}$. (Recall that there are no degree-1 invariants since we are not using the trivial representation $\ell = 0$).

In Section A.6 we give a conjectured formula for the exact value of $\dim(U^T_2) + \dim(U^T_3)$ for all $S \geq 1$, $F \geq 2$. As a result we can determine for any given $S \geq 1$ and $F \geq 2$, the exact condition on $K$ for which we believe generic list recovery is possible. For $S$ and $F$ large, this condition is approximately $K \leq S^2/4$.

### 6 Open questions

We leave the following as directions for future work.

1. Our methods require testing the rank of the Jacobian on a computer for each problem size. It would be desirable to have analytic results for e.g. (variants of) MRA in any dimension $p$.

2. We have given an efficient test for whether generic list recovery is possible, but have not given a similarly efficient test for generic unique recovery. In cases where unique recovery is impossible, it would be nice to give a tight bound on the size of the list; for instance, for MRA with projection, we conjecture that the list has size exactly 2 (due to “chirality”), but we lack a proof for this fact. Our algorithms for testing generic unique recovery are based on Gröbner bases, the calculation of which is known to be computationally hard in the worst case [Hu86]. Unfortunately, the algorithms we have proposed are also extremely slow in practice, though a faster implementation may be possible.

3. Our procedure for recovering $\theta$ from the samples involves solving a polynomial system of equations. While solving polynomial systems is NP-hard in general, the fact that the polynomials used in the orbit recovery problem have special structure leaves open the possibility of finding an efficient (polynomial time) method with rigorous guarantees. Possible methods include tensor decomposition [PWB+17] and non-convex optimization [BBLST17].

4. We have addressed the statistical limits of orbit recovery problems. However, prior work has indicated the presence of statistical-to-computational gaps in related synchronization problems [PWBM16a], and we expect such gaps to appear in orbit recovery problems too. As discussed in Section 5.3.2 the results of [BBLST17] suggest a possible gap of this kind for heterogeneous MRA.
7 Proofs for Section 3: statistical results

We first prove Theorem 3.2. This theorem in fact holds for more general mixture problems, not merely those arising from the orbit recovery problems defined in Problem 2.3. For convenience, we will state and prove the theorem in its general form.

**Problem 7.1** (mixture recovery). Let $V = \mathbb{R}^p$, and let $\Theta \subset V$ be compact. For $\theta \in \Theta$, let $\mu_\theta$ be a measure on $\mathbb{R}^p$ whose support is contained in the unit ball, and assume the map $\theta \mapsto \mu_\theta$ is continuous with respect to the weak topology. Let $D$ be a known distribution on $\mathbb{R}$ with finite moments of all orders, and let $\sigma \geq 1$. For $i \in [n] = \{1, 2, \ldots, n\}$, we observe

$$y_i = x_i + \sigma \xi_i,$$

where $x_i \sim \mu_\theta$ and the entries of $\xi_i$ are independently drawn from $D$. The goal is to estimate $\theta$.

Write $P_\theta$ for the distribution arising from the parameter $\theta$, and let $E_\theta$ be expectation with respect to this distribution. We denote by $E_\theta^n$ the expectation taken with respect to $n$ i.i.d. samples from $P_\theta$. Where there is no confusion, we also write $E_\theta$ for expectation with respect to the distribution $\mu_\theta$.

We require that $\mu_\theta$ have bounded support; the requirement that it be supported in the unit ball is for normalization purposes only. We assume throughout that $\sigma \geq 1$. The following definition gives the generalization of Definition 3.1 to the mixture recovery problem.

**Definition 7.2.** Given a positive integer $d$ and $\theta \in V$, the order-$d$ matching set $M_{\theta, d}$ is the set consisting of all $\phi \in V$ such $E_\theta[x^\otimes k] = E_\phi[x^\otimes k]$ for $k = 1, \ldots, d$, where $E_\phi$ represents expectation with respect to $x \sim \mu_\phi$.

**Problem 7.1** generalizes Problem 2.3 by allowing the random vector $x_i$ to arise from more general mixtures than those arising from group actions. Note that when the mixtures do arise from a generalized orbit recovery problem, i.e., when $x_i = \Pi(g_i \cdot \theta_k)$, where $g_i$ and $k_i$ are distributed as in Problem 2.3, then Definition 7.2 reduces to Definition 3.1.

Having made these definitions, our goal in this section is to show that Theorem 3.2 holds word-for-word in the setting of mixture recovery. To do so, we show that entries of the moment tensors $E_\theta[x^\otimes k]$ can be estimated on the basis of $O(\sigma^{2k})$ samples from $P_\theta$.

7.1 Estimation of moments

Our estimators will be based on a system of orthogonal univariate polynomials under the measure corresponding to $D$. Let $H_0(x) = 1$, and for $k \geq 1$, define

$$H_k(x) = x^k - \sum_{j=0}^{k-1} E_{\xi \sim D}[\xi^k H_j(\xi)] E_{\xi \sim D}[H_j(\xi)^2] H_j(x).$$

It is easy to check that these polynomials are orthogonal under the inner product given by $\langle f, g \rangle = E_{\xi \sim D}[f(\xi)g(\xi)]$ and that the polynomials $H_0, \ldots, H_k$ form a basis for the space of polynomials of degree at most $k$. We denote them by $H_k$ because they coincide with the classic Hermite polynomials when $D$ is Gaussian.

Like the Hermite polynomials, they satisfy the identity

$$E_{\xi \sim D}[H_k(x + \xi)] = x^k. \tag{4}$$

Indeed, we can expand $H_k(x + \xi)$ in the basis of the orthogonal polynomials as

$$H_k(x + \xi) = \sum_{j=0}^{k} \alpha_j(x) H_j(\xi),$$

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where \( \alpha_j(x) \) is a polynomial in \( x \) of degree at most \( k - j \). Since \( H_j(\xi) \) has zero mean for \( j \geq 1 \) by construction, we obtain
\[
\mathbb{E}[H_k(x + \xi)] = \alpha_0(x),
\]
and since \( H_k \) is a monic polynomial of degree \( k \), we must have \( \alpha_0(x) = x^k \).

We briefly review multi-index notation.

**Definition 7.3.** A \( p \)-dimensional multi-index is a tuple \( \alpha = (\alpha_1, \ldots, \alpha_p) \) of nonnegative integers. For \( x \in \mathbb{R}^p \), let \( x^\alpha = \prod_{j=1}^p x_j^{\alpha_j} \).

For any multi-index \( \alpha \), we write \( |\alpha| = \sum_{j=1}^p \alpha_j \). Given independent samples \( y_1, \ldots, y_n \) from \( P_\theta \), consider the estimate for \( \mathbb{E}_{x \sim P_\theta}[x^\alpha] \) given by
\[
\hat{x}^\alpha := \frac{1}{n} \sum_{i=1}^n \prod_{j=1}^p \sigma^{\alpha_j} H_{\alpha_j}(\sigma^{-1} y_i).
\]

We first show that \( \hat{x}^\alpha \) is unbiased.

**Lemma 7.4.** For all \( \theta \in \Theta \), \( \mathbb{E}_\theta[\hat{x}^\alpha] = \mathbb{E}_\theta[x^\alpha] \).

**Proof.** Since \( \hat{x}^\alpha \) is a sum of i.i.d. terms, it suffices to prove the claim for a single sample. By \( \mathbb{E}_\theta \),
\[
\mathbb{E}_\theta \left[ \prod_{j=1}^p \sigma^{\alpha_j} H_{\alpha_j}(\sigma^{-1} y_j) \right] = \mathbb{E}_{x \sim P_\theta} \left[ \prod_{j=1}^p \sigma^{\alpha_j} H_{\alpha_j}(\sigma^{-1} (x_j + \sigma \xi_j))|x| \right]
\]
\[
= \mathbb{E}_{x \sim P_\theta} \left[ \prod_{j=1}^p \sigma^{\alpha_j} H_{\alpha_j}(\sigma^{-1} x_j + \xi_j)|x| \right]
\]
\[
= \mathbb{E}_{x \sim P_\theta} \left[ \prod_{j=1}^p \sigma^{\alpha_j} (\sigma^{-1} x_j)^{\alpha_j} \right] = \mathbb{E}_\theta[x^\alpha].
\]

It remains to bound the variance.

**Proposition 7.5.** For any multi-index \( \alpha \), there exists a constant \( c_\alpha \) such that for all \( \theta \in \Theta \), \( \text{Var}_\theta[\hat{x}^\alpha] \leq c_\alpha n^{-1} \sigma^{2|\alpha|} \).

**Proof.** Since \( \hat{x}^\alpha \) is a sum of i.i.d. terms, it suffices to prove the claim for \( n = 1 \). Given a multi-index \( \alpha \), let \( c_\alpha = \prod_{j=1}^p \sup_{x_j \in [-1,1]} \mathbb{E}_{\xi_j \sim \mathcal{D}}[H_{\alpha_j}(x_j + \xi_j)^2] \), and note that \( c_\alpha \) is independent of \( \sigma \). We obtain
\[
\text{Var}_\theta[\hat{x}^\alpha] \leq \mathbb{E}_{x \sim P_\theta} \left[ \prod_{j=1}^p \mathbb{E}_{\xi_j \sim \mathcal{D}} \left[ \sigma^{2\alpha_j} H_{\alpha_j}(\sigma^{-1} x_j + \xi_j)^2 \right] \right]
\]
\[
\leq \sup_{x : |x| \leq 1} \prod_{j=1}^p \mathbb{E}_{\xi_j \sim \mathcal{D}} \left[ \sigma^{2\alpha_j} H_{\alpha_j}(\sigma^{-1} x_j + \xi_j)^2 \right]
\]
\[
\leq c_\alpha \sigma^{2|\alpha|},
\]
as claimed.

Finally, we apply the “median-of-means” trick \( \text{[NY83]} \) to show that we can combine the estimators defined above to obtain estimates for the moment tensors \( \mathbb{E}_\theta[x^{\otimes k}] \) for \( k \leq d \) which are close to their expectation with high probability.
**Proposition 7.6.** Let \( y_1, \ldots, y_n \) be i.i.d. samples from \( P_\theta \). For any degree \( d \) and accuracy parameter \( \delta \), there exist estimators \( \hat{x}^\alpha = \hat{x}^\alpha(y_1, \ldots, y_n) \) for all \( \alpha \) with \( |\alpha| \leq d \) such that with probability at least \( 1 - \delta \),

\[
\max_{\alpha:|\alpha| \leq d} \left| \mathbb{E}_\theta[x^\alpha] - \hat{x}^\alpha \right| \leq c_d \sigma^d \sqrt{\frac{\log(p/\delta)}{n}},
\]

for some constant \( c_d \).

**Proof.** Split the samples into \( m \) subsamples of equal size, for some \( m \) to be specified, and for each \( \alpha \) construct the \( m \) estimators \( \hat{x}_1^\alpha, \ldots, \hat{x}_m^\alpha \) on the basis of the \( m \) subsamples. (We assume for convenience that \( m \) divides \( n \).) Let \( \hat{x}_m^\alpha \) be the median of \( \hat{x}_1^\alpha, \ldots, \hat{x}_m^\alpha \).

Chebyshev’s inequality together with Proposition 7.5 implies that there exists a constant \( c_d \) such that, for each \( j = 1, \ldots, m \) and multi-index \( \alpha \),

\[
\Pr \left[ \left| \hat{x}_j^\alpha - \mathbb{E}_\theta[x^\alpha] \right| > c_d \sigma^d \sqrt{\frac{m}{n}} \right] \leq \frac{1}{4},
\]

and since the estimators \( \hat{x}_1^\alpha, \ldots, \hat{x}_m^\alpha \) are independent, a standard concentration argument shows that

\[
\Pr \left[ \left| \hat{x}_j^\alpha - \mathbb{E}_\theta[x^\alpha] \right| > c_d \sigma^d \sqrt{\frac{m}{n}} \right] \leq e^{-m/4}.
\]

By a “stars-and-bars” counting argument [Fel68], there are \( (p+d)^m \) multi-indices \( \alpha \) satisfying \( |\alpha| \leq d \), so taking a union bound over all choices of \( \alpha \) yields

\[
\max_{\alpha:|\alpha| \leq d} \left| \mathbb{E}_\theta[x^\alpha] - \hat{x}^\alpha \right| \leq c_d \sigma^d \sqrt{\frac{m}{n}}
\]

with probability at least \( 1 - \frac{1}{m} (p+d)^m e^{-m/4} \). Choosing \( m = 4 \log((p+d)/\delta) \) and taking \( c_d \) sufficiently large in the statement of the theorem yields the claim.

Note that the constant \( c_d \) in the statement of Proposition 7.6 can be made explicit, given knowledge of the distribution \( D \).

### 7.2 Robust solutions to polynomial systems

We now show that approximate knowledge of the moment tensors \( \mathbb{E}_\theta[x^\otimes k] \) for \( k = 1, \ldots, d \) suffices to approximately recover \( \theta \).

**Lemma 7.7.** For all \( \theta \in \Theta \) and \( \varepsilon > 0 \), there exists a \( \varepsilon' > 0 \) such that, if \( \phi \in \Theta \) satisfies \( \max_{k \leq d} \| \mathbb{E}_\theta[x^\otimes k] - \mathbb{E}_\phi[x^\otimes k] \|_\infty < \varepsilon' \), then there exists a \( \tau \in \mathcal{M}_{\theta,d} \) such that \( \| \phi - \tau \| < \varepsilon \).

**Proof.** We employ a simple compactness argument. Consider the set \( F = \{ \phi \in \Theta : \forall \tau \in \mathcal{M}_{\theta,d} \| \phi - \tau \| \geq \varepsilon \} \). Since \( \Theta \) is compact, so is \( F \). Set

\[
\varepsilon' = \min_{\phi \in F} \max_{k \leq d} \| \mathbb{E}_\theta[x^\otimes k] - \mathbb{E}_\phi[x^\otimes k] \|_\infty.
\]

Clearly if \( \max_{k \leq d} \| \mathbb{E}_\theta[x^\otimes k] - \mathbb{E}_\phi[x^\otimes k] \|_\infty < \varepsilon' \) for some \( \phi \in \Theta \), then there exists a \( \tau \in \mathcal{M}_{\theta,d} \) such that \( \| \phi - \tau \| < \varepsilon \), so it remains to check that \( \varepsilon' > 0 \).

Since \( \theta \mapsto \mu_\theta \) is continuous with respect to the weak topology and \( \mu_\theta \) is supported on a compact set for all \( \theta \in \Theta \), the moment map \( \theta \mapsto \mathbb{E}_\theta[x^\otimes k] \) is also continuous for all \( k \leq d \). If \( \phi \in F \), then in particular \( \phi \notin \mathcal{M}_{\theta,d} \), so there exists a \( k \leq d \) for which \( \mathbb{E}_\phi[x^\otimes k] \neq \mathbb{E}_\phi[x^\otimes k] \). Therefore \( \varepsilon' > 0 \), as desired.

Lemma 7.7 is simply stating that the function \( \phi \mapsto \min_{\tau \in \mathcal{M}_{\theta,d}} \| \phi - \tau \| \) is continuous at \( \theta \) with respect to the topology induced by the moment maps. Note that, for generic \( \theta \) when \( \mu_\theta \) arises from an orbit recovery problem, the moment map will be continuously differentiable with a nonsingular Jacobian, so the inverse function theorem implies \( \varepsilon' \) can be taken to be \( \Omega(\varepsilon) \). In general, however, the dependence could be worse.
7.3 Proof of Theorem 3.2

Construct the estimators \( \hat{\Theta}_n \) as in Proposition 7.6 and let

\[
\hat{\Theta}_n = \left\{ \phi \in \Theta : \max_{\alpha:|\alpha| \leq d} |E_\phi[\phi^\alpha] - \tilde{x}^\alpha| \leq c_d \sigma d \sqrt{\frac{\log(p/\delta)}{n}} \right\}
\]

Applying Proposition 7.6, we have with probability at least \( 1 - \delta \) that \( \Theta_{\theta,d} \subseteq \hat{\Theta}_n \) and that, for all \( \phi \in \hat{\Theta}_n, \)

\[
\max_{k \leq d} \|E_{\phi}[\phi^{\otimes k}] - E_\theta[\phi^{\otimes k}]\| = \max_{\alpha:|\alpha| \leq d} \|E_{\phi}[\phi^\alpha] - E_\theta[\phi^\alpha]\| \leq 2c_d \sigma d \sqrt{\frac{\log(p/\delta)}{n}}.
\]

By Lemma 7.7, there exists an \( \varepsilon_{\theta,\varepsilon} \) such that, as long as \( 2c_d \sigma d \sqrt{\frac{\log(p/\delta)}{n}} < \varepsilon_{\theta,\varepsilon}' \), then with probability at least \( 1 - \delta \), we have the desired inclusion \( \hat{\Theta}_n \subseteq \Theta_{\theta,d} \).

Therefore taking \( n > (2c_d/2)^2 \log(p/\delta) \sigma^2 d = c_{\theta,d} \log(1/\delta) \sigma^2 d \) suffices.

\[ \square \]

7.4 Information geometry of gaussian mixtures

In this section, we establish an upper bound on the Kullbeck-Leibler divergence between different gaussian mixtures, which we denote by \( D(\cdot \| \cdot) \).

The proof follows the outline used in [BRW17], based on a technique developed in [LNS99, CL11].

**Proposition 7.8.** Let \( \theta, \phi \in \Theta \), let the distribution \( D \) be \( N(0,1) \) for some \( \sigma \geq 1 \), and let \( d \) be any positive integer.

There exist universal constants \( C \) and \( c \) such that if \( E_\phi[\phi^{\otimes k}] = E_\theta[\phi^{\otimes k}] \) for \( k \leq d - 1 \), then

\[
D(P_\theta \| P_\phi) \leq C \frac{(\sigma c)^{d-2d}}{d!}.
\]

**Proof.** We first establish the claim when \( d = 1 \). Note that the condition on the moment tensors is vacuous in this case. By the convexity of the divergence,

\[
D(P_\theta \| P_\phi) \leq \mathbb{E}_{x \sim P_\theta, \phi \sim P_\phi} D(N(x, \sigma^2), N(x', \sigma^2)) = \mathbb{E}_{x \sim P_\theta, \phi \sim P_\phi} \frac{||x - x'||^2}{2\sigma^2} \leq 2\sigma^{-2},
\]

where in the last step we used the fact that \( x \) and \( x' \) lie in the unit ball almost surely.

Now, assume \( d > 1 \), so in particular \( E_\phi[x] = E_\theta[x] \). Denote their common mean by \( v \). For \( \zeta \in \{\theta, \phi\} \) denote by \( \overline{P}_\zeta \) the distribution of \( x - v \) when \( x \sim P_\zeta \), and let \( \overline{P}_\zeta \) denote distribution of \( y \) when \( y = x + \xi \) for \( x \sim P_\zeta \) and \( \xi \sim N(0, \sigma^2 I) \). Since this transformation is a deterministic bijection, the data processing inequality implies \( D(P_\theta \| P_\phi) = D(\overline{P}_\theta \| \overline{P}_\phi) \).

Note that \( E_{\overline{P}_\theta}[x] = E_{\overline{P}_\phi}[x] = 0 \) and \( E_{\overline{P}_\theta}[x^{\otimes k}] = E_{\overline{P}_\phi}[x^{\otimes k}] \) for \( k \leq d - 1 \). Hence without loss of generality we can reduce to the case where \( \mu_\theta \) and \( \mu_\phi \) are both centered and are supported in a ball of radius \( 2 \).

We bound the \( \chi^2 \)-divergence between \( P_\theta \) and \( P_\phi \). Let \( f \) be the density of a standard \( p \)-dimensional Gaussian and for \( \zeta \in \Theta \), let \( f_\zeta \) be the density of \( P_\zeta \), which can be written explicitly as

\[
f_\zeta(y) = E_{x \sim \mu_\zeta} \sigma^{-p} f(\sigma^{-1}(y - x)) = \sigma^{-p} f(\sigma^{-1} y)e^{-\frac{1}{2\sigma^2}((1-2y^\top E_\zeta x)^2 - \sigma^2 x^\top x)}.
\]

Since \( ||x|| \leq 2 \) almost surely with respect \( \mu_\zeta \), Jensen’s inequality implies that

\[
f_\zeta(y) \geq \sigma^{-p} f(\sigma^{-1} y)e^{-\frac{1}{2\sigma^2}((1-2y^\top E_\zeta x)^2 - \sigma^2 x^\top x)} = \sigma^{-p} f(\sigma^{-1} y)e^{-\frac{2}{\sigma^2} x^\top x}.
\]

Recall that the \( \chi^2 \) divergence is defined by

\[
\chi^2(P_\theta, P_\phi) = \int \frac{(f_\theta(y) - f_\phi(y))^2}{f_\theta(y)} dy.
\]

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Applying (5) to the denominator, expanding the definitions of \( f_\theta \) and \( f_\phi \), and applying a change of variables yields

\[
\chi^2(P_\theta, P_\phi) \leq e^{2/\sigma^2} \int \left( e^{-\frac{1}{2\sigma^2} x^T D(P_{\theta, \phi}^2)} - e^{-\frac{1}{2\sigma^2} (x^T - 2\theta^T x)^2} \right)^2 \sigma^2 f(x) \, dx
\]

\[
= e^{2/\sigma^2} \int \left( e^{-\frac{1}{2\sigma^2} y^T (\sigma^{-1} x) - \frac{1}{2\sigma^2} \|\sigma^{-1} x\|^2} - e^{-\frac{1}{2\sigma^2} y^T (\sigma^{-1} x) - \frac{1}{2\sigma^2} \|\sigma^{-1} x\|^2} \right)^2 f(y) \, dy
\]

\[
= e^{2/\sigma^2} \int \left( e^{-\frac{1}{2\sigma^2} y^T (\sigma^{-1} x) - \frac{1}{2\sigma^2} \|\sigma^{-1} x\|^2} - e^{-\frac{1}{2\sigma^2} y^T (\sigma^{-1} x) - \frac{1}{2\sigma^2} \|\sigma^{-1} x\|^2} \right)^2 f(y) \, dy
\]

\[
= e^{2/\sigma^2} \mathbb{E}[e^{\phi_\theta^T (\sigma^{-1} x) - \frac{1}{2\sigma^2} \|\sigma^{-1} x\|^2}] - e^{2/\sigma^2} \mathbb{E}[e^{\phi_\phi^T (\sigma^{-1} x) - \frac{1}{2\sigma^2} \|\sigma^{-1} x\|^2}]
\]

\[
g \sim \mathcal{N}(0, I).
\]

Given \( \zeta, \zeta' \in \Theta \), let \( x \sim \mu_\zeta \) and \( x' \sim \mu_{\zeta'} \) be independent. Then interchanging the order of expectation and using the expression for the moment generating function of a standard Gaussian random variable, we obtain

\[
\mathbb{E}[\zeta_\zeta' e^{\phi_\zeta^T (\sigma^{-1} (x + x')) - \frac{1}{2\sigma^2} \|\sigma^{-1} x\|^2 + \|\sigma^{-1} x'\|^2}] = \mathbb{E}[\nu_\zeta' e^{\nu_\zeta^T x'}].
\]

Applying this expression to (6) after expanding the square produces

\[
\chi^2(P_\theta, P_\phi) \leq e^{2/\sigma^2} \sum_{k=0}^{\infty} \frac{\sigma^{-2k}}{k!} \left( \mathbb{E}_x [x^T \xi^k] - 2 \mathbb{E}_x [x^T \xi^k] + \mathbb{E}_x [x^T \xi^k] \right)
\]

where in each expectation the random variables \( x \) and \( x' \) are independent. Since \( \mu_\theta \) and \( \mu_\phi \) are compactly supported, Fubini’s theorem implies we can expand each term as a power series and interchange expectation and summation to produce

\[
\chi^2(P_\theta, P_\phi) \leq e^{2/\sigma^2} \sum_{k=0}^{\infty} \frac{\sigma^{-2k}}{k!} \left( \mathbb{E}_\theta [\xi^k] - 2 \mathbb{E}_\theta [\xi^k] + \mathbb{E}_\phi [\xi^k] \right)
\]

\[
= e^{2/\sigma^2} \sum_{k=0}^{\infty} \frac{\sigma^{-2k}}{k!} \left( \mathbb{E}_\theta [\xi^k] - 2 \mathbb{E}_\theta [\xi^k] + \mathbb{E}_\phi [\xi^k] \right)
\]

\[
= e^{2/\sigma^2} \sum_{k=0}^{\infty} \frac{\sigma^{-2k}}{k!} \left( \mathbb{E}_\theta [\xi^k] - 2 \mathbb{E}_\theta [\xi^k] + \mathbb{E}_\phi [\xi^k] \right)
\]

\[
\leq e^{2/\sigma^2} \sum_{k=0}^{\infty} \frac{\sigma^{-2k}}{k!} \left( \mathbb{E}_\theta [\|x\|^2] - 2 \mathbb{E}_\theta [\|x\|^2] + \mathbb{E}_\phi [\|x\|^2] \right)
\]

\[
= e^{2/\sigma^2} \sum_{k=0}^{\infty} \frac{\sigma^{-2k}}{k!} \left( \mathbb{E}_\theta [\|x\|^2] - 2 \mathbb{E}_\theta [\|x\|^2] + \mathbb{E}_\phi [\|x\|^2] \right)
\]

where \( \langle \cdot, \cdot \rangle \) denotes the Frobenius inner product between tensors and \( \| \cdot \|_\text{HS} \) denotes the Hilbert-Schmidt norm. Since under both \( \mu_\theta \) and \( \mu_\phi \), \( \|x\| \leq 2 \) almost surely, we have for all \( k \geq 2 \),

\[
\mathbb{E}_\theta [\|x\|^k] - \mathbb{E}_\phi [\|x\|^k] \leq 2 \mathbb{E}_\theta [\|x\|^k] + 2 \mathbb{E}_\phi [\|x\|^k] \leq 2k + 1
\]

Therefore

\[
\chi^2(P_\theta, P_\phi) \leq 4e^{2/\sigma^2} \sum_{k=0}^{\infty} \frac{4^k \sigma^{-2k}}{k!} \leq 4e^{6/\sigma^2} \frac{4^d \sigma^{-2d}}{d!},
\]

and applying the inequality \( D(P_\theta \| P_\phi) \leq \chi^2(P_\theta, P_\phi) \) \cite{Tsy09} proves the claim.

\[\square\]

### 7.5 Proof of Theorem 3.4

If \( \tau_1 \) and \( \tau_2 \) are both in \( \mathcal{M}_{\theta, d-1} \), then by Proposition 7.8 the corresponding distributions \( P_{\tau_1} \) and \( P_{\tau_2} \) satisfy \( D(P_{\tau_1} \| P_{\tau_2}) \leq \frac{C}{(1+\sigma)^2\sigma^d} \). By the Neyman-Pearson lemma, for any test \( \psi \) using \( n \) samples,

\[
\Pr(\tau_1) = 2 + \Pr(\tau_2) = 1 - d_{TV}(P_{\tau_1}^n, P_{\tau_2}^n) \geq 1 - \sqrt{\frac{1}{2} D(P_{\tau_1}^n \| P_{\tau_2}^n) = 1 - \sqrt{\frac{Cn}{2(1+\sigma)^2\sigma^d}}}.
\]

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where we have applied Pinsker’s inequality and the chain rule for divergence. Therefore, to achieve an error probability of at most 1/3, we must have \( n \geq 2(c_0) d (2d)! / (9C) = c_d d^{2d} \), as claimed.

\[ \square \]

8 Proofs for Section 4: algebraic results

8.1 Algorithm for generators of \( R[x] \)

We know that \( R[x] \) is finitely generated as an \( R \)-algebra (Theorem 4.23). There are various algorithms to compute a finite set of generators for \( R[x] \). However, some require the group to be finite or to be reductive over an algebraically-closed field. One algorithm that certainly works in our context (compact groups) is Algorithm 2.2.5 in [Stu08]. As input it requires the Hilbert series of \( R[x] \) (which can be computed by Proposition 4.14) and a procedure to compute a basis for \( R[x] \) (which can be done with the Reynolds operator by Observation 4.2). The idea is as follows. We keep a set of proposed generators \( f_1, \ldots, f_m \). At each step we compare the Hilbert series of \( f \) with the Hilbert series of \( R[x] \) computed using Gröbner bases. If these series differ at the \( t^d \) term, this means we are missing an invariant at degree \( d \). To remedy this, we create a new homogeneous invariant of degree \( d \) using the Reynolds operator, and add it to our set of proposed generators. We repeat until the Hilbert series match.

8.2 Bounding the list size for generic signals

In this section we prove Theorem 4.24 and the first part of Theorem 4.9 (see Section 8.3 for the second part). Recall the following basic definitions and facts from field theory.

**Definition 8.1.** If \( F_2 \) is a subfield of \( F_1 \), we write \( F_1 / F_2 \) and call this a field extension. The degree of the extension, denoted \([F_1 : F_2]\), is the dimension of \( F_1 \) as a vector space over \( F_2 \).

**Proposition 8.2.** Let \( \mathbb{R} \subseteq \mathbb{F} \subseteq \mathbb{F}_1 \) with \( \mathbb{F}_1 \) finitely generated (as a field) over \( \mathbb{R} \). Let \( r \) be the transcendence degree of \( \mathbb{F}_1 \) (over \( \mathbb{R} \)). The field extension \( \mathbb{F}_1 / \mathbb{F}_2 \) has finite degree if and only if \( \mathbb{F}_1 \) contains \( r \) algebraically independent elements.

**Proof.** This is a basic fact of field theory. If \( \mathbb{F}_1 \) contains \( r \) algebraically independent elements then the extension \( \mathbb{F}_1 / \mathbb{F}_2 \) is algebraic and finitely generated, and therefore has finite degree. Otherwise, the extension is transcendental and has infinite degree.

In light of the above (and using the fact that \( R[x] \) is finitely generated), Theorem 4.24 implies the first part of Theorem 4.9 (i.e. list size is bounded by \( D := [G : \mathbb{R}(U)] \)).

**Proof of Theorem 4.24.**

Write \( V := \mathbb{R}(U) \). In characteristic zero, every algebraic extension is separable, so by the primitive element theorem, \( F_G = F_U(\alpha) \) for some \( \alpha \in F_G \). Since \( \alpha \) generates a degree-\( D \) extension, \( \alpha \) is the root of a degree-\( D \) polynomial

\[
\alpha^D + b_D - 1 \alpha^{D-1} + \cdots + b_1 \alpha + b_0
\]

with coefficients \( b_i \in F_U \). Furthermore, every element of \( F_G \) can be expressed as

\[
c_0 + c_1 \alpha + \cdots + c_{D-1} \alpha^{D-1}
\]

with \( c_i \in F_U \). In particular, let \( g_1, \ldots, g_k \) be generators for \( R[x] \) (as an \( R \)-algebra) and write

\[
g_i = c^{(i)}_0 + c^{(i)}_1 \alpha + \cdots + c^{(i)}_{D-1} \alpha^{D-1}.
\]

Let \( S \subseteq V \) be the subset for which \( \alpha \) and all the (finitely-many) coefficients \( b_i, c^{(i)}_j \) have nonzero denominators; \( S \) is a non-empty Zariski-open set and thus has full measure. Now fix \( \theta \in S \). Given the values \( f(\theta) \) for all \( f \in U \), each \( b_i \) takes a well-defined value in \( \mathbb{R} \) and so from (7) there are at most \( D \) possible values that \( \alpha(\theta) \) can take. From (8), each value of \( \alpha(\theta) \) uniquely determines all the values \( g_i(\theta) \) and thus uniquely determines all the values \( f(\theta) \) for \( f \in R[x] \). Since \( \mathbb{R}[x] \) resolves \( \theta \) (Theorem 4.4), this completes the proof.

\[ \square \]
8.3 Generic list recovery converse

In this section we prove the second part of Theorem 4.13 (the converse).

Let \( p = \dim(V) \), \( \operatorname{trdeg}(U) = q \), and \( \operatorname{trdeg}(\mathbb{R}[x]^G) = r \) so that \( q < r \leq p \). Let \( f = \{f_1, \ldots, f_m\} \) be a basis for \( U \), and let \( g = \{g_1, \ldots, g_r\} \) be a transcendence basis for \( \mathbb{R}[x]^G \). Let \( S \subseteq V \) be the set of points \( \theta \) for which the Jacobian \( J_x(f)|_{x=\theta} \) has row rank \( q \) and the Jacobian \( J_x(g)|_{x=\theta} \) has row rank \( r \); by the Jacobian criterion (see Corollary 4.14), \( S \) is a non-empty Zariski-open set and thus has full measure.

Fix \( \theta \in S \). For a sufficiently small open neighborhood \( X \subseteq S \) containing \( \theta \) we have the following. The Jacobian criterion on \( f \) implies that \( \{\tau \in X : f(\tau) = f(\theta)\} \) has dimension \( p - q \). The Jacobian criterion on \( g \) implies that every \( z \in g(X) \) has a preimage \( g^{-1}(z) := \{\tau \in X : g(\tau) = z\} \) of dimension \( p - r \). Since \( p - q > p - r \) it follows that there are infinitely many \( \theta_1, \theta_2, \ldots \in X \) such that \( f(\theta_i) = f(\theta) \) but the values \( g(\theta_1), g(\theta_2), \ldots \) are all distinct (and thus the \( \theta_i \) belong to distinct orbits). Therefore \( U \) does not list-resolve \( \theta \).

8.4 Hilbert series and Hironaka decomposition

In this section we prove Proposition 4.14 on extracting the transcendence degree from the Hilbert series (as the pole order at \( t = 1 \)). While this is a general property of finitely generated algebras over a field, there is an easy proof for invariant rings stemming from a key structural property of such rings called the Cohen-Macaulay property or Hironaka decomposition.

Theorem 8.3 ([DK15] Section 2.6). The invariant ring \( \mathbb{R}[x]^G \) has the following structure. There exist homogeneous primary invariants \( f_1, \ldots, f_r \in \mathbb{R}[x]^G \) and homogeneous secondary invariants \( g_1, \ldots, g_s \in \mathbb{R}[x]^G \) such that

- \( \{f_1, \ldots, f_r\} \) are algebraically independent, and
- any element of \( \mathbb{R}[x]^G \) can be written uniquely as a linear combination of \( g_1, \ldots, g_s \) with coefficients from \( \mathbb{R}[f_1, \ldots, f_r] \).

The proof can be found in Section 2.6 of [DK15]: note that the only property of the group that is used is the existence of a Reynolds operator (and so the proof is valid for compact groups).

Proof of Proposition 4.14

The Hironaka decomposition above implies that the Hilbert series takes the form

\[
\frac{\sum_{j=1}^s \mu_{\deg(g_j)}}{\prod_{i=1}^r (1 - t\deg(f_i))}
\]

(this is equation (2.7.3) in [DK15]). It is now clear that the order of the pole at \( t = 1 \) is precisely \( r \). But we can see as follows that \( f_1, \ldots, f_r \) is a transcendence basis for \( \mathbb{R}[x]^G \) and so \( r = \operatorname{trdeg}(\mathbb{R}[x]^G) \). As in the proof of Theorem 4.12, since \( \mathbb{R}[x]^G \) is a finitely generated \( \mathbb{R}[f_1, \ldots, f_r] \)-module, every \( h \in \mathbb{R}[x]^G \) satisfies a polynomial with coefficients in \( \mathbb{R}[f_1, \ldots, f_r] \), which is an algebraic dependence among \( \{f_1, \ldots, f_r, h\} \).

8.5 Transcendence degree for heterogeneity

In this section we prove Proposition 4.15. To recall the setup, we have \( \tilde{G} \) acting on \( \tilde{V} \) with associated variables \( \tilde{x} \). We also have \( G = \tilde{G} \times S_K \) acting on \( V = \tilde{V} \otimes \mathbb{K} \oplus \sum_{k=1}^{K-1} \mathbb{K} \) with associated variables \( x \). Let us also introduce an intermediate group: \( G' = \tilde{G}^K \), acting on \( V \) (with associated variables \( x \)).

Partition the variables \( x \) as follows. For \( k = 1, \ldots, K \), let \( x^{(k)} = (x_1^{(k)}, \ldots, x_p^{(k)}) \) be the variables corresponding to signal \( k \). Let \( z = (z_1, \ldots, z_{K-1}) \) be the variables corresponding to the mixing weights \( \omega_1, \ldots, \omega_{K-1} \). Whenever we refer to \( z_K \), this is just shorthand for \( -\sum_{k=1}^{K-1} z_k \).

We first prove a simpler version of the result without the action of \( S_K \).
Lemma 8.4. Let \( \tilde{r} = \text{trdeg}(\mathbb{R}[x \! G]) \) and let \( r = K \tilde{r} + K - 1 \). Then
\[
\text{trdeg}(\mathbb{R}[x \! G]) = r.
\]

Proof. To show ‘\( \geq \)’ we need to exhibit \( r \) algebraically independent elements of \( \mathbb{R}[x \! G] \). Letting \( f_1, \ldots, f_\tilde{r} \) be a transcendence basis for \( \mathbb{R}[x \! G] \), it suffices to take
\[
I := \{ f_i(x^{(k)}) \}_{1 \leq i \leq \tilde{r}, 1 \leq k \leq K} \cup \{ z_1, \ldots, z_{K-1} \}.
\]
To show ‘\( \leq \)’ we first recall that we can obtain a spanning set for the subspace \( \mathbb{R}[x \! G'] \) by applying the Reynolds operator \( R \) (for \( G' \)) to each degree-\( d \) monomial (in the variables \( x \)). Such a monomial takes the form
\[
m(x) = M(z) \prod_{k=1}^{K} m_k(x^{(k)})
\]
where \( M, m_k \) are monomials. Applying the Reynolds operator yields
\[
R(m(x)) = \bigoplus_{g_1, \ldots, g_{\tilde{r}} \rightarrow \tilde{G}} M(z) \prod_{k=1}^{K} m_k(g_k \cdot x^{(k)}) = M(z) \prod_{k=1}^{K} \bigoplus_{g_k \sim \tilde{G}} m_k(g_k \cdot x^{(k)}).
\]
Note that \( R(m(x)) \) is the product of pure invariants, i.e. invariants that only involve variables from a single one of the blocks \( x^{(1)}, \ldots, x^{(K)}, z \). It is clear that \( I \) (from above) is a maximal set of algebraically independent pure invariants. It is now easy to show using the Jacobian criterion (Proposition 4.22) that if any \( R(m(x)) \) is added to \( I \), it will no longer be algebraically independent. The result now follows using basic properties of algebraic independence (Proposition 4.22 and Lemma 4.23). \( \square \)

Proof of Proposition 4.15
Since \( \mathbb{R}[x \! G] \subseteq \mathbb{R}[x \! G'] \), it is clear (in light of the above) that \( \text{trdeg}(\mathbb{R}[x \! G]) \leq r \). Thus we need only to show \( \text{trdeg}(\mathbb{R}[x \! G]) \geq r \) by demonstrating \( r \) algebraically independent invariants. Let \( e_1, \ldots, e_K \) be the elementary symmetric functions in \( K \) variables. With \( f_i \) as above, we take the invariants
\[
\{ e_k(f_i(x^{(1)}), \ldots, f_i(x^{(K)})) \}_{1 \leq i \leq \tilde{r}, 1 \leq k \leq K} \cup \{ e_2(z_1, \ldots, z_K), \ldots, e_K(z_1, \ldots, z_K) \}.
\]
Note that \( e_1(z_1, \ldots, z_K) \) is not included because it is equal to 0. The fact that \( e_k(f_i(x^{(1)}), \ldots, f_i(x^{(K)})) \) are algebraically independent can be seen because \( \{ e_1, \ldots, e_K \} \) is algebraically independent and \( \{ f_i(x^{(k)}) \}_{i,k} \) is algebraically independent. We can see that \( \{ e_k(z_1, \ldots, z_K) \}_{k \geq 2} \) are algebraically independent as follows. An algebraic dependence would be a polynomial \( P \) such that \( P(e_2(z_2, \ldots, z_K), \ldots, e_K(z_1, \ldots, z_K)) \) (now treating \( z_K \) as a separate variable) has a root \( z_K = -\sum_{k=1}^{K-1} z_k \) and thus has \( e_1(z_1, \ldots, z_K) \) as factor. But this contradicts the fact that any symmetric polynomial has a unique representation in terms of the elementary symmetric polynomials. \( \square \)

8.6 Gröbner bases

In this section we show how to use Gröbner bases to test various algebraic conditions. In particular, we prove Theorems 4.26 and 4.28. The ideas from this section are mostly standard in the theory of Gröbner bases; see e.g. [CLLO07] for a reference.

Definition 8.5. A monomial order on \( \mathbb{R}[x] \) is a well-ordering on the set \( M \) of all (monic) monomials, satisfying \( M \subseteq N \iff MP \leq NP \) for all \( M, N, P \in M \). We will say that a monomial order favors a variable \( x_i \) if the monomial \( x_i \) is larger (with respect to the monomial order) than any monomial not involving \( x_i \). We write \( LM(f) \) to denote the leading monomial of a polynomial \( f \), i.e. the monomial occurring in \( f \) that is largest (with respect to the monomial order); \( LM(f) \) does not include the coefficient.
**Definition 8.6.** A Gröbner basis of an ideal \( I \subseteq \mathbb{R}[x] \) is a finite subset \( B \subseteq I \) such that for every \( f \in I \) there exists \( b \in B \) such that \( \text{LM}(f) \) is a multiple of \( \text{LM}(b) \). We call \( B \) a reduced Gröbner basis if all its elements are monic and it has the additional property that for every pair of distinct \( b, b' \in B \), no monomial occurring in \( b \) is a multiple of \( \text{LM}(b') \).

The following basic facts about Gröbner bases are proved in [CLO07]. A Gröbner basis is indeed a basis, in that it generates the ideal. Every ideal \( I \subseteq \mathbb{R}[x] \) has a Gröbner basis, and has a unique reduced Gröbner basis. Buchberger’s algorithm computes the reduced Gröbner basis of an ideal \( I = \langle f_1, \ldots, f_m \rangle \), given a list of generators \( f_i \). (It is not a polynomial-time algorithm, however.)

Suppose we are interested in the relations between polynomials \( f_1, \ldots, f_m \in \mathbb{R}[x] \). Introduce additional variables \( t = (t_1, \ldots, t_m) \) and consider the ideal \( I := \langle f_1(x) - t_1, \ldots, f_m(x) - t_m \rangle \subseteq \mathbb{R}[x, t] \). Given \( f_1, \ldots, f_m \) there is an algorithm to compute a Gröbner basis for the elimination ideal

\[ J := \langle f_1(x) - t_1, \ldots, f_m(x) - t_m \rangle \cap \mathbb{R}[t]. \]

In fact, the algorithm is simply to compute a Gröbner basis for \( I \) using a particular monomial order and then keep only the elements that depend only on \( t \) (see Chapter 3 of [CLO07]). The elimination ideal consists precisely of the polynomial relations among \( f_1, \ldots, f_m \):

**Lemma 8.7.** For any polynomial \( P \in \mathbb{R}[t] \) we have: \( P \in J \) if and only if \( P(f_1(x), \ldots, f_m(x)) = 0 \).

**Proof.** The direction ‘\( \Rightarrow \)’ is clear because if we let \( t_i = f_i(x) \) for all \( i \) then the generators of \( I \) vanish and so every element of \( I \) vanishes. To show the converse, it suffices to show that for any polynomial \( P \in \mathbb{R}[t] \),

\[ P(f_1(x), \ldots, f_m(x)) - P(t_1, \ldots, t_m) \in I. \]

This can be shown inductively using the following key idea:

\[ x_1x_2 - t_1t_2 = \frac{1}{2}(x_1 - t_1)(x_2 + t_2) + \frac{1}{2}(x_2 - t_2)(x_1 + t_1) \]

and so \( x_1x_2 - t_1t_2 \in \langle x_1 - t_1, x_2 - t_2 \rangle. \)

**Generation as an \( \mathbb{R} \)-algebra.** Suppose we want to know whether \( f_m \in \mathbb{R}[f_1, \ldots, f_{m-1}] \). This is equivalent to asking whether there exists \( P \in J \) of the form

\[ P(t) = t_m - Q(t_1, \ldots, t_{m-1}) \]  

for some \( Q \in \mathbb{R}[t_1, \ldots, t_{m-1}] \). Suppose that \( J \) contains an element \( P \) of the form \((9)\). Compute a Gröbner basis \( B \) for \( J \) with respect to a monomial order that favors \( t_m \). The leading monomial of \( P \) is \( t_m \) so by the definition of a Gröbner basis there must be an element \( b \in B \) whose leading monomial divides \( t_m \). Since \( 1 \notin J \) (by Lemma 8.7), the leading monomial of \( b \) is exactly \( t_m \) and so \( b \) takes the form \((9)\). Therefore, \( f_m \in \mathbb{R}[f_1, \ldots, f_{m-1}] \) if and only if \( B \) contains an element of the form \((9)\).

We can now prove Theorem 12.28 to test whether \( \mathbb{R}[f_1, \ldots, f_m] = \mathbb{R}[x]^G \), compute generators \( g_1, \ldots, g_s \) for \( \mathbb{R}[x]^G \) (see Section 8.1) and use the above to test whether each \( g_i \) is in \( \mathbb{R}[f_1, \ldots, f_m] \).

**Generation as a field.** Suppose we want to know whether \( f_m \in \mathbb{R}(f_1, \ldots, f_{m-1}) \). This is equivalent to asking whether \( f_m \) can be expressed as a rational function of \( f_1, \ldots, f_{m-1} \) (with coefficients in \( \mathbb{R} \)), which is equivalent (by multiplying through by the denominator) to asking whether there exists \( P \in J \) of the form

\[ P(t) = t_mQ_1(t_1, \ldots, t_{m-1}) - Q_2(t_1, \ldots, t_{m-1}) \quad \text{with} \quad Q_1 \notin J. \]

Suppose that \( J \) contains an element \( P \) of the form \((10)\). Compute a reduced Gröbner basis \( B \) for \( J \) with respect to a monomial order that favors \( t_m \). It is a basic property of Gröbner bases that \( P \) can be written as

\[ P(t) = \sum_i p_i(t)b_i(t) \]

where \( p_i \in \mathbb{R}[t] \) and \( b_i \in B \) with \( \text{LM}(p_i) \leq \text{LM}(P) \) and \( \text{LM}(b_i) \leq \text{LM}(P) \). If no \( b_i \) involves the variable \( t_m \) then \( Q_1 \in J \), a contradiction. Therefore some \( b_j \) must have degree 1 in \( t_m \). Since \( B \) is a reduced Gröbner basis it cannot contain any element of the form \((10)\) with \( Q_1 \in J \). This completes the proof that \( f_m \in \mathbb{R}(f_1, \ldots, f_{m-1}) \) if and only if \( B \) contains an element of the form \((10)\).
Degree of field extension. Consider the setup from Theorem 124 given a finite set \( U = \{ f_1, \ldots, f_m \} \subseteq \mathbb{R}[x]^G \), we want to compute \( [F_G : F_U] \) where \( F_U = \mathbb{R}(U) \) and \( F_G \) is the field of fractions of \( \mathbb{R}[x]^G \). We can assume \( [F_G : F_U] \) is finite (since we can efficiently test whether this is the case using Proposition S2 and the methods of Section 112). Let \( d \) be such that \( \mathbb{R}[x]^G \) generates \( F_G \) as a field (over \( \mathbb{R} \)). (It is sufficient for \( \mathbb{R}[x]^G \) to generate \( \mathbb{R}[x]^G \) as an \( \mathbb{R} \)-algebra; such a \( d \) can be computed via Section S11.) If \( G \) is finite then \( d = |G| \) is sufficient; see Section 113. A generic element of \( \mathbb{R}[x]^G \) will generate the field extension:

**Lemma 8.8.** For all but a measure-zero set of \( \alpha \in \mathbb{R}[x]^G \), \( F_G = F_U(\alpha) \).

This fact is related to the primitive element theorem. We include a proof for completeness.

**Proof.** The field extension \( F_G/F_U \) is finite and separable (since we’re in characteristic zero), so by the fundamental theorem of Galois theory, there are only finitely many intermediate fields. (Take the normal closure of \( F_G/F_U \); then the intermediate fields are in bijection with a finite group, and only some of them lie inside \( F_G \).) Let \( \mathcal{L} \) be the collection of intermediate fields of \( F_G/F_U \) that are proper subfields of \( F_G \). We know \( \mathbb{R}[x]^G \) is a subspace of \( F_G \) that generates \( F_G \) and therefore is not contained by any field in \( \mathcal{L} \). This means each field \( \mathcal{L} \in \mathcal{L} \) intersects \( \mathbb{R}[x]^G \) at a proper subspace \( V_L \) of \( \mathbb{R}[x]^G \). The finite union \( \cup_{L \in \mathcal{L}} V_L \) is a measure-zero subset of \( \mathbb{R}[x]^G \) and any \( \alpha \) outside of it satisfies \( F_G = F_U(\alpha) \).

Let \( \alpha \) be a generic element of \( \mathbb{R}[x]^G \). In light of the above, \( [F_G : F_U] \) is equal to the smallest positive integer \( D \) for which there exists a relation

\[
Q_D(f_1, \ldots, f_m) \alpha^D + \cdots + Q_1(f_1, \ldots, f_m) \alpha + Q_0(f_1, \ldots, f_m) = 0
\]

for polynomials \( Q_i \) with \( Q_D(f_1, \ldots, f_m) \neq 0 \). This can be tested similarly to field generation. Compute a reduced Gröbner basis \( B \) for the elimination ideal \( J \subseteq \mathbb{R}[t_1, \ldots, t_m, \tau] \) consisting of the relations among \( f_1, \ldots, f_m, \tau \); use a monomial order that favors \( \tau \). Then \( [F_G : F_U] \) is equal to the smallest positive integer \( D \) for which \( B \) contains an element of degree \( D \) in \( \tau \) (or \( \infty \) if \( B \) contains no element that involves \( \tau \)). This proves Theorem 120.

**Remark 8.9.** An alternative to using Gröbner bases for the above tasks is to solve a (very large) linear system in order to find the minimal relation among a set of polynomials. There are bounds on the maximum possible degree of such a relation (if one exists) \([\text{Kay09}]\).

### 9 Proofs for \( S^2 \) registration

#### 9.1 Formula for Hilbert series of \( \mathbb{R}[x]^G \)

We can derive the Hilbert series of \( \mathbb{R}[x]^G \) for \( S^2 \) registration using the methods in Section 4.6 of \([\text{DK15}]\).

**Proposition 9.1.** Consider \( S^2 \) registration with frequencies \( \mathcal{F} \). For \( |t| < 1 \), the Hilbert series of \( \mathbb{R}[x]^G \) is given by

\[
H(t) = \sum_{z \in \mathcal{P}} \text{Res}(f, z)
\]

where

\[
f(z) = \frac{1 - \frac{1}{2}(z + 1/z)}{z \prod_{\ell \in \mathcal{F}} \prod_{m=-\ell}^{\ell}(1 - tz^m)} = \frac{-z^{N-2}(1-z^2)}{2 \prod_{\ell \in \mathcal{F}} \prod_{m=1}^{\ell}(z^m - t) \prod_{m=0}^{\ell}(1 - tz^m)}
\]

with \( N = \frac{1}{2} \sum_{\ell \in \mathcal{F}} \ell(\ell + 1) \). Here \( \text{Res}(f, z) \) denotes the residue (from complex analysis) of the function \( f \) at the point \( z \), and \( \mathcal{P} \) is the set of poles of \( f(z) \) inside the unit circle (in \( \mathbb{C} \)). Namely, \( \mathcal{P} \) contains \( t^{1/m} e^{\frac{2\pi ik}{m}} \) for all \( m \in \{1, 2, \ldots, \max_{\ell \in \mathcal{F}} \ell \} \) and for all \( k \in \{0, 1, \ldots, m-1\} \). If \( N \leq 1 \), \( \mathcal{P} \) also contains 0.
Proof. Recall Molien’s formula (Proposition 4.13):

\[ H(t) = \prod_{g \sim \text{Haar}(G)} \det(I - t \rho(g))^{-1}. \]

Note that \( \det(I - t \rho(g)) \) depends only on the conjugacy class of \( g \). In \( \text{SO}(3) \), two elements are conjugate if and only if they rotate by the same angle \( \phi \). When \( g \sim \text{Haar}(\text{SO}(3)) \), the angle \( \phi = \phi(g) \) is distributed with density function \( \frac{1}{\pi}(1 - \cos \phi) \) on \([0, \pi]\) (see e.g. [Sal79]). If \( g \) has angle \( \phi \), the matrix \( \rho(g) \) by which it acts on the irreducible representation \( V_\ell \) has eigenvalues \( e^{-i\ell\phi}, e^{-i(\ell-1)\phi}, \ldots, e^{i\ell\phi} \) (see e.g. [vYc01]). The matrix \( \rho(g) \) by which \( g \) acts on \( V = \bigoplus_{\ell \in \mathbb{F}} V_\ell \) is block diagonal with blocks \( \rho_\ell(g) \). Using the above we write an expression for the Hilbert series:

\[ H(t) = \frac{1}{\pi} \int_0^\pi \prod_{\ell \in \mathbb{F}} \prod_{m = -\ell}^{\ell} (1 - te^{im\phi}) \, d\phi = \frac{1}{2\pi} \int_0^{2\pi} \prod_{\ell \in \mathbb{F}} \prod_{m = -\ell}^{\ell} (1 - te^{im\phi}) \, d\phi. \]

Now write this as a complex contour integral around the unit circle in \( \mathbb{C} \) and apply the residue theorem from complex analysis to arrive at the result. \( \square \)

### 9.2 Formula for dimension of \( \mathbb{R}[x]^G \)

The dimension of \( \mathbb{R}[x]^G \) can be extracted as the coefficient of \( t^d \) in the Hilbert series from the previous section, but here we give a different formula based on character theory from representation theory. The character of a representation \( \rho : G \to \text{GL}(V) \) (where \( V \) is a finite-dimensional real vector space) is the function \( \chi_V : G \to \mathbb{R} \) defined by \( \chi_V(g) = \text{tr}(\rho(g)) \).

In our case, using the eigenvalues of \( \rho_\ell(g) \) from the previous section, we have

\[ \chi_{V_\ell}(g) = 1 + 2 \sum_{m=1}^{\ell} \cos(m \phi(g)) \]

where \( \phi(g) \) is the angle of rotation of \( g \). For \( V = \bigoplus_{\ell \in \mathbb{F}} V_\ell \) we then have \( \chi_V(g) = \sum_{\ell \in \mathbb{F}} \chi_{V_\ell}(g) \).

As a representation of \( G = \text{SO}(3) \), \( \mathbb{R}[x]_d \) is (isomorphic to) the \( d \)th symmetric power of \( V \), denoted \( S^d(V) \). (This is using the fact that a real representation is isomorphic to its dual.) There is a recursive formula for the character of \( S^d(V) \):

\[ \chi_{S^d(V)}(g) = \frac{1}{d} \sum_{i=1}^{d} \chi_V(g^i) \chi_{S^{d-i}(V)}(g). \]

This comes from the Newton–Girard formula for expressing complete homogeneous symmetric polynomials in terms of power sum polynomials.

The representation \( \mathbb{R}[x]_d = S^d(V) \) decomposes as the direct sum of irreducible representations \( V_\ell \). The subspace of \( \mathbb{R}[x]_d \) consisting of all copies of the trivial representation \( V_0 \) (the 1-dimensional representation on which every group element acts as the identity) is precisely \( \mathbb{R}[x]_d^G \). Thus, \( \dim(\mathbb{R}[x]_d^G) \) is the number of copies of the trivial representation in the decomposition of \( \mathbb{R}[x]_d \). This can be computed using characters: \( \dim(\mathbb{R}[x]_d^G) = \langle \chi_{S^d(V)}, \chi_V \rangle = \langle \chi_{S^d(V)}, 1 \rangle \) where \( \langle f_1, f_2 \rangle := \int_{g \sim \text{Haar}(G)} [f_1(g)f_2(g)] \). Since characters are class functions (i.e. they are constant on conjugacy classes), we can compute this inner product by integrating over the angle \( \phi \) (as in the previous section). This yields the formula stated in Proposition 5.7.

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### A Spherical harmonics and SO(3) invariants

#### A.1 Spherical harmonics

We follow the conventions of [BF97]. Parametrize the unit sphere by angular spherical coordinates \((\theta, \phi)\) with \(\theta \in [0, \pi]\) and \(\phi \in [0, 2\pi]\). (Here \(\theta = 0\) is the north pole and \(\theta = \pi\) is the south pole.) For integers \(\ell \geq 0\) and \(-\ell \leq m \leq \ell\), define the complex spherical harmonic

\[
Y_{\ell m}(\theta, \phi) = (-1)^m N_{\ell m} P^m_\ell (\cos \theta) e^{im\phi}
\]

with normalization factor

\[
N_{\ell m} = \sqrt{\frac{(2\ell + 1)(\ell - m)!}{4\pi(\ell + m)!}}
\]

where \(P^m_\ell(x)\) are the associated Legendre polynomials

\[
P^m_\ell(x) = \frac{1}{2\ell!} (1 - x^2)^{\ell/2} \frac{d^{\ell+m}}{dx^{\ell+m}}(x^2 - 1)^\ell.
\]

In the \(S^2\) registration problem we are interested in representing a real-valued function on the sphere, in which case we use an expansion (with real coefficients) in terms of the real spherical harmonics:

\[
S_{\ell m}(\theta, \phi) = \begin{cases} 
\frac{(-1)^m}{\sqrt{2}} (Y_{\ell m}(\theta, \phi) + Y_{\ell m}(\theta, \phi)) = \sqrt{2} N_{\ell m} P^m_\ell (\cos \theta) \cos(m\phi) & m > 0, \\
Y_{00}(\theta, \phi) = N_{00} P^0_0 (\cos \theta) & m = 0, \\
\frac{(-1)^m}{\sqrt{2}} (Y_{\ell |m|}(\theta, \phi) - Y_{\ell |m|}(\theta, \phi)) = \sqrt{2} N_{\ell |m|} P^{|m|}_\ell (\cos \theta) \sin(|m|\phi) & m < 0.
\end{cases}
\]
Here $\overline{Y_{\ell m}}$ is the complex conjugate of $Y_{\ell m}$, which satisfies the identity
\[ \overline{Y_{\ell m}(\theta, \phi)} = (-1)^m Y_{\ell(-m)}(\theta, \phi). \]  
(11)

Above we have also used the identity $P^{-m}_\ell = (-1)^m \frac{(\ell - m)!}{(\ell + m)!} P^m_\ell$, which implies $N_{\ell(-m)} P^{-m}_\ell = (-1)^m N_{\ell m} P^m_\ell$.

In the cryo-EM problem we are instead interested in representing the Fourier transform of a real-valued function. Such a function $f$ has the property that if $\vec{r}$ and $-\vec{r}$ are antipodal points on the sphere, $f(-\vec{r}) = \overline{f(\vec{r})}$. For this type of function we use an expansion (with real coefficients) in terms of a new basis of spherical harmonics:
\[ H_{\ell m}(\theta, \phi) = \begin{cases} \frac{1}{\sqrt{2}}(Y_{\ell m}(\theta, \phi) + (-1)^{\ell+m} Y_{\ell(-m)}(\theta, \phi)) & m > 0, \\ i^{\ell} Y_{\ell 0}(\theta, \phi) & m = 0, \\ \frac{1}{\sqrt{2}}(Y_{\ell|m|}(\theta, \phi) - (-1)^{\ell+m} Y_{\ell(-|m|)}(\theta, \phi)) & m < 0. \end{cases} \]

One can check that $H_{\ell m}(\vec{r}) = \overline{H_{\ell m}(\vec{r})}$ using (11) along with the fact $Y_{\ell m}(\vec{r}) = (-1)^{\ell} Y_{\ell m}(\vec{r})$ which comes from $P^m_\ell(-x) = (-1)^{\ell+m} P^m_\ell(x)$.

### A.2 Wigner D-matrices

We will mostly work in the basis of complex spherical harmonics $Y_{\ell m}$ since the formulas are simpler. The analogous results for the other bases can be worked out by applying the appropriate change of basis.

Let $V_\ell \simeq \mathbb{C}^{2\ell+1}$ be the vector space consisting of degree-$\ell$ complex spherical harmonics represented in the basis $\{Y_{\ell m}\}_{-\ell \leq m \leq \ell}$, i.e. $v \in \mathbb{C}^{2\ell+1}$ encodes the spherical harmonic $\sum_{m=-\ell}^{\ell} v_m Y_{\ell m}$. These $V_\ell$ (for $\ell = 0, 1, 2, \ldots$) are the irreducible representations of $\text{SO}(3)$. Each can also be defined over the real numbers by changing basis to the real spherical harmonics $S_{\ell m}$.

A group element $g \in \text{SO}(3)$ acts on a (spherical harmonic) function $f : S^2 \to \mathbb{R}$ via $(g \cdot f)(x) = f(g^{-1}x)$. The action of $g$ on $V_\ell$ is given by the Wigner D-matrix $D^\ell(g) \in \mathbb{C}^{(2\ell+1) \times (2\ell+1)}$ defined as in [BFB97].

We will need the following orthogonality properties of the Wigner D-matrices. First, the standard Schur orthogonality relations from representation theory yield
\[ \mathbb{E}_{g \sim \text{Haar}(\text{SO}(3))} D^\ell_{mk}(g) D^\ell_{m'k'}(g) = \frac{1}{2\ell + 1} \mathbb{I}_{\ell = \ell'} \mathbb{I}_{m = m'} \mathbb{I}_{k = k'}. \]

We also have [Ros57]
\[ D^\ell_{mk}(g) D^{\ell'}_{m'k'}(g) = \sum_{L = |L|} \langle \ell \ell' m m' | L (m + m') \rangle \langle L k k' | L (k + k') \rangle D^L_{(m + m')(k + k')}(g) \]

where $\langle \ell_1 m_1 \ell_2 m_2 | \ell m \rangle$ is a Clebsch-Gordan coefficient. There is a closed-form expression for these coefficients [Böhm13]:
\[ \langle \ell_1 m_1 \ell_2 m_2 | \ell m \rangle = \mathbb{I}_{m = m_1 + m_2} \sqrt{\frac{(2\ell + 1)(\ell + \ell_1 - \ell_2)!(\ell - \ell_1 + \ell_2)!(\ell_1 + \ell_2 - \ell)!(\ell_1 + \ell_2 + \ell + 1)!}{(\ell_1 + \ell_2 - \ell_1)!}} \times \sqrt{(\ell + m)!(\ell - m)!(\ell_1 - m_1)!(\ell_1 + m_1)!(\ell_2 + m_2)!(\ell_2 - m_2)!} \times \sum_k \frac{(-1)^k}{k!(\ell + \ell_2 - \ell - k)!((\ell_1 - m_1 - k)!(\ell_2 + m_2 - k)!((\ell - \ell_2 + m_1 + k)!(\ell - \ell_1 - m_2 + k)!}} \]

where the sum is over all $k$ for which the argument of every factorial is nonnegative.
A.3 Moment tensor

Let $\mathcal{F}$ be a multi-set of frequencies from $\{1, 2, \ldots\}$ and consider the action of $G = \text{SO}(3)$ on $V = \oplus_{\ell \in \mathcal{F}} V_\ell$. Recall that we want an explicit formula for $T_d(x) = E_g[(\Pi(g \cdot x))^\otimes d]$ with $g \sim \text{Haar}(G)$ (where $\Pi$ can be the identity in the case of no projection). We have

$$E_g[(\Pi(g \cdot x))^\otimes d] = \Pi^\otimes d E_g[\rho(g)^\otimes d] x^\otimes d$$

(where $x^\otimes d$ is a column vector of length $\dim(V)^d$) and so we need an explicit formula for the matrix $E_g[\rho(g)^\otimes d]$. Here $\rho(g)$ is block diagonal with blocks $D^\ell(g)$ for $\ell \in \mathcal{F}$. There are no degree-1 invariants since we have excluded the trivial representation. We have

$$T_d = \text{the above orthogonality relations} \text{ (and using } E_g)$$

Similarly, for degree 3 we have

$$E_g[(D^\ell_1(g))_{m_1,k_1}(D^\ell_2(g))_{m_2,k_2}](D^\ell_3(g))_{m_3,k_3}] =$$

using the special case $\langle \ell_1, \ell_2, m_2 | 0 \rangle = 1, \ell_1 = \ell_2, m_1 = -m_2$.

$$= \langle \ell_1, \ell_2, m_1 = -m_2 | \ell_1 m_1 \ell_2 m_2 | 0 \rangle$$

A.4 Projection

Let $V = \oplus_{\ell \in \mathcal{F}} V_\ell$ with $\mathcal{F}$ a subset of $\{1, 2, \ldots\}$. Let $\Pi : V \rightarrow W$ be the projection that takes a complex spherical harmonic function and reveals only its values on the equator $\theta = \pi/2$. In cryo-EM this projection is applied separately to each shell (see Section 5.3). Letting $L = \max_{\ell \in \mathcal{F}} \ell$, the functions $b_{-L}, b_{-L+1}, \ldots, b_L$ (from the circle $S^1$ to $\mathbb{R}$) form a basis for $W$, where $b_m(\phi) = e^{im\phi}$. The projection $\Pi$ takes the form

$$\Pi(Y_{\ell m}) = (-1)^m N_{\ell m} P^m_\ell (0)b_m$$

extended by linearity. By taking a binomial expansion of $(x^2 - 1)^\ell$ it can be shown that

$$P^m_\ell (0) = \begin{cases} 0, & (\ell + m) \text{ odd,} \\ \frac{(-1)^{(\ell-m)/2} \ell! (\ell + m)!}{2^\ell \ell! (\ell + m)!}, & (\ell + m) \text{ even.} \end{cases} \quad (12)$$

For cryo-EM, if we use the basis $H_{\ell m}$ so that the expansion coefficients are real, the output of the projection can be expressed (with real coefficients) in the basis

$$h_m(\phi) = \begin{cases} \frac{1}{\sqrt{2}}(e^{im\phi} + (-1)^m e^{-im\phi}) & m > 0, \\ 1 & m = 0, \\ \frac{1}{\sqrt{2}}(e^{im\phi} - (-1)^m e^{-im\phi}) & m < 0, \end{cases}$$

where the projection $\Pi$ takes the form

$$\Pi(H_{\ell m}) = (-1)^m N_{\ell |m|} P^{|m|}_\ell (0)h_m$$

extended by linearity.
A.5 Explicit construction of invariants

Consider the cryo-EM setup (see Section A.3) with $S$ shells and $F$ frequencies. We will cover $S^2$ registration as the special case $S = 1$ (without projection). Use the basis of complex spherical harmonics, with corresponding variables $x_{s,l}$ with $1 \leq s \leq S$, $1 \leq l \leq F$, and $-l \leq m \leq l$. One can change variables to $S_{l,m}$ or $H_{l,m}$ but for our purposes of testing the rank of the Jacobian it is sufficient to just work with $Y_{l,m}$ (since the change of variables has no effect on the rank of the Jacobian).

Recall that in Section A.3 we computed expressions for the matrices $E_g[D^f_1(g) \otimes D^f_2(g)]$ and $E_g[D^f_1(g) \otimes D^f_2(g) \otimes D^f_3(g)]$, and in particular they are rank-1. Using this we can explicitly compute the entries of $T_d(x)$ and thus extract a basis for $U_2^T$ and $U_3^T$. We present the results below.

A.5.1 Degree-2 invariants

Without projection, the degree-2 invariants are

$$I_2(s_1, s_2, \ell) = \frac{1}{2\ell + 1} \sum_{|k| \leq \ell} (-1)^k x_{s_1,\ell k} x_{s_2,\ell(-k)}$$

for $s_1, s_2 \in \{1, \ldots, S\}$ and $\ell \in \{1, \ldots, F\}$. Swapping $s_1$ with $s_2$ results in the same invariant, so take $s_1 \leq s_2$ to remove redundancies.

With projection, the degree-2 invariants are

$$P_2(s_1, s_2, m) = (-1)^m \sum_{\ell \geq |m|} N_{l,m} P_m^{\ell}(0) P_m^{-\ell}(0) I_2(s_1, s_2, \ell)$$

with $s_1, s_2 \in \{1, \ldots, S\}$ and $m \in \{-F, \ldots, F\}$. Negating $m$ or swapping $s_1$ with $s_2$ results in the same invariant (up to sign) so take $s_1 \leq s_2$ and $m \geq 0$ to remove redundancies. Recall the expression (12) for $P_m^{\ell}(0)$.

A.5.2 Degree-3 invariants

Let $\Delta(\ell_1, \ell_2, \ell_3)$ denote the predicate $|\ell_2 - \ell_3| \leq \ell_1 \leq \ell_2 + \ell_3$ (which captures whether $\ell_1, \ell_2, \ell_3$ can be the side-lengths of a triangle). Without projection, the degree-3 invariants are

$$I_3(s_1, \ell_1, s_2, \ell_2, s_3, \ell_3) = \frac{1}{2\ell_1 + 1} \sum_{k_1 + k_2 + k_3 = 0, |k_i| \leq \ell} (-1)^{k_1} \langle \ell_2 k_2 \ell_3 k_3 | \ell_1 (-k_1) \rangle x_{s_1,\ell_1 k_1} x_{s_2,\ell_2 k_2} x_{s_3,\ell_3 k_3}$$

for $s_i \in \{1, \ldots, S\}$ and $\ell_i \in \{1, \ldots, F\}$ satisfying $\Delta(\ell_1, \ell_2, \ell_3)$. There are some redundancies here. First, permuting the three $(s_i, \ell_i)$ pairs (while keeping each pair in tact) results in the same invariant (up to scalar multiple). Also, some of the above invariants are actually zero; specifically, this occurs when $(s_1, \ell_1) = (s_2, \ell_2) = (s_3, \ell_3)$ with $\ell_1$ odd, or when $(s_1, \ell_1) = (s_2, \ell_2) \neq (s_3, \ell_3)$ with $\ell_3$ odd (or some permutation of this case).

With projection, the degree-3 invariants are

$$P_3(s_1, m_1, s_2, m_2, s_3, m_3) =$$

$$(-1)^{m_1} \sum_{\ell_1, \ell_2, \ell_3 : \Delta(\ell_1, \ell_2, \ell_3)} N_{\ell_1 m_1} N_{\ell_2 m_2} N_{\ell_3 m_3} P_{\ell_1}^{m_1}(0) P_{\ell_2}^{m_2}(0) P_{\ell_3}^{m_3}(0) \langle \ell_2 m_2 \ell_3 m_3 | \ell_1 (-m_1) \rangle I_3(s_1, \ell_1, s_2, \ell_2, s_3, \ell_3)$$

for $s_i \in \{1, \ldots, S\}$ and $m_i \in \{-F, \ldots, F\}$ such that $m_1 + m_2 + m_3 = 0$. There are again redundancies under permutation: permuting the three $(s_i, m_i)$ pairs results in the same invariant. Negating all three $m$’s also results in the same invariant. There are additional non-trivial linear relations (see Section A.6 below).
A.6 Counting the number of invariants

A.6.1 $S^2$ registration

For the case of $S^2$ registration ($S = 1$) the above degree-2 and degree-3 invariants without projection (with redundancies removed as discussed above) form a basis for $\mathbb{R}[x_1^G] \oplus \mathbb{R}[x_3^G]$ (although we have not made this rigorous). Thus, counting these invariants gives a combinatorial analogue of Proposition 5.7.

A.6.2 Cryo-EM

In this section we give a formula for $\text{trdeg}(U^T_{\leq 3})$ for (heterogeneous) cryo-EM (with projection), valid for all $K \geq 1$, $S \geq 1$ and $F \geq 2$. The formula is conjectural but has been tested (via the Jacobian criterion) for various small values of $K, S, F$.

The number of algebraically independent degree-2 invariants turns out to be the number of distinct $\mathcal{I}_2$ invariants (i.e. without projection), since the projected invariants $\mathcal{P}_2$ are linear combinations of these. The number of such invariants is $\frac{1}{2}S(S + 1)F$.

For degree 3, things are more complicated because the projected invariants $\mathcal{P}_3$ have smaller dimension than the $\mathcal{I}_3$. We start by counting the number of distinct (up to scalar multiple) $\mathcal{P}_3$ invariants. To this end, let $\mathcal{X}(S, F)$ be the set of equivalence classes of tuples $(s_1, m_1, s_2, m_2, s_3, m_3)$ with $s_i \in \{1, \ldots, S\}$ and $m_i \in \{-F, \ldots, F\}$, modulo the relations

$$(s_1, m_1, s_2, m_2, s_3, m_3) \sim (s_2, m_2, s_1, m_1, s_3, m_3) \sim (s_1, m_1, s_3, m_3, s_2, m_2) \quad \text{(permutation)}$$

$$(s_1, m_1, s_2, m_2, s_3, m_3) \sim (s_1, -m_1, s_2, -m_2, s_3, -m_3) \quad \text{(negation)}.$$ 

There are some non-trivial linear relations among the distinct $\mathcal{P}_3$ invariants, which we must now account for. The number of such relations is

$$E(S) := 2S + 4S(S - 1) + S(S - 1)(S - 2).$$

This can be broken down as follows. For each $k \in \{1, 2, 3\}$ there are $2k$ relations for each size-$k$ multiset $\{s_1, s_2, s_3\}$ of $\{1, \ldots, S\}$ with exactly $k$ distinct elements. (We do not currently have a thorough understanding of what exactly the linear relations are, but we have observed that the above pattern holds.)

We can now put it all together and state our conjecture. We will also use the formula (3) for $\text{trdeg}(\mathbb{R}[x]^G)$, extended to the heterogeneous case via Proposition 4.15.

**Conjecture A.1.** Consider cryo-EM with $F \geq 2$ frequencies.

- $\text{trdeg}(\mathbb{R}[x]^G) = K[S(F^2 + 2F) - 3] + K - 1$,

- $\text{dim}(U^T_2) = \frac{1}{2}S(S + 1)F$,

- $\text{dim}(U^T_3) = |\mathcal{X}(S, F)| - E(S),$

- generic list recovery is possible at degree 3 if and only if $\text{dim}(U^T_2) + \text{dim}(U^T_3) \geq \text{trdeg}(\mathbb{R}[x]^G)$.

When $S$ and $F$ are large, the dominant term in $\text{dim}(U^T_2) + \text{dim}(U^T_3)$ is $|\mathcal{X}(S, F)| \approx S^3F^2/4$ and so generic list recovery is possible when (roughly) $K \leq S^2/4$.

B Unique recovery for the regular representation

Let $G$ be a finite abelian group. Let $V$ be the regular representation of $G$ over $\mathbb{R}$, i.e. $V = \mathbb{R}[G]$ with basis indexed by the elements of $G$, and the action of $G$ permutes the basis elements $v_g$ according to group multiplication: $h \cdot v_g = v_{hg}$. Note that for the cyclic group $G = \mathbb{Z}/p$, this is precisely the MRA problem. We will show that with this setup, generic unique recovery is possible at degree 3:
Theorem B.1. Let $G$ be a finite abelian group and let $V$ be the regular representation of $G$ over $\mathbb{R}$. Then $\mathbb{R}(U_{\leq 3}^T)$ is equal to the field of fractions of $\mathbb{R}[x]^G$.

Recall that the equality of the two fields above implies generic unique recovery at degree 3 by Corollary\textsuperscript{125}. Generic unique recovery at degree 3 is actually true in the more general setting where $V$ is the regular representation over $\mathbb{R}$ of any finite group [Kak09].

Proof. It is sufficient to show $\mathbb{C}(U_{\leq 3}^T) = \mathbb{C}(\mathbb{R}[x]^G)$. Let $p = |G| = \dim(V)$. The polynomial algebra on $V$ gets an action of $G$ in the usual way and the degree-1 component is isomorphic to the regular representation.

Over $\mathbb{C}$, the regular representation decomposes as a direct sum of all the characters $\chi^{(1)}, \ldots, \chi^{(p)}$ of $G$ (each of which is a group homomorphism $G \to \mathbb{C}^\times = \mathbb{C} \setminus \{0\}$). (Here we have used the fact that $G$ is finite and abelian, and so its irreducible representations are 1-dimensional.)

Let $\hat{G} = \{\chi^{(1)}, \ldots, \chi^{(p)}\}$ be the set of characters. For each $\chi \in \hat{G}$ let $y_\chi \in \mathbb{C}[V]$ be the associated eigenvector (in the degree-1 component of the polynomial algebra) so that $g \cdot y_\chi = \chi(g)y_\chi$ for all $g \in G$. $\hat{G}$ forms an abelian group (the character group or Pontryagin dual of $G$) under pointwise multiplication: $(\chi_1 \chi_2)(g) = \chi_1(g)\chi_2(g)$.

Observe that for any $\chi \in \hat{G}$, $y_\chi y_{\chi^{-1}}$ is a degree-2 invariant, and for any $\chi_1, \chi_2 \in \hat{G}$, $y_{\chi_1} y_{\chi_2} y_{(\chi_1 \chi_2)^{-1}}$ is a degree-3 invariant. For each $\chi \in \hat{G}$ we have

$$y_\chi^p \prod_{\chi' \in \hat{G}} \frac{y_{\chi'}}{y_{\chi}} = \prod_{\chi' \in \hat{G}} y_{\chi} y_{\chi'} y_{(\chi'\chi)^{-1}}$$

and so $y_\chi^p$ lies in the field generated by the invariants of degree $\leq 3$.

The field extension $\mathbb{C}(y_{\chi^{(1)}}, \ldots, y_{\chi^{(p)}})/\mathbb{C}(y_{\chi^{(1)}}, \ldots, y_{\chi^{(p)}})$ is Galois with Galois group $H = (\mathbb{Z}/p)^p$; the generator of the $i$th copy of $\mathbb{Z}/p$ acts by multiplying $y_{\chi^{(i)}}$ by a fixed primitive $p$th root of unity. (Recall that the Galois group is the automorphisms of the larger field that fix the smaller field pointwise.)

By the fundamental theorem of Galois theory, intermediate extensions of the above Galois extension are in bijection with subgroups of $H$. The correspondence maps a field to the group that fixes it (pointwise) and maps a group to the field that it fixes. The field $\mathbb{C}(\mathbb{R}[x]^G)$ is an intermediate extension with corresponding group $G$. The field $\mathbb{C}(U_{\leq 3}^T)$ is also an intermediate extension, and we will show that its corresponding group is also $G$, thus proving $\mathbb{C}(U_{\leq 3}^T) = \mathbb{C}(\mathbb{R}[x]^G)$ as desired.

Clearly $G$ fixes $\mathbb{C}(U_{\leq 3}^T)$ (since $U_{\leq 3}$ are invariants), so it remains to show that there are no other automorphisms of $\mathbb{C}(y_{\chi^{(1)}}, \ldots, y_{\chi^{(p)}})$ that fix $U_{\leq 3}$. Let $\phi \in H$. As an element of $(\mathbb{Z}/p)^p$, we can write $\phi = (\phi_1, \ldots, \phi_p)$. If $\chi = \chi^{(i)}$ we will also write $\phi_\chi$ for $\phi_i$. If $\phi$ fixes the degree-2 invariant $y_{\chi} y_{\chi^{-1}}$, we must have $\phi_{\chi^{-1}} = \phi_{\chi}^{-1}$. If $\phi$ also fixes the degree-3 invariant $y_{\chi_1} y_{\chi_2} y_{(\chi_1 \chi_2)^{-1}}$, we must have $\phi_{\chi_1} \phi_{\chi_2} = \phi_{(\chi_1 \chi_2)^{-1}} = \phi_{\chi_1} \phi_{\chi_2}$. In particular, the map $\hat{G} \to \mathbb{C}^\times$ given by $\chi \mapsto \phi_\chi$ is a group homomorphism. Thus, any $\phi$ fixing $U_{\leq 3}$ can be identified with an element of the Pontryagin double dual $\hat{\hat{G}}$, which is isomorphic to $G$; in particular there are only $p$ such elements $\phi$, which completes the proof. \qed