

000 001 002 003 004 005 006 007 008 009 010 011 012 013 014 015 016 017 018 019 020 021 022 023 024 025 026 027 028 029 030 031 032 033 034 035 036 037 038 039 040 041 042 043 044 045 046 047 048 049 050 051 052 053 LEARNING EQUIVARIANT TENSOR FUNCTION REPRESENTATIONS VIA COVARIANT ALGEBRA OF BINARY FORMS

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ABSTRACT

Representing tensor-valued functions of tensor arguments is fundamental in many modeling problems. Tensor functions play a central role in constructing reduced-order approximations and are particularly useful for nonlinear anisotropic constitutive modeling of physical phenomena, such as fluid turbulence and material deformation among others. By imposing equivariance under the orthogonal group, tensor functions can be finitely and minimally generated by using the isomorphism between binary forms and symmetric trace-free tensors. After determining minimal generators, their coefficients can be learned as functions of the invariants of the tensor arguments by training on data which facilitates generality of the models. The algebraic nature of the learned models makes them interpretable by revealing underlying dynamics, and it keeps the models economical as they contain the theoretically minimum required number of terms. Determining minimal representations of higher-order tensor functions has remained computationally intractable in many cases of interest until now. The current work overcomes this limitation. Numerically efficient algorithms for generating tensor functions and reducing them to minimal sets are presented. A few classical tensor function representations and an approach to a bottleneck in modeling turbulence are worked out to showcase the practical applicability of our framework.

1 INTRODUCTION

Tensor function representations are important for building models of tensors using tensors arguments. They are useful for many applications in physics, particularly fluid turbulence (Alfonsi (2009); Speziale et al. (1991); Speziale (1990)) and continuum mechanics (Olive et al. (2017); Boehler & Boehler (1987); Boehler (1979)), and also modeling problems dealing with image and video data as tensors of order 2 and 3 (Vasilescu & Terzopoulos (2002); Shashua & Hazan (2005)). It is a much more intricate modeling problem than while working with scalars due to the complexity of the structure imposed by tensor symmetries.

For learning physically meaningful tensor function representations, in addition to maintaining consistent symmetry in index permutations, it is also important to preserve proper rotational or orthogonal equivariance, i.e., rotating or reflecting the inputs should also rotate or reflect the outputs predictably (Zheng (1994)).

$$\mathbf{T} : \mathbb{V} \rightarrow \mathbb{T}^m, \quad \text{where} \quad \mathbb{V} := \mathbb{T}^{n_1} \oplus \mathbb{T}^{n_2} \oplus \mathbb{T}^{n_3} \cdots \oplus \mathbb{T}^{n_k} \quad (1)$$

In this work, a new strategy is presented for building equivariant tensor functions of tensor of the type shown in Eq. 1. These functions can be modeled as a linear combination of Invariant scalar coefficients (**C**s) and equivariant tensor monomials (**B**s) which depend on some tensor arguments (**A**s) as shown in Eq. 2. The **C**s are functions of joint invariants (λ_i) of **A**s and the tensor monomials are *einsum* type tensor products of **A**s.

$$\mathbf{T}(\mathbf{A}_1, \mathbf{A}_2, \dots, \mathbf{A}_k) = \sum_{i=1}^{\gamma} C_i(\lambda_1, \lambda_2, \dots, \lambda_m) \mathbf{B}_i(\mathbf{A}_1, \mathbf{A}_2, \dots, \mathbf{A}_k) \quad (2)$$

054 The model in Eq. 2 is *complete* if 1) all invariants of \mathbb{V} are *generated* by (functions of) λ s and
 055 2) all tensor monomials in \mathbb{V} are linear *combinations* of \mathbf{B} s under scalar coefficient functions of
 056 the joint invariants. Additionally, the model is *minimal* if removing any tensor monomial or joint
 057 invariant makes the model incomplete. Working with minimal generator sets significantly reduces
 058 the number of terms involved in modeling. In many cases it is not just preferable, but necessary to
 059 make computations tractable. The goal of the current work is to develop a framework for determining
 060 minimally complete tensor function representations which are equivariant under the $SO(3, \mathbb{R})$
 061 group, and to establish their applicability in modeling any generic physical tensor in 3 dimensions.
 062 From a modeling perspective, the structure (or the coded versions) of \mathbf{B}_i 's and the λ_i 's can be de-
 063 rived *apriori*, while the exact coefficients C_i s are *learned* using domain-specific data from \mathbf{T} and
 064 $(\mathbf{A}_1, \mathbf{A}_2, \dots, \mathbf{A}_k)$. Eq. 2 shows a general model with γ terms. Algebraically, the joint invariants
 065 form an algebra (say, **Inv**), and for completeness of the model $\lambda_1, \lambda_2, \dots, \lambda_m$ should be algebra gen-
 066 erators for **Inv**. Meanwhile, equivariant tensor monomials form a submodule (say, **Cov**) of tensors
 067 (in which \mathbf{T} exists) over **Inv**, and $(\mathbf{B}_1, \mathbf{B}_2, \dots, \mathbf{B}_\gamma)$ should be module generators for **Cov**.
 068

069 One of the earliest works in this vein is by Robertson (1940), which was widely used for developing
 070 isotropic tensor functions for closure modeling in turbulence. Motivated by some use cases in linear
 071 elasticity theory, other authors derived several minimally complete isotropic tensor function repre-
 072 sentations in Wang (1970); Smith (1971); Zheng (1993a; 1994; 1993b). However, these results were
 073 restricted to tensors of order less than or equal to 2. After significant dormancy, recently Olive &
 074 Auffray (2014) gave a minimal set of isotropic invariants of a symmetric third order tensor. These re-
 075 sults are scalar function representations, but an extension to general tensor function representations
 076 was not made, until now. There has been considerable interest in learning such tensor function re-
 077 presentations using Equivariant Neural Networks (ENNs) Villar et al. (2021); Gasteiger et al. (2020);
 078 Geiger & Smidt (2022) which have been used successfully in a range of applications (for example,
 079 Jumper et al. (2021); Satorras et al. (2021); Gregory et al. (2024)). We develop a new methodology
 080 for deriving algebraically minimal equivariant functions with more interpretability than black box
 081 ENNs architectures, which could be useful for similar applications.
 082

083 The workflow for the current work is summarized in Fig. 3. A central idea is to work with binary
 084 forms for deriving the tensor monomials and the invariants, then learn the coefficient functions
 085 using neural networks. This is possible because: 1) every tensor can be irreducibly decomposed into
 086 a direct sum of symmetric trace free (i.e., harmonic) tensors (Zou et al. (2001); Spencer (1970));
 087 and 2) There is an isomorphism (Smith & Bao (1997); Boehler et al. (1994)) between harmonic
 088 tensors and binary forms, by which tensor monomials can be derived in the space of binary forms.
 089 Another advantage of working with binary forms is that the equivariant polynomials in binary forms
 090 naturally form an *algebra* (and not a module), which can be finitely generated (Gordan (1868);
 091 Hilbert (1993)). Our results thus arise from the invariant theory of binary forms, which is a very
 092 mature field (Hilbert (1993); Olver (1999); Kung & Rota (1984)) and reliable algorithms (Sturmfels
 093 (2008); Bruns et al. (2017); Eisenbud et al. (2001)) for effective computations. Working in the binary
 094 forms space is not only convenient, but we found it essential for making computations tractable.
 095

096 The rest of the paper is laid out as follows. Some background for invariant theory is introduced in §2.
 097 This will be used in §3 to discuss the overall methodology for deriving minimal tensor monomials
 098 and invariants. A supervised learning problem is discussed with tensor invariants as inputs and the
 099 monomial coefficients as outputs, which will complete the learning framework for general tensor
 100 function representations. In §4, the approach is verified by deriving symmetric tensor function rep-
 101 resentations of one and two symmetric second order tensors, for which we compare against classical
 102 results of Wang (1970). In §5, the fourth order Rapid Pressure Strain Rate (RPSR) correlation tensor
 103 (Pope (2001)), a well-known bottleneck (Kassinos et al. (2001)) in modeling turbulence, is explored
 104 using the current methodology. We present numerical results showing a substantial improvement
 105 over existing modeling approaches.
 106

107 Contributions of the current work:
 108

1. A new paradigm for learning equivariant tensor functions from tensor tuple inputs to tensor outputs is developed by first deriving the underlying algebraic structure, and next learning scalar coefficient functions using neural networks and problem specific data. This paradigm also enforces tensor trace constraints exactly the the final models.
2. Minimally complete tensor function representations are derived using covariant algebra of binary forms in an interpretable learning based setting.

- 108 3. Efficient numerical algorithms are developed for generating covariant modules and finding
 109 minimal module generators.
 110 4. *Nonlinear* RSPR tensor models are built using turbulence structure tensors (Kassinos
 111 (1995)) for the first time and tested on a wide variety of turbulent flow configurations.
 112

113 **2 MATHEMATICAL BACKGROUND AND PREREQUISITES**
 114

115 Groups describe symmetries Olver (1999). We recall that a *group* G is a set with a binary operation
 116 that is associative, has an identity element, and admits inverses. $GL(n, \mathbb{F}) = \{M \in \mathbb{F}^{n \times n}\}$ is the
 117 **general linear group**. Main examples in this work are the matrix groups $SO(3, \mathbb{R}) = \{R \in \mathbb{R}^{3 \times 3} : R R^\top = R R^\top = I\}$ and $SL(2, \mathbb{C}) = \{M \in \mathbb{C}^{2 \times 2} : \det(M) = 1\}$, where the group operation is
 118 matrix multiplication.
 119

120 Representations encode how symmetries operate on spaces. A **W-representation** of G is a finite-
 121 dimensional vector space (real or complex) on which G acts by linear maps. That is, there exists a
 122 group homomorphism $\rho : G \rightarrow GL(\mathbf{W})$ from G to invertible linear transformations of \mathbf{W} . Often
 123 we abbreviate $\rho(g)w$ as $g \cdot w$ for $g \in G$ and $w \in \mathbf{W}$ with ρ being tacitly understood. Key examples
 124 of representations are spaces of tensors, 3-dimensional in each direction, under the action of 3D
 125 rotations. For instance, the space \mathbf{W} of 3×3 real matrices is a representation of $SO(3, \mathbb{R})$ where
 126 the action is by conjugation: $R \cdot W := R W R^\top$ for $R \in SO(3, \mathbb{R})$ and $W \in \mathbf{W}$.
 127

128 **Definition 2.1** (G -equivariant and G -invariant functions¹). Let \mathbf{W} and \mathbf{V} be representations of some
 129 group G . A function $B : \mathbf{W} \rightarrow \mathbf{V}$ is said to be *equivariant* with respect to G if:

$$130 \quad B(g \cdot W) = g \cdot B(W), \quad \forall g \in G, \quad \forall W \in \mathbf{W}. \quad (3)$$

131 Further, let \mathbf{X} be any set. A function $\lambda : \mathbf{W} \rightarrow \mathbf{X}$ is said to be *invariant* with respect to G if:

$$132 \quad \lambda(g \cdot W) = \lambda(W), \quad \forall g \in G, \quad \forall W \in \mathbf{W}. \quad (4)$$

133 **Definition 2.2** (G -covariant module and G -invariant algebra). Let \mathbf{W} and \mathbf{V} be K -representations
 134 of some group G , where $K = \mathbb{R}$ or $K = \mathbb{C}$. Then the *covariant module* is $\mathbf{Cov}_G(\mathbf{W}, \mathbf{V})$ is the
 135 set of all G -equivariant polynomial functions over K from \mathbf{W} to \mathbf{V} . Further, the *invariant algebra*
 136 $\mathbf{Inv}_G(\mathbf{W})$ is the set of all G -invariant polynomial functions over K from \mathbf{W} to K .
 137

138 We note that $\mathbf{Inv}_G(\mathbf{W})$ is closed under multiplication and addition, while $\mathbf{Cov}_G(\mathbf{W}, \mathbf{V})$ is closed
 139 under addition and scalar multiplication by elements of $\mathbf{Inv}_G(\mathbf{W})$. This makes $\mathbf{Inv}_G(\mathbf{W})$ into an
 140 algebra, and $\mathbf{Cov}_G(\mathbf{W}, \mathbf{V})$ into a module over this algebra. We are interested in this paper chiefly
 141 in $SO(3, \mathbb{R})$ -equivariant and -invariant functions between tensor spaces.
 142

143 A helpful relationship exists between the groups $SO(3, \mathbb{R})$ and $SL(2, \mathbb{C})$. Namely, there is a double
 144 cover (see Appendix D for explicit details):

$$145 \quad \Psi : SL(2, \mathbb{C}) \rightarrow SO(3, \mathbb{C}), \quad (5)$$

146 where $SO(3, \mathbb{C})$ is the complexification of $SO(3, \mathbb{R})$. Double cover here means that Ψ is a surjective
 147 homomorphism that is 2-to-1. This relationship lets us identify real representations of $SO(3, \mathbb{R})$ with
 148 complex representations of $SL(2, \mathbb{C})$, via $\mathbf{W} \mapsto \mathbf{W} \otimes_{\mathbb{R}} \mathbb{C}$.
 149

150 **Definition 2.3.** Let S_n denote the complex vector space of *binary forms* of order n . For $\mathbf{f} \in S_n$, it
 151 can be written

$$152 \quad \mathbf{f}(x, y) = \sum_{i=0}^n \binom{n}{i} a_i x^{n-i} y^i, \quad \text{for } (x, y) \in \mathbb{C}^2. \quad (6)$$

153 A space of binary forms, \mathbf{V} , is defined as follows (where \oplus denotes direct sum):
 154

$$155 \quad \mathbf{V} = \bigoplus_{i=0}^s S_{n_i}, \quad n_i \in \mathbb{N}. \quad (7)$$

156 Spaces of binary forms are representations of $SL(2, \mathbb{C})$ under change of variables. A binary form
 157 covariant is an $SL(2, \mathbb{C})$ -equivariant function between two binary form spaces. It can be written as
 158

159 ¹The terms functions and maps are used interchangeably.
 160

162 a polynomial in x, y and the coefficients of binary forms. Similarly, a binary form *invariant* is an
 163 $SL(2, \mathbb{C})$ -invariant polynomial function. Gordan (1868) and Hilbert (1993) proved that the *algebra*
 164 of covariants for a binary form space, $\mathbf{Cov}(\mathbf{V}) := \bigoplus_{n=0}^{\infty} \mathbf{Cov}_{SL(2, \mathbb{C})}(\mathbf{V}, S_n)$, is finitely generated.
 165

166 There is a natural *bi-grading* in covariant algebra, i.e., each covariant can be graded using two
 167 integers: the *order* and the *degree*. The order refers to the sum of powers of \mathbf{x}, \mathbf{y} and the degree
 168 refers to the sum of powers of coefficients of any term in the binary forms. For a bihomogeneous
 169 binary form, the degree and order on all terms will be the same, hence can be used for uniquely
 170 grading them. For example, $\mathbf{f} \in S_4$ is an order 4, degree 1 covariant, while \mathbf{f}^2 is an order 8, degree
 171 2. The order 0 covariants coincide with the invariants (Hilbert (1993)), hence the invariant algebra
 172 is contained in the covariant algebra.

173 It is known that the space of S_n is an $SL(2, \mathbb{C})$ *irreducible* representation, which cannot be further
 174 decomposed into direct sum of representations. The $SL(2, \mathbb{C})$ irreducible decomposition of a tensor
 175 product is given by *Clebsch-Gordan decomposition* (Olive (2017)),

$$176 \quad S_n \otimes S_p \cong \bigoplus_{r=0}^{\min(n,p)} S_{n+p-2r}, \quad (8)$$

177 where \bigoplus indicates a direct sum over the binary form spaces. For each $0 \leq r \leq \min(n, p)$, up to
 178 nonzero scalar, there is a unique *transvectant*. Let $\mathbf{f} \in S_m, \mathbf{g} \in S_n$, their transvectant of index r , is
 179 denoted by $(\mathbf{f}, \mathbf{g})_r$, and given as follows where π_r denotes $SL(2, \mathbb{C})$ -equivariant projection:
 180

$$181 \quad \pi_r : S_m \otimes S_n \rightarrow S_{m+n-2r}, \quad \mathbf{f} \otimes \mathbf{g} \mapsto (\mathbf{f}, \mathbf{g})_r := \pi_r(\mathbf{f} \otimes \mathbf{g}). \quad (9)$$

182 **Lemma 2.1.** Olive & Auffray (2014) *The transvectant operation of index r between two binary
 183 forms $\mathbf{f} \in S_m$ and $\mathbf{g} \in S_n$ is given by*

$$184 \quad (\mathbf{f}, \mathbf{g})_r = \frac{(m-n)!}{m!} \frac{(n-r)!}{n!} \sum_{i=0}^r (-1)^i \binom{r}{i} \frac{\partial^r \mathbf{f}}{\partial^{r-i} x \partial^i y} \frac{\partial^r \mathbf{g}}{\partial^i x \partial^{r-i} y}. \quad (10)$$

185 **Remark.** Let d_f, o_f be the degree and orders of \mathbf{f} , then for $(\mathbf{f}, \mathbf{g})_r$, the degree is $d_f + d_g$ and its
 186 order is $o_f + o_g - 2r$.

193 3 TENSOR REPRESENTATION METHODS

195 Let $\mathbb{T}^n = (\mathbb{R}^3)^{\otimes n}$ and let $\mathbf{T} \in \mathbb{T}^n$ be a general order n tensor. Equation 2 shows a general tensor
 196 function representation of \mathbf{T} using $(\mathbf{A}_1, \mathbf{A}_2, \dots, \mathbf{A}_k)$ where $\mathbf{A}_i \in \mathbb{T}^{o(i)}$,
 197

$$198 \quad \mathbf{T}(\mathbf{A}_1, \mathbf{A}_2, \dots, \mathbf{A}_k) = \sum_{i=1}^{\gamma} C_i(\lambda_1, \lambda_2, \dots, \lambda_m) \mathbf{B}_i(\mathbf{A}_1, \mathbf{A}_2, \dots, \mathbf{A}_k).$$

201 For completeness of this model, λ_i 's must generate the invariant algebra $\mathbf{Inv}_{SO(3, \mathbb{R})}(\mathbb{T}^{o(1)} \oplus \mathbb{T}^{o(2)} \oplus$
 202 $\dots \oplus \mathbb{T}^{o(k)})$ and \mathbf{B}_i 's must generate $\mathbf{Cov}_{SO(3)}(\mathbb{T}^{o(1)} \oplus \mathbb{T}^{o(2)} \oplus \dots \oplus \mathbb{T}^{o(k)}, \mathbb{T}^n)$ as an module over
 203 the invariant ring. From [definition 2.2](#), it follows that if λ_i 's and the \mathbf{B}_i 's are minimal generators,
 204 then the model $\mathbf{T}(\mathbf{A}_1, \mathbf{A}_2, \dots, \mathbf{A}_k)$ is minimally complete. Once the model is developed, the
 205 coefficients functions C_i 's must be learned as functions([Robertson \(1940\)](#)) of the invariant ring
 206 generators (λ_i 's) using neural networks and domain-specific training data. Here, we first show the
 207 link between general tensors and harmonic tensors. Then we show how to accomplish the three
 208 major steps involved in deriving tensor function representations: 1) Using Harmonic Tensors (§3.1)
 209 to derive the minimal invariant algebra generators (§3.2); 2) Obtaining the minimal covariant module
 210 generators (§3.2); and 3) learning coefficient functions using neural networks (§3.4). Additionally,
 211 §3.3 shows an algorithm to reduce to *minimal* module generators.

213 3.1 IRREDUCIBLE DECOMPOSITION INTO HARMONIC TENSORS

215 The space of harmonic (i.e., symmetric and trace free) tensors $\mathbb{H}^n \subset \mathbb{T}^n$ is an $SO(3, \mathbb{R})$ irreducible
 216 representation. For the space of general order n tensors, \mathbb{T}^n , the following theorem holds:

216 **Theorem 3.1.** \mathbb{T}^n irreducibly decomposes as $\mathbb{H}^n \oplus \mathbb{H}^{n-1} \oplus \cdots \oplus \mathbb{H}^0$. (Spencer (1970); Zou et al.
 217 (2001))

218 **Corollary 3.1.1.** Covariant spaces between general tensor spaces can be expressed in terms of
 219 covariant spaces between harmonic tensor spaces.

221 *Proof.* From Theorem 3.1,

$$\begin{aligned} \mathbf{Cov}_G\left(\bigoplus_{i=1}^k \mathbb{T}^{o(i)}, \mathbb{T}^n\right) &\cong \mathbf{Cov}_G(\mathbb{T}^{o(1)} \oplus \mathbb{T}^{o(2)} \oplus \cdots \oplus \mathbb{T}^{o(k)}, \mathbb{T}^n) \\ &\cong \mathbf{Cov}_G\left(\bigoplus_{l=0}^{o(1)} \mathbb{H}^l \oplus \bigoplus_{l=0}^{o(2)} \mathbb{H}^l \oplus \cdots \oplus \bigoplus_{l=0}^{o(k)} \mathbb{H}^l, \bigoplus_{i=0}^n \mathbb{H}^i\right) \\ &\cong \mathbf{Cov}_G\left(\bigoplus_{j=1}^k \bigoplus_{l=0}^{o(j)} \mathbb{H}^l, \bigoplus_{i=0}^n \mathbb{H}^i\right) \cong \bigoplus_{i=0}^n \mathbf{Cov}_G\left(\bigoplus_{j=1}^k \bigoplus_{l=0}^{o(j)} \mathbb{H}^l, \mathbb{H}^i\right). \end{aligned}$$

232 This completes the proof. \square

234 For example, the symmetric order 2 tensor space $\text{Sym}^2 \subset \mathbb{T}^2$ can be decomposed into:

$$\begin{aligned} \text{Sym}^2 &\cong \mathbb{H}^2 \oplus \mathbb{H}^0 \\ \mathbf{Cov}_{SL(2,\mathbb{C})}(\text{Sym}^2, \text{Sym}^2) &\cong \mathbf{Cov}_{SL(2,\mathbb{C})}(\mathbb{H}^2 \oplus \mathbb{H}^0, \mathbb{H}^2 \oplus \mathbb{H}^0) \\ \mathbf{Cov}_{SL(2,\mathbb{C})}(\text{Sym}^2, \text{Sym}^2) &\cong \mathbf{Cov}_{SL(2,\mathbb{C})}(\mathbb{H}^2 \oplus \mathbb{H}^0, \mathbb{H}^2) \oplus \mathbf{Cov}_{SL(2,\mathbb{C})}(\mathbb{H}^2 \oplus \mathbb{H}^0, \mathbb{H}^0). \end{aligned} \quad (11)$$

240 To develop complete tensor function representations for $\mathbf{Cov}_{SO(3,\mathbb{R})}(\text{Sym}^2, \text{Sym}^2)$, the invariant
 241 generators of $\mathbb{H}^2 \oplus \mathbb{H}^0$ and the $\mathbf{Cov}_{SO(3,\mathbb{R})}(\mathbb{H}^2 \oplus \mathbb{H}^0, \mathbb{H}^2)$ and $\mathbf{Cov}_{SO(3,\mathbb{R})}(\mathbb{H}^2 \oplus \mathbb{H}^0, \mathbb{H}^0)$ are
 242 required. This example is revisited and worked out in §4.1. Corollary 3.1.1 is a useful result which
 243 implies that **Inv** and **Cov** for harmonic tensors are sufficient to build tensor function representations
 244 for any general tensor. Below we show that a finite set of generators can be derived.

245 3.2 HARMONIC TENSORS AND BINARY FORMS

247 There is an association (Zheng (1994); Boehler et al. (1994)) from real irreducible representations
 248 of $SO(3, \mathbb{R})$ to complex irreducible representations of $SL(2, \mathbb{C})$. Via equation 5, there is an isomorphism
 249 as $SL(2, \mathbb{C})$ representations:

$$\mathbb{H}^n \otimes \mathbb{C} \cong S_{2n}. \quad (12)$$

251 This link is well known in the field of constitutive modeling and used to derive the isotropic invariants
 252 of traceless symmetric order 3 and order 4 tensors (Smith & Bao (1997)) and more recently a
 253 symmetric order 3 tensor Olive & Auffray (2014). It was also used to derive the minimal integrity
 254 basis for the order 4 elasticity tensor (Olive et al. (2017)). We use this link to show two important
 255 results.

256 **Theorem 3.2.** Complete $SO(3, \mathbb{R})$ equivariant tensor function representations can be derived from
 257 $SL(2, \mathbb{C})$ covariant modules² of binary forms.

259 *Proof.* Using Eq. 12,

$$\mathbf{Inv}_{SO(3,\mathbb{R})}\left(\bigoplus_{i=1}^k \mathbb{H}^{n_i}\right) \otimes \mathbb{C} \cong \mathbf{Inv}_{SL(2,\mathbb{C})}\left(\bigoplus_{i=1}^k S_{2n_i}\right) \quad (13)$$

263 In addition to these two invariant rings are isomorphic, we can say that for any order m , the following
 264 covariant modules are isomorphic:

$$\mathbf{Cov}_{SO(3,\mathbb{R})}\left(\bigoplus_{i=1}^k \mathbb{H}^{n_i}, \mathbb{H}^m\right) \otimes \mathbb{C} \cong \mathbf{Cov}_{SL(2,\mathbb{C})}\left(\bigoplus_{i=1}^k S_{2n_i}, S_{2m}\right) \quad (14)$$

\square

²The direct finite sum of covariant modules gives the covariant algebra.

270 **Remark.** This concludes theoretical development in the current work and brings about an important
 271 comment. Using Theorem 3.2 and Corollary 3.1.1, the tensor function representations in Eq. 2 can
 272 be built, provided the invariant and covariant generators of binary forms are known:
 273

$$274 \quad \mathbf{Cov}_{SO(3, \mathbb{R})} \left(\bigoplus_{i=1}^k \mathbb{T}^{o(i)}, \mathbb{T}^n \right) \cong \bigoplus_{i=0}^n \mathbf{Cov}_{SL(2, \mathbb{C})} \left(\bigoplus_{j=1}^k \bigoplus_{l=0}^{o(j)} S_{2l}, S_{2i} \right). \quad (15)$$

277 3.3 EFFECTIVE NUMERICAL COMPUTATIONS

280 The generators for \mathbf{Inv}_G and \mathbf{Cov}_G of binary forms can be finitely obtained using the Gordan's
 281 Algorithm (Gordan (1868); Olive (2017) which is explained in detail in Appendix E. For
 282 any space of binary forms $\mathbf{V} := \bigoplus_{i=1}^k S_{2i}$, the algorithm gives finite generators for any S_n
 283 covariant module, $\mathbf{Cov}_{SL(2, \mathbb{C})}(\mathbf{V}, S_n)$. It can also be used to generate the invariant algebra as
 284 $\mathbf{Inv}_G(\mathbf{V}) \simeq \mathbf{Cov}_G(\mathbf{V}, S_0)$. Results for covariant algebra of $S_6 \oplus S_2, S_4 \oplus S_4, S_6 \oplus S_4 \oplus S_2$ and
 285 several others are computed using Gordan's algorithm and readily available in literature. We note
 286 that the generators computed by Gordan's algorithm are in the form of iterated transvectants as
 287 defined in equation 10, which facilitates their efficient evaluation. The results can be used to develop
 288 complete $SO(3, \mathbb{R})$ equivariant tensor functions. But these representations will not be minimal,
 289 because Gordan's algorithm does not provide minimal generators, only complete ones.
 290

291 **Algorithm 1:** Identifying the minimal generating set for an R-module

292 **Inputs:** Generators of R-Module M, Generators of Ring R

293 **Result:** Minimal generating set of R-Module

```

1 begin
2   Initialize p ← 65521                                // Some large prime
3   Initialize K ← ZZ/p                                  // Galois (Finite) Field
4   Initialize R ← K[c1, c2, ..., ck, x, y]      // Poly Ring with Coefs and Vars
5   Initialize I ← {i1, i2, ..., im}                // Ring Generators
6   Initialize F ← {f1, f2, ..., fn}                // Module Generators
7   I+ ← {il | degree(il) > 0}
8   m ← ideal(I+)                                     // The Irrelevant (maximal) Ideal
9   for ∀fl ∈ F do
10    | flm ← fl%m                                // Viewing M gens as M/mM gens
11   end
12   Fm ← {f1m, f2m, ..., fnm}
13   γ ← Linearly Independent Row Indices (Fm) // Using Gaussian Elimination
14   return F(min) ← {fγ(1), fγ(2), ..., fγ(s)} // Minimal Gen. Set
15 end

```

309 In order to remedy this, the *minimal* generator subsets of Gordan's generators for \mathbf{Inv} and \mathbf{Cov}
 310 must be identified. For reducing generators of \mathbf{Inv} to a minimal set, Olive (2017) gives a degree-
 311 per-degree approach using the Hilbert series (Bedratyuk (2010)). As far as the authors are aware,
 312 there are fewer readily implemented methods for identifying minimal generators of a module over a
 313 ring (like \mathbf{Cov} over \mathbf{Inv}) from a finite generating set. So, the Algorithm 1 is proposed. This uses
 314 the graded version of Nakayama's Lemma (Eisenbud (2013)) which expresses module generation in
 315 terms of vector space generation over a field, so that linear algebra can be used for minimal generator
 316 identification. The lemma says that if \mathbf{m} is the homogeneous maximal ideal of the graded ring R ,
 317 then $M/\mathbf{m}M$ is a vector space over the field R/\mathbf{m} and $\{f_1, f_2, \dots\}$ form a module generating set
 318 for M if and only if the reductions $\{f_1^{\mathbf{m}}, f_2^{\mathbf{m}}, \dots\}$ form a vector space spanning set for $M/\mathbf{m}M$
 319 over R/\mathbf{m} . Further, since the polynomials in our computations have rational coefficients, the linear
 320 algebra calculations can be done over a finite field by working modulo a prime number. We choose
 321 a few large primes and repeat the computations to ensure that the results are accurate.

322 The algorithm is as follows. Load the generators of the invariant ring and the covariant module
 323 **upto some fixed degree using Gordan's algorithm**. Create the maximal ideal I^+ (\mathbf{m}) using positively
 graded ring elements. View the module generators, \mathbf{f} , of M in $M/\mathbf{m}M$ by taking the remainder

against \mathfrak{m} , denoted by $\mathfrak{f}\% \mathfrak{m}$. Now, implement reduced row echelon form and identify the linearly independent entries which correspond to R -linearly independent \mathfrak{f} 's; these are the minimal generators. If the invariant ring is not too large, the $\mathfrak{f}\% \mathfrak{m}$ step could be computed using a Gröbner basis (Sturmfels (2008)). If that is too restrictive, the numerical linear algebra algorithm proposed in Appendix F can be used. These computations were done using Macaulay2 (Eisenbud et al. (2001)).

3.4 LEARNING THE COEFFICIENTS

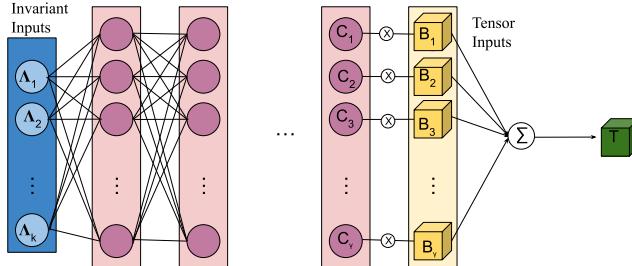


Figure 1: Schematic of the architecture for learning tensor representations as shown in Eq. 2. Circles are scalars (\mathbb{H}^0) and cubes are tensors (\mathbb{H}^n). Λ 's are the invariants, C_i 's are scalar functions of invariants, B_i 's are the tensor monomials, T is the tensor function representation.

The minimal generators of Inv_G and Cov_G complete the learning architecture. The minimal generators will all be iterated polynomial transvectants, which must be converted back into \mathbb{H}^n using the mapping shown in Appendix B. A schematic of the proposed architecture is shown in Fig. 3. The model has two input layers, the invariant algebra generator, labelled Λ_i and the covariant module generators labeled B_i in yellow. The scalar coefficient functions are learned using a hidden layers, with appropriate size, based on the complexity of the problem. We can visualize the contributions from each each tensor input towards the modeling opening new possibilites for discovering insights about the modeling process. The covariant module computations can be reused for every run after the first time. An example is worked out in §5.

4 COMPUTATIONS AND RESULTS

4.1 MODELING A SYMMETRIC ORDER 2 TENSOR IN TERMS OF A SYMMETRIC ORDER 2 TENSOR

To model $\mathbf{A}(\mathbf{B})$, where, $\mathbf{A}, \mathbf{B} \in \text{Sym}^2$, following Eq. 11, this problem is split into two sub parts. The covariant algebra of S_4 is well known(Olive (2017)). It is summarized in Table. 2 First minimal generators of $\text{Inv}(S_4 \oplus S_0)$ are computed minimally. They are $(\mathbf{v}, \mathbf{v})_4$ and $(\mathbf{v}, (\mathbf{v}, \mathbf{v})_2)_4$, which correspond to $\text{tr}(\mathbf{B}^2)$ and $\text{tr}(\mathbf{B}^3)$ from S_4 , and S_0 corresponds to $\text{tr}(\mathbf{B})$. These 3 invariants are inputs to coefficients and also used to create an R-module. Minimal generators of $\text{Cov}(S_4 \oplus S_0, S_4)$ are \mathbf{v} and the transvectant $(\mathbf{v}, \mathbf{v}_2)$, which correspond to \mathbf{B} and \mathbf{B}^2 . Putting all these together,

$$\begin{aligned} \mathbf{A}(\mathbf{B}) &\in \text{Cov}_{\text{SO}(3, \mathbb{R})}(\mathbb{H}^2 \oplus \mathbb{H}^0, \mathbb{H}^2 \oplus \mathbb{H}^0) \simeq \text{Cov}_{\text{SL}(2, \mathbb{C})}(S_4 \oplus S_0, S_4 \oplus S_0) \\ &\simeq \text{Cov}_{\text{SL}(2, \mathbb{C})}(S_4 \oplus S_0, S_4) \oplus \text{Cov}_{\text{SL}(2, \mathbb{C})}(S_4 \oplus S_0, S_0) \end{aligned}$$

$$\mathbf{A}(\mathbf{B}) = (c_1 \mathbf{B} + c_2 \mathbf{B}^2) + c_3 \mathbf{I}.$$

where $c_i = c_i(\text{tr}(\mathbf{B}), \text{tr}(\mathbf{B}^2), \text{tr}(\mathbf{B}^3))$ are to be learned using data from \mathbf{A} and \mathbf{B} , in most cases using neural networks. These results can be verified from the results of Smith (1971); Zheng (1993a).

4.2 MODELING A SYMMETRIC ORDER 2 TENSOR USING TWO SYMMETRIC ORDER 2 TENSOR

The previous result is extended in this example. Let, $\mathbf{A}, \mathbf{B}, \mathbf{C} \in \text{Sym}^2$, then $\mathbf{A}(\mathbf{B}, \mathbf{C})$ is derived. Irreducible decomposition shows,

Deg	Covs	Harmonic Tensors
1	\mathbf{q}, \mathbf{p}	$\mathbf{H}_{1a} := \mathbf{B}, \mathbf{H}_{1b} := \mathbf{C}$
2	$(\mathbf{p}, \mathbf{q})_2$ $(\mathbf{q}, \mathbf{q})_2, (\mathbf{p}, \mathbf{p})_2$	$\mathbf{H}_{2a} := (\mathbf{B}\mathbf{C} + \mathbf{C}\mathbf{B}) - \frac{1}{3}\text{tr}(\mathbf{B}\mathbf{C} + \mathbf{C}\mathbf{B})\mathbf{I}$ $\mathbf{H}_{2b} := \mathbf{B}^2 - \frac{1}{3}\text{tr}(\mathbf{B}^2)\mathbf{I}, \mathbf{H}_{2c} := \mathbf{C}^2 - \frac{1}{3}\text{tr}(\mathbf{C}^2)\mathbf{I}$
3	$(\mathbf{q}, (\mathbf{p}, \mathbf{p})_2)_2$ $(\mathbf{p}, (\mathbf{q}, \mathbf{q})_2)_2$	$\mathbf{H}_{3a} := (\mathbf{B}\mathbf{C}^2 + \mathbf{C}^2\mathbf{B}) - \frac{2}{3}\text{tr}(\mathbf{C}^2)\mathbf{H}_{1a} - \frac{1}{3}\text{tr}(\mathbf{H}_{2c}\mathbf{H}_{1a} + \mathbf{H}_{1a}\mathbf{H}_{2c})\mathbf{I}$ $\mathbf{H}_{3b} := (\mathbf{C}\mathbf{B}^2 + \mathbf{B}^2\mathbf{C}) - \frac{2}{3}\text{tr}(\mathbf{B}^2)\mathbf{H}_{1b} - \frac{1}{3}\text{tr}(\mathbf{H}_{2b}\mathbf{H}_{1b} + \mathbf{H}_{1b}\mathbf{H}_{2b})\mathbf{I}$
4	$[(\mathbf{p}, \mathbf{q})_3]^2$	$\mathbf{H}_4 := 6(\mathbf{B}^2\mathbf{C}^2 + \mathbf{C}^2\mathbf{B}^2) + 10\mathbf{H}_{1a}^2\text{tr}(\mathbf{C}^2) +$ $10\mathbf{H}_{1b}^2\text{tr}(\mathbf{B}^2) + 2\text{tr}(\mathbf{C}^2)\text{tr}(\mathbf{B}^2)\mathbf{I}$ $-\frac{1}{3}(6\text{tr}(\mathbf{C}^2\mathbf{B}^2) + 6\text{tr}(\mathbf{B}^2\mathbf{C}^2) + 26\text{tr}(\mathbf{B}^2)\text{tr}(\mathbf{C}^2))\mathbf{I}$

Table 1: Minimal module generators of order 4 covariant polynomials expressed as iterated transvectants and their corresponding expressions as harmonic tensors in \mathbb{H}^2 .

$$\mathbf{A}(\mathbf{B}, \mathbf{C}) \in \mathbf{Cov}_{\text{SO}(3, \mathbb{R})}(2\mathbb{H}^2 \oplus 2\mathbb{H}^0, \mathbb{H}^2 \oplus \mathbb{H}^0)$$

$$\simeq \mathbf{Cov}_{\text{SL}(2, \mathbb{C})}(2S_4, S_4) \oplus \mathbf{Cov}_{\text{SL}(2, \mathbb{C})}(2S_4, S_0) \oplus \mathbf{Cov}_{\text{SL}(2, \mathbb{C})}(2S_0, S_4) \oplus \mathbf{Cov}_{\text{SL}(2, \mathbb{C})}(2S_0, S_0)$$

$\mathbf{Cov}_{\text{SL}(2, \mathbb{C})}(2S_0, S_4)$ will have no terms. The terms from $\mathbf{Cov}_{\text{SL}(2, \mathbb{C})}(2S_4, S_0)$, and $\mathbf{Cov}_{\text{SL}(2, \mathbb{C})}(2S_0, S_0)$ will be reduced to $c\mathbf{I}$ in the model, for some coefficient function c . To build the tensor function representations for $\mathbf{Cov}_{\text{SL}(2, \mathbb{C})}(2S_4, S_4)$, the order 4 module generators are build using the non-invariant covariant algebra of $S_4 \oplus S_4$, whose covariant algebra is derived in Olive (2017) is summarized in Table. 3. By solving a linear Diophantine system for every degree, 43 order 4 module generators were identified. Using Algorithm 1, they are reduced to a linearly independent minimal set of 8 polynomials. The linearly independent covariant polynomials and the corresponding harmonic tensors are written in Table 1. Using these generators, a model for a symmetric tensor can be written as,

$$\mathbf{A}(\mathbf{B}, \mathbf{C}) = c_1\mathbf{I} + c_2\mathbf{B} + c_3\mathbf{C} + c_4(\mathbf{B}\mathbf{C} + \mathbf{C}\mathbf{B}) + c_5\mathbf{B}^2 + c_6\mathbf{C}^2 + c_7(\mathbf{B}\mathbf{C}^2 + \mathbf{C}^2\mathbf{B}) + c_8(\mathbf{C}\mathbf{B}^2 + \mathbf{B}^2\mathbf{C}) + c_9(\mathbf{C}^2\mathbf{B}^2 + \mathbf{B}^2\mathbf{C}^2) \quad (16)$$

These 9 terms are consistent with the terms given by Wang (1970) and also noted in Smith (1970).

5 RESULTS FOR TURBULENCE MODELING

5.1 MODELING THE RAPID PRESSURE STRAIN RATE CORRELATION

Direct numerical simulations of fluid turbulence is prohibitively expensive in complex geometries. In practice, it is common to simulate by approximately modeling the effects of turbulence. One particularly difficult aspect to model is the Rapid Pressure Strain Rate (RSPR, Π) tensor plays a central role in re-distributing the turbulence stresses. It has been extensively studied (Lauder et al. (1975); Johansson & Hallbäck (1994); Girimaji (2000)) and it is a well-known bottleneck in turbulence modeling. The RSPR tensor is defined in Eq. 17 using the mean velocity gradient $U_{i,j} := \frac{\partial U_i}{\partial x_j}$ and an order $\mathbf{M} \in \mathbb{T}^4$ tensor.

$$\Pi_{ij} = 2U_{n,m}(M_{imnj} + M_{jmni}) \quad (17)$$

The mean velocity gradients are generally known apriori and the modeling is only focused on the \mathbf{M} tensor. It is hypothesized that the \mathbf{M} tensor depends on three turbulence structure tensors Kassinos et al. (2001): Reynolds Stress ($\mathbf{R} \in \text{Sym}^2$), Dimensionality ($\mathbf{D} \in \text{Sym}^2$), Stropholysis ($\mathbf{Q}^h \in \mathbb{H}^3$). Physically, \mathbf{R} quantifies the anisotropy in the velocity components, \mathbf{D} quantified the anisotropy in

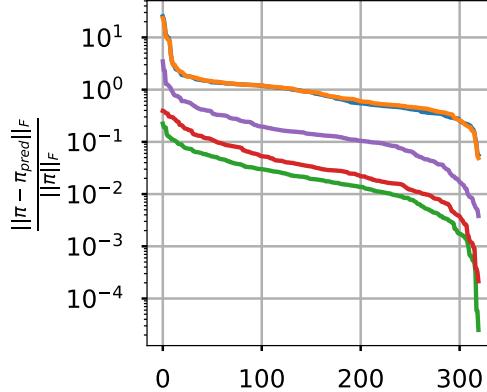
432 the turbulent length scales and \mathbf{Q}^h quantifies how strongly flow rotation breaks reflectional symmetry. Consequently, a model for $\mathbf{M}(\mathbf{R}, \mathbf{D}, \mathbf{Q}^h)$ is valuable for turbulence modeling. This is first reformulated as a problem of modeling $\mathbf{M}^h(\mathbf{R}^h, \mathbf{D}^h, \mathbf{Q}^h)$ where, \mathbf{R}^h and \mathbf{D}^h are the harmonic projections of \mathbf{R} and \mathbf{D} , which are commonly known as Reynolds Stress anisotropy ($\mathbf{R}^h \in \mathbb{H}^2$) and Dimensionality anisotropy ($\mathbf{D}^h \in \mathbb{H}^2$) in the field turbulence modeling Choi & Lumley (2001).
 433 First, the exact decomposition of \mathbf{M} carried out by KassinosKassinos (1995) is noted:
 434

$$435 \quad M_{ijkl} = M_{(ijkl)} + \frac{1}{8} [4M_{ijkl} - 4M_{klij}] + \frac{1}{12} [4M_{lkij} - 4M_{kjil} - 4M_{ilkj} \\ 436 \quad - M_{l j k i} - M_{i k l j} - M_{k i l j}] \quad (18)$$

437 \mathbf{M} must satisfy some constraints on its traces: $M_{iikl} = D_{kl}$, $M_{klli} = R_{kl}$, $\epsilon_{its} M_{sptj} = Q_{ipj}$.
 438 These are introduced in Eq. 18 which simplifies to Eq. 19. By modeling the \mathbf{M}^h and substituting in
 439 the harmonic decomposition (Eq. 19), trace constraints are satisfied *exactly* for the model of \mathbf{M} .
 440

$$441 \quad M_{ijkl} = \left[M_{ijkl}^h + \frac{1}{7} (\delta_{(ij} R_{kl)} + \delta_{(ij} D_{kl)}) - \frac{1}{35} \delta_{(ij} \delta_{kl)} R_{ii} \right] + \frac{1}{2} [\epsilon_{z k j} Q_{z i l}^h - \epsilon_{z i l} Q_{z k j}^h] + \\ 442 \quad \frac{1}{6} [(\delta_{il} \delta_{jk} + \delta_{ik} \delta_{lj} - 2\delta_{ij} \delta_{kl}) R_{ii} + 3(\delta_{kl} R_{ij} + \delta_{kl} D_{ij}) + (\delta_{kl} D_{ij} + \delta_{ij} R_{kl})] \\ 443 \quad - \frac{1}{6} [\delta_{il} (R_{kj} + D_{kj}) - \delta_{kj} (R_{il} + D_{lj}) - \delta_{ik} (R_{lj} + D_{lj}) - \delta_{lj} (R_{ki} + D_{ki})] \quad (19)$$

444 $\mathbf{M}(\mathbf{R}, \mathbf{D}, \mathbf{Q}^h)$ can be modeled using $\mathbf{M}^h(\mathbf{R}^h, \mathbf{D}^h, \mathbf{Q}^h) \in \text{Cov}(\mathbb{H}^2 \oplus \mathbb{H}^2 \oplus \mathbb{H}^3, \mathbb{H}^4)$. The difficulty
 445 in modeling $\mathbf{M}(\mathbf{R}, \mathbf{D}, \mathbf{Q}^h)$ is due to \mathbf{Q}^h which is in \mathbb{H}^3 . So, historically models were either ad-hoc
 446 (Lauder et al. (1975)), only used a subset of tensor dependencies (Johansson & Hallbäck (1994))
 447 built $\mathbf{M}(\mathbf{R})$, or simply linear (Kassinos et al. (2001)). We present a complete $\mathbf{M}(\mathbf{R}, \mathbf{D}, \mathbf{Q}^h)$ model
 448 (using \mathbf{M}^h) non-linear up to degree 2 and 3 for the first time. The explicit models are shown in
 449



450 Figure 2: Error in the rapid term. Legend: — Degree 3 model, — Degree 2 model, — Linear
 451 Model (Kassinos et al. (2001)), — LRR Model (Lauder et al. (1975)), — IP Model (Lauder
 452 (1989))

453 Appendix G.2. Computations show that a degree 2 \mathbf{M} model can be built using 4 invariants and 6
 454 tensor monomials and a degree 3 term is constructed with 11 Invariants and 27 tensor monomials.
 455 This is the underlying algebraic structure. For these two models, simple MLPs with 2 hidden layers
 456 with 128 neurons were used with input-output layer sizes of (4, 6) and (11, 27) respectively to learn
 457 coefficients for each tensor monomial as a function of the Invariants. In Fig. 2, these new models
 458 are compared against two classical LRR (Lauder et al. (1975)) and IP (Lauder (1989)), models
 459 and the linear $\mathbf{M}(\mathbf{R}, \mathbf{D}, \mathbf{Q}^*)$ model by Kassinos (1995). To learn the scalar coefficient functions for
 460 the representation functions of \mathbf{M} tensor, 320 different flow scenarios were simulated using Rapid
 461 Distortion theory (Pope (2001)) and a dataset is curated with $\mathbf{M}, \mathbf{R}, \mathbf{D}, \mathbf{Q}^*$ tensors. A 75:20:5 split
 462 was used for train, validation and testing split, while ensuring that the testing data was the most
 463 anisotropic, which would make modeling most difficult. The results in Fig. 2 shows the error in
 464 modeling the $\mathbf{\Pi}$ tensor using different models. The models we propose give – for the first time – an
 465 error which is lower than 10% in most flow scenarios. They perform an order of magnitude better
 466 than the linear model and almost two orders of magnitude better than the classical models.

486 **6 REPRODUCIBILITY**
 487

488 All theoretical, computational, and numerical results in this paper are readily reproducible by the the
 489 methods described in the paper and/or by using the code included in out supplement. Specifically,
 490 three different cases were considered to showcase the applicability of the current work. In §4.1, and
 491 §4.2 the results were purely algebraic. For the first of these, the results do not require extensive
 492 computations. Following the second remark in the Appendix E, and using the covariant algebra
 493 in Table 2, the covariant module generators can be computed by hand. For the second case, we
 494 follow the same outline but use the covariant algebra in Table 3, but this needs explicitly invocation
 495 the Algorithm 1, because it has 4 invariants and Gröbner basis calculations are not trivial by hand.
 496 Source code is attached in the supplementary files, where this example is worked out end-to-end. In
 497 §5, an extensive numerical example is worked out. The primary result in minimal covariant module
 498 generators and the generators of the invariant algebra, which are summarized in Table 6 and Table 5.
 499 These results require covariant algebra generators of $S_6 \oplus S_4 \oplus S_4$ which is not readily available in
 500 literature. But, S_6 and $S_4 \oplus S_4$ are available separately. This can be used to create the joint covariant
 501 algebra by Gordan’s algorithm as described in Appendix E, and then we proceed in the same way as
 502 before to identify the invariant generators and the covariant Module generators of S_8 . In this case, we
 503 impose limits on the degrees to 2 and 3 to obtain quadratic and cubic models. Then, the covariants
 504 are converted back to tensors using Appendix B and trained using two simple feedforward neural
 505 networks whose descriptions are mentioned in Appendix G.2.

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648 A LARGE LANGUAGE MODEL USAGE
649650 LLMs were not used to generate or research any parts of this paper.
651652 B TENSOR COVARIANTS
653654
655 **Lemma B.1.** *Let $\mathbf{H}_1 \in \mathbb{H}^n(\mathbb{R}^3)$ and $\mathbf{H}_2 \in \mathbb{H}^p(\mathbb{R}^3)$ be two harmonic tensors. Let r be the order of
656 the transvectant, then*

657
658
$$\{\phi^*\mathbf{H}_1, \phi^*\mathbf{H}_2\}_{2r} = \frac{1}{2^r} \phi^*((\mathbf{H}_1 \cdot \mathbf{H}_2)_0^s),$$

659

660
661
$$\{\phi^*\mathbf{H}_1, \phi^*\mathbf{H}_2\}_{2r+1} = \kappa(n, p, r) \phi^*((\text{tr}^r(\mathbf{H}_1 \times \mathbf{H}_2))_0),$$

662

663 where,

664
665
$$\kappa(n, p, r) = \frac{1}{2^{2r+1}} \frac{(n+p-1)! (n-r-1)! (p-r-1)!}{(n+p-1-2r)! (n-1)! (p-1)!}.$$

666

667 The tensor contraction is defined as
668

669
670
$$(\mathbf{T}^{1(r)} \mathbf{T}^2)_{i_1 i_2 \dots i_{p-r} j_{r+1} j_{r+1} \dots j_q} = \delta_{i_{p-r+1} j_1} \dots \delta_{i_p j_q} T_{i_1 i_2 \dots i_p}^1 T_{j_1 j_2 \dots j_q}^2,$$

671

672 the symmetrization operation is
673

674
675
$$\mathbf{T}^s = \frac{1}{n!} \sum_{\sigma \in \mathfrak{S}_n} T_{\sigma(1)\sigma(2)\dots\sigma(n)},$$

676

677 and \mathbf{P}_0 is the harmonic projection of the tensor \mathbf{P} . The generalized cross product between two
678 totally symmetric tensors $\mathbf{S}^1 \in \mathbb{S}^p(\mathbb{R}^3)$ and $\mathbf{S}^2 \in \mathbb{S}^q(\mathbb{R}^3)$ is
679

680
681
$$\mathbf{S}^1 \times \mathbf{S}^2 = (S^1 \times S^2)_{i_1 \dots i_{p+1-1}} = (\epsilon_{i_1 j_k} S_{j i_2 \dots p}^1 S_{k i_{p+1} \dots i_{p+q-1}}^2)^s$$

682 Finally, $\phi^* : \mathcal{H}_n(\mathbb{C}^3) \rightarrow S_{2n}$ is a unique equivariant isomorphism (up to a nonzero scale factor).
683684 C HARMONIC DECOMPOSITION OF ANY TENSOR
685686 From a representation theory perspective, the harmonic decomposition is an irreducible decomposi-
687 tion. One of the earliest works which showed harmonic decomposition is by Spencer (1970; 1987).
688 A more refined version is developed by Zou et al. (2001), harmonic decomposition is referred to
689 as deviatoric decomposition, and a recursive formula is shown which is particularly conducive for
690 working with computer algebra software. Most works on harmonic decomposition occur in two
691 steps. First, the tensor is decomposed into its symmetric components, then each symmetric compo-
692 nent is decomposed into trace-less components. For example, a general order 2 tensor ($\mathbf{T} \in \mathbb{T}^2$) can
693 be decomposed as,
694

695
$$T_{ij} = \delta_{ij} p + \epsilon_{ijk} u_k + b_{ij}$$

696 where, $p = \frac{1}{3} T_{kk}$, $u_k = \frac{1}{2} \epsilon_{ijk} T_{jk}$, $b_{ij} = \frac{1}{2} (T_{ij} + T_{ji}) - \frac{1}{3} \delta_{ij} T_{kk}.$ (20)
697

698 Here, δ_{ij} is the kronecker-delta and ϵ_{ijk} is the alternating tensor. Here, $p \in \mathbb{H}^0$, $u \in \mathbb{H}^1$, and $b \in \mathbb{H}^2$
699 are irreducible representations. Outside of the complete harmonic decomposition, the symmetric and
700 traceless decompositions have also been studied. The theory of Young tableau (Fulton (1997)) can
701 help with effective symmetric decomposition. More recently, the result given by Toth & Turyshev

(2022) can be adapted for the current context to begin with a symmetric tensor and decompose it into trace-less component. For $\mathbf{Q} \in \mathbb{S}^m$, an iterative formula can be written as

$$\mathbf{Q}_0 = Q_{i_1 i_2 \dots i_k} + \sum_{p=1}^{\lfloor k/2 \rfloor} (-1)^p \frac{k! (n+2k-2(p+2))!!}{2^p p! (k-2p)! (n+2k-4)!!} \delta_{(i_1 i_2} \delta_{i_3 i_4} \dots \delta_{i_{2p-1} i_{2p}} Q_{i_{2p+1} \dots i_k)},$$

where the n^{th} trace is defined as

$$Q_{i_1 i_2 \dots i_{k-2n}} = \delta_{i_{k+1} i_{k+2}} \dots \delta_{i_{k-1} i_k} Q_{i_1 i_2 \dots i_k}.$$

Here n is the number of dimensions, and k is the order of the tensor \mathbf{Q} . Also,

$$a!! = \begin{cases} a(a-2)(a-4) \dots 2, & \text{if } a \text{ is even,} \\ a(a-2)(a-4) \dots 1, & \text{if } a \text{ is odd,} \end{cases} \quad \text{with } 0!! = 1, 1!! = 1.$$

Using this formula, some common harmonic projection formulae are worked out below, for 3 dimensions. Here, $\mathbf{T}_n \in \mathbb{S}^n$ and $\mathbf{T}_n^0 \in \mathbb{H}^n$ is its corresponding harmonic projection.

$$\mathbf{T}_2^0 = T_{ij} - \frac{1}{3} \delta_{ij} T_{mm}$$

$$\mathbf{T}_4^0 = T_{ijkl} - \frac{6}{7} (\delta_{ij} T_{mmkl})^s + \frac{3}{35} (\delta_{ij} \delta_{kl})^s T_{mmnn}$$

$$\mathbf{T}_7^0 = T_{ijklmnp} - \frac{21}{13} (\delta_{ij} T_{qqklmnp})^s + \frac{105}{143} (\delta_{ij} \delta_{kl} T_{qqrrmnp})^s - \frac{105}{1287} (\delta_{ij} \delta_{kl} \delta_{mn} T_{qqrrtpp})^s$$

D ISOMORPHISM BETWEEN BINARY FORMS AND HARMONIC TENSORS

The isomorphism which links S_{2n} and \mathbb{H}^n is crucial for the results established in §3. Let $\mathbf{T} \in \mathbb{H}^n[\mathbb{R}^3]$ which is an irreducible representation of $\text{SO}(3, \mathbb{R})$. It can be complexified with $\otimes \mathbb{C}$ to get $\mathbb{H}^n[\mathbb{C}^3]$, which is an irreducible representation of $\text{SO}(3, \mathbb{C})$. The *polarization* (see Appendix A in Olive et al. (2017)) map can be used to convert a order n harmonic (or any symmetric) tensor into a homogeneous polynomial $p(x, y, z)$:

$$\psi : \mathbb{H}^n(\mathbb{C}^3) \rightarrow \mathbb{C}_n[\mathbb{C}^3]. \quad (21)$$

Here $\mathbb{C}_n[\mathbb{C}^3]$ is the space of homogeneous ternary polynomials (in 3 variables) of order n . This map is invertible so any polynomial $p(x, y, z)$ can also be mapped to a harmonic tensor³. There is an isomorphism between the ternary polynomial forms and binary forms which can be written using the Cartan map:

$$\mathbf{f}(u, v) = p \left(\frac{u^2 - v^2}{2}, \frac{u^2 + v^2}{2i}, uv \right), \quad (22)$$

where $\mathbf{f} \in S_{2n}$. The ternary form ($p \in \mathbb{C}_n[\mathbb{C}^3]$) can be recovered with the map below:

$$u^{2n-k} v^k \longrightarrow \begin{cases} z^k (x + iy)^{n-k}, & \text{if } 0 \leq k \leq n, \\ z^{2n-k} (-x + iy)^{k-n}, & \text{if } n \leq k \leq 2n. \end{cases}$$

This finishes the description of the isomorphism. The implementation of the isomorphism can be altered based on the application. For a more detailed treatment we refer to the works of Olive et al. (2017) and Olive et al. (2018).

³Now, if the tensor is symmetric and also trace free, then the laplacian of the corresponding homogeneous polynomial is zero, hence they are appropriately referred to as harmonic tensors.

756 E GORDAN'S ALGORITHM
757

758 Gordan's algorithm is used for generating the covariant algebra of binary forms. It was originally
759 proposed Gordan (1868) first showed that the covariant algebra is finitely generated (even before
760 Hilbert). Olive (2017) provides a reformulation of the algorithm using the language of modern
761 representation and invariant theories. The Gordan's algorithm has two form. The first form is to
762 derive $\mathbf{Cov}(S_n)$ using $\mathbf{Cov}(S_k)$ for $k < n$. The second form is to derive the covariant algebra of joint
763 binary forms, i.e., $\mathbf{Cov}(S_{n_1} \oplus S_{n_2} \oplus \dots \oplus S_{n_k})$. The Covariant algebra of simple binary forms is
764 already derived for several orders. S_5, S_6 are derived by Gordan (1875), S_7 by Dixmier & Lazard
765 (1985); Bedratyuk (2009), S_8 by Draisma (2014); Bedratyuk (2006), S_9 and S_{10} by Lercier & Olive
766 (2015). Using these equivariant tensor functions using dependencies upto T^5 can be computed
767 following the current work. Results for $\mathbf{Cov}(S_4)$, as an example, are shown in Table 2, where
768 $\mathbf{v} \in S_4$.

Degree / Order	0	4	6
1		\mathbf{v}	$(\mathbf{v}, (\mathbf{v}, \mathbf{v})_2)_1$
2	$(\mathbf{v}, \mathbf{v})_4$	$(\mathbf{v}, \mathbf{v})_2$	
3	$(\mathbf{v}, (\mathbf{v}, \mathbf{v})_2)_4$		

775
776 Table 2: Covariant Algebra of S_4 ($\mathbf{v} \in S_4$).

777 The second form of Gordan's algorithm uses the $\mathbf{Cov}(S_n)$ and $\mathbf{Cov}(S_m)$ to derive $\mathbf{Cov}(S_n \oplus S_m)$. If
778 $\mathbf{f}_i \in S_n, \mathbf{g}_j \in S_m$ for $1 \leq i \leq p, 1 \leq j \leq q$ then let a_i, b_j be the orders of $\mathbf{f}_i, \mathbf{g}_j$, a new transvectant
779 can be constructed using $\alpha \in \mathbb{N}^p, \beta \in \mathbb{N}^q$ as $(\mathbf{f}_1^{\alpha_1} \mathbf{f}_2^{\alpha_2} \dots \mathbf{f}_p^{\alpha_p}, \mathbf{g}_1^{\beta_1} \mathbf{g}_2^{\beta_2} \dots \mathbf{g}_q^{\beta_q})_r$ for some r . Gordan's
780 algorithm gives a finite set of (α, β, r) 's using which the covariant algebra can be generated. They
781 are obtained as irreducible solutions (cannot be decomposed into sum of non-trivial solutions) of the
782 linear Diophantine equation:
783

$$a_1\alpha_1 + a_2\alpha_2 + \dots + a_p\alpha_p = u + r \\ b_1\beta_1 + b_2\beta_2 + \dots + b_q\beta_q = v + r \quad (23)$$

d/o	0	2	4	6
1			\mathbf{p}, \mathbf{q}	
2	$(\mathbf{p}, \mathbf{p})_4, (\mathbf{q}, \mathbf{q})_4$ $(\mathbf{p}, \mathbf{q})_4$	$(\mathbf{p}, \mathbf{q})_3$	$(\mathbf{p}, \mathbf{p})_2, (\mathbf{q}, \mathbf{q})_2$ $(\mathbf{p}, \mathbf{q})_2$	$(\mathbf{p}, \mathbf{q})_1$
3	$(\mathbf{p}, (\mathbf{p}, \mathbf{p})_2)_4$ $(\mathbf{q}, (\mathbf{q}, \mathbf{q})_2)_4$ $(\mathbf{p}, (\mathbf{q}, \mathbf{q})_2)_4$ $(\mathbf{q}, (\mathbf{p}, \mathbf{p})_2)_4$	$(\mathbf{p}, (\mathbf{q}, \mathbf{q})_2)_3$ $(\mathbf{q}, (\mathbf{p}, \mathbf{p})_2)_3$	$(\mathbf{p}, (\mathbf{q}, \mathbf{q})_2)_2$ $(\mathbf{q}, (\mathbf{p}, \mathbf{p})_2)_2$	$(\mathbf{p}, (\mathbf{p}, \mathbf{p})_2)_1$ $(\mathbf{q}, (\mathbf{q}, \mathbf{q})_2)_1$ $(\mathbf{p}, (\mathbf{q}, \mathbf{q})_2)_1$ $(\mathbf{q}, (\mathbf{p}, \mathbf{p})_2)_1$
4	$((\mathbf{p}, \mathbf{p})_2, (\mathbf{q}, \mathbf{q})_2)_4$	$((\mathbf{p}, \mathbf{p})_2, (\mathbf{q}, \mathbf{q})_2)_3$ $((\mathbf{p}, (\mathbf{p}, \mathbf{p})_2)_1, \mathbf{q})_4$ $(\mathbf{p}, (\mathbf{q}, (\mathbf{q}, \mathbf{q})_2)_1)_4$		
5		$(\mathbf{p}^2, (\mathbf{q}, (\mathbf{q}, \mathbf{q})_2)_1)_6$ $((\mathbf{p}, (\mathbf{p}, \mathbf{p})_2)_1, \mathbf{q}^2)_6$		

806
807 Table 3: Covariant Algebra of $S_4 \oplus S_4$ ($\mathbf{p}, \mathbf{q} \in S_4$)

808 Using this algorithm, the $\mathbf{Cov}(S_6 \oplus S_2)$, $\mathbf{Cov}(S_4 \oplus S_4)$, $\mathbf{Cov}(S_6 \oplus S_4)$, $\mathbf{Cov}(S_6 \oplus S_4 \oplus S_2)$ are
809 derived by Olive (2017). $\mathbf{Cov}(S_4 \oplus S_4)$ is shown in Table 3 for reference, by ordering them degree
and order wise. Here, $\mathbf{p} \in S_4, \mathbf{q} \in S_4$.

810
 811 **Remark.** Solutions to linear Diophantine equations can become expensive when the number of
 812 variables is large. In the current work, the Gordan’s algorithm and also numerical polynomial re-
 813 mainder algorithm proposed in Appendix F can involve linear Diophantine equations with hundreds
 814 (if not thousands) of variables. In practice, the fastest strategy to obtain solutions is by first creating
 815 a convex cone and computing its lattice points. The algorithms described in the Normaliz (Bruns
 et al. (2017)) Package are recommended.

816
 817 **Remark.** It should be noted that the Gordan’s algorithm attempts to produce a finite covariant
 818 algebra and not a finite covariant module basis which is what we need. So, after the algebra (for ex-
 819 ample, \mathbf{V}) is generated by Gordan’s algorithm, the covariant module generators of $\text{Cov}_{\mathbf{G}}(\mathbf{V}, \mathbf{S}_n)$
 820 are generated by multiplying the polynomials in the algebra together with one another such that
 821 they match the order of \mathbf{S}_n and some degree. This process can be repeated degree-per-degree to
 822 find covariant generators in each degree. Since, the algebra is finitely generated, after some degree,
 823 new generators will not be identified. This problem of finding all possible combinations of poly-
 824 nomial multiplication for a particular degree and order can also be achieved by solving a linear
 825 Diophantine equation.

826 F POLYNOMIAL REMAINDER

827
 828 In Algorithm 15, the operation $f_i \% \mathbf{m}$ involves calculating the polynomial remainder after dividing
 829 by an ideal. This can be significantly expensive. It is convenient to use Gröbner basis calculations.
 830 In Macaulay2, creating an Ideal pre-computes the Gröbner basis. Also, since the ideal \mathbf{m} is homo-
 831 geneous, degree limits can be imposed on S-pairs that are used in the basis computations, which
 832 tremendously reduces the expenditure. However, if the maximum degree under consideration is too
 833 high, the calculation of Gröbner basis might be too expensive. So, a numerical linear algebra based
 834 algorithm is desirable to avoid symbolic computations altogether.

835
 836 Instead of computing the polynomial reminders for every generator and then computing the linearly
 837 independence, the linear independence test can be done in a degree by degree, order by order manner.
 838 An intermediate degree, order (d, o) stage computations would involve the following steps. Let
 839 $\mathcal{H}_{(d,o)}$ be the non-minimal module generators who have a degree d , and order o . Let the R linearly
 840 independent module generators identified up to (d, o) be $\mathcal{H}_{(< d, < o)}^{\text{LI}}$. By multiplying polynomials in
 841 $\mathcal{H}_{(< d, < o)}^{\text{LI}}$ together among themselves and using the generators of R , the (d, o) piece can be spanned,
 842 by solving an appropriate linear Diophantine equation for the degree and order. The polynomials in
 843 $\mathcal{H}_{(d,o)}$ which are linearly among themselves and also linearly independent with this newly spanned
 844 set can be added to $\mathcal{H}_{(< d, < o)}^{\text{LI}}$ to complete the calculation for the degree, order (d, o) pair. Next,
 845 the calculation could focus either on $(d + 1, o)$ or $(d, o + 1)$ piece until the module generators are
 846 exhausted.

847 G MINIMAL ANVARIANT ALGEBRA AND COVARIANT MODULE GENERATORS

848 G.1 MODELING A SYMMETRIC ORDER 2 TENSOR USING TWO SYMMETRIC ORDER 2 849 TENSORS

Deg	$2\mathbb{H}^2$	$2\mathbb{H}^0$
1		$\text{tr}(\mathbf{B}), \text{tr}(\mathbf{C})$
2	$\text{tr}(\mathbf{B}^2), \text{tr}(\mathbf{C}^2), \text{tr}(\mathbf{BC} + \mathbf{CB})$	
3	$\text{tr}(\mathbf{CH}_{2c} + \mathbf{H}_{2c}\mathbf{C}), \text{tr}(\mathbf{BH}_{2b} + \mathbf{H}_{2b}\mathbf{B}), \text{tr}(\mathbf{CH}_{2b} + \mathbf{H}_{2b}\mathbf{C}), \text{tr}(\mathbf{BH}_{2c} + \mathbf{H}_{2c}\mathbf{B})$	
4	$\text{tr}(\mathbf{H}_{2c}\mathbf{H}_{2b} + \mathbf{H}_{2b}\mathbf{H}_{2c})$	

862
 863 Table 4: Invariants of $2\mathbb{H}^2 \oplus 2\mathbb{H}^0$.

864 G.2 NON-LINEAR RAPID PRESSURE STRAIN RATE TENSOR MODELS
865

866 To model the Π tensor, the order 4 \mathbf{M} tensor must be modeled. Eq. 19 shows this requires modeling
867 a \mathbb{H}^4 using $\mathbb{H}^2 \oplus \mathbb{H}^2 \oplus \mathbb{H}^3$. This requires identifying the minimal generators of the order 8 covariant
868 module of $S_6 \oplus S_4 \oplus S_4$. Using the Covariant Algebra of S_6 and $S_4 \oplus S_4$ (Olive (2017)), Gordan's
869 algorithm can be used to get the module generators of $S_6 \oplus S_4 \oplus S_4$. From those the order 8 and
870 degree ≤ 3 covariant modules generators are identified and minimized (using Algorithm 1). There
871 are 4 degree 2 invariants and 7 degree 3 invariants which are shown in Table 6. There are 6 degree
872 2 and 21 degree 3 minimal covariant generators shown in Table 5, which will be converted to tensor
873 monomials. The coefficients to these monomials will be learned as scalar functions of invariants,
874 which will be learned using neural networks. The coefficients of the degree 2 and degree 3 models
875 are learned using two neural networks with similar architectures. The networks have two hidden
876 layers with 128 neurons and have 18k and 20k parameters respectively. We used AdamW for
877 regularization and dropout was used for regularization.
878

d/o	8
2	$(\mathbf{f}, \mathbf{p})_1, (\mathbf{f}, \mathbf{q})_1, (\mathbf{f}, \mathbf{f})_2, \mathbf{p}^2, (\mathbf{q}, \mathbf{p})_0, \mathbf{q}^2$
3	$(\mathbf{f}, (\mathbf{p}, \mathbf{p})_2)_1, (\mathbf{f}, (\mathbf{q}, \mathbf{q})_2)_1, (\mathbf{f}, (\mathbf{p}, \mathbf{q})_2)_1, (\mathbf{f}, (\mathbf{p}, \mathbf{q})_1)_2, (\mathbf{f}, (\mathbf{f}, \mathbf{p})_4)_0, (\mathbf{f}, (\mathbf{f}, \mathbf{q})_4)_0,$ $((\mathbf{f}, \mathbf{f})_2, \mathbf{p})_2, ((\mathbf{f}, \mathbf{f})_2, \mathbf{q})_2, ((\mathbf{f}, \mathbf{f})_4, \mathbf{f})_1, (\mathbf{p}, (\mathbf{f}, \mathbf{f})_4)_0, (\mathbf{p}, (\mathbf{f}, \mathbf{p})_3)_0, (\mathbf{p}, (\mathbf{f}, \mathbf{q})_3)_0,$ $(\mathbf{q}, (\mathbf{f}, \mathbf{f})_4)_0, (\mathbf{q}, (\mathbf{f}, \mathbf{p})_3)_0, (\mathbf{q}, (\mathbf{f}, \mathbf{q})_3)_0, ((\mathbf{p}, \mathbf{p})_2, \mathbf{p})_0, ((\mathbf{p}, \mathbf{p})_2, \mathbf{q})_0, ((\mathbf{q}, \mathbf{q})_2, \mathbf{p})_0,$ $((\mathbf{q}, \mathbf{q})_2, \mathbf{q})_0, ((\mathbf{p}, \mathbf{q})_2, \mathbf{p})_0, ((\mathbf{p}, \mathbf{q})_2, \mathbf{q})_0$

887 Table 5: Order 8 Covariant module generators of $S_6 \oplus S_4 \oplus S_4$ up to degree 3. ($\mathbf{p}, \mathbf{q} \in S_4, \mathbf{f} \in S_6$)
888

d/o	0
2	$(\mathbf{f}, \mathbf{f})_6, (\mathbf{p}, \mathbf{p})_4, (\mathbf{q}, \mathbf{q})_4, (\mathbf{p}, \mathbf{q})_4$
3	$(\mathbf{p}, (\mathbf{p}, \mathbf{p})_2)_4, (\mathbf{q}, (\mathbf{q}, \mathbf{q})_2)_4, (\mathbf{p}, (\mathbf{q}, \mathbf{q})_2)_4, (\mathbf{q}, (\mathbf{p}, \mathbf{p})_2)_4,$ $(\mathbf{f}, (\mathbf{p}, \mathbf{q})_1)_6, ((\mathbf{f}, \mathbf{f})_4, \mathbf{q})_4, ((\mathbf{f}, \mathbf{f})_4, \mathbf{p})_4$

896 Table 6: Invariant ring generators of $S_6 \oplus S_4 \oplus S_4$ up to degree 3. ($\mathbf{p}, \mathbf{q} \in S_4, \mathbf{f} \in S_6$)
897898 H OVERVIEW
900901 The Fig. 3 shows the overall workflow for learning function representations developed in this work.
902903 I EXTENSIONS TO OTHER GROUPS
905906 The following general formula is used in the current work:
907

$$908 \mathbf{T}(\mathbf{A}_1, \mathbf{A}_2, \dots, \mathbf{A}_k) = \sum_{i=1}^{\gamma} C_i(\lambda_1, \lambda_2, \dots, \lambda_m) \mathbf{B}_i(\mathbf{A}_1, \mathbf{A}_2, \dots, \mathbf{A}_k)$$

911 For mappings between any representation of any group G , this ansatz holds. The generators for the
912 Invariant ring and the Covariant module over that ring are necessary for building functions between
913 representations of any general group. In this work tensor representations over $SO(3)$ were
914 considered, and algorithms were developed for identifying generators of Invariants and Covariant modules.
915 For extension of this work to other representations of different groups, appropriate algorithms for
916 generators must be identified, which can then be used with Algorithm 1 to build the representation
917 maps. There is extensive literature for efficient computation of invariant rings and covariant module
918 generators (Derksen & Kemper (2015); Goodman et al. (2009)).

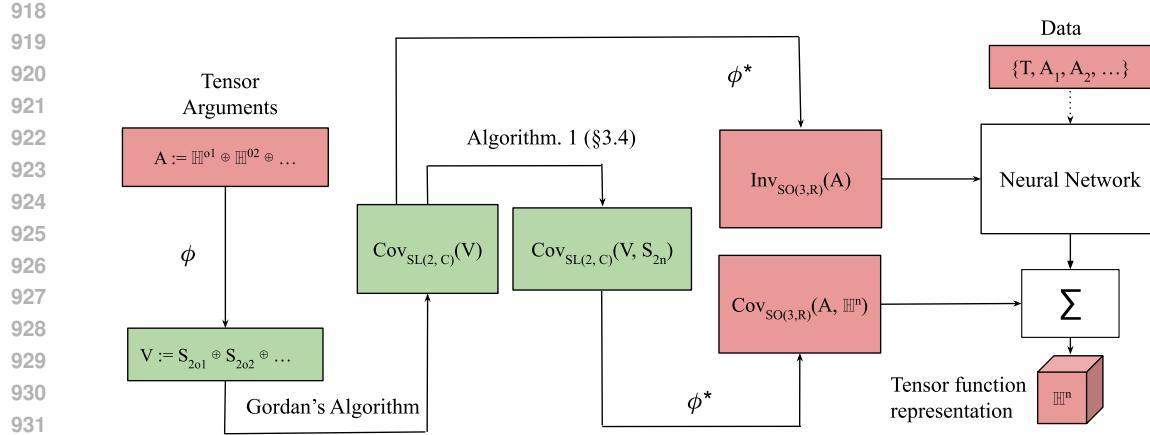


Figure 3: Workflow for learning tensor function representations of order n harmonic tensor \mathbf{T} using $(\mathbb{H}^{o1} \oplus \mathbb{H}^{o2} \oplus \dots)$. Red blocks work with tensors, and green blocks work with binary forms. ϕ is the isomorphism between them and ϕ^* is the inverse map of the isomorphism.

Let $\mathcal{V} := \mathbb{T}^{n_1} \oplus \mathbb{T}^{n_2} \oplus \dots \mathbb{T}^{n_k}$ be a tensor space. Then the G -equivariant tensor function representations over $\mathcal{T} := \mathbb{T}^t$ can be derived as covariant module, $\text{Cov}_G(\mathcal{T})$ generators over the Invariant ring $\text{Inv}_G(\mathcal{V})$. This work focused on the $G = \text{SO}(3, \mathbb{R})$ extensively, but the results can be extended to the $\text{O}(3, \mathbb{R})$ in a straight forward manner.

I.1 $\text{O}(3, \mathbb{R})$ -EQUIVARIANT TENSOR FUNCTIONS

The $\text{O}(3, \mathbb{R})$ group contains both reflections and rotations, unlike $\text{SO}(3, \mathbb{R})$ which only contains proper rotation matrices ($\text{SO}(3) \subset \text{O}(3)$). Since, $\text{O}(3)$ is a bigger group, $\text{O}(3)$ -equivariance is more restrictive than $\text{SO}(3)$ -equivariance. Once, the $\text{SO}(3)$ -equivariant functions are derived using the Gordan's algorithm, the following Lemma can be used to filter out the $\text{O}(3)$ -equivariant tensor functions.

Lemma I.1. *Let $\mathbf{T}(\mathbf{A}_1, \mathbf{A}_2, \dots, \mathbf{A}_k)$ be a tensor function of order, $o(\mathbf{T})$ and degree, $d(\mathbf{T})$, then \mathbf{T} is an $\text{O}(3)$ equivariant function representation, iff:*

$$o(\mathbf{T}) \cong \sum_{i=1}^n o(\mathbf{A}_i)d(\mathbf{A}_i) + d(\epsilon) \pmod{2} \quad (24)$$

Where, $d(\epsilon)$ is degree (number of copies) of levi-civita tensors in \mathbf{T} . In its general form, the expression takes the following form including the degree of kroncker-deltas, $d(\delta)$ as:

$$\begin{aligned} o(\mathbf{T}) &\cong \sum_{i=1}^n o(\mathbf{A}_i)d(\mathbf{A}_i) + o(\delta)d(\delta) + o(\epsilon)d(\epsilon) \pmod{2} \\ o(\mathbf{T}) &\cong \sum_{i=1}^n o(\mathbf{A}_i)d(\mathbf{A}_i) + 2d(\delta) + 3d(\epsilon) \pmod{2} \\ o(\mathbf{T}) &\cong \sum_{i=1}^n o(\mathbf{A}_i)d(\mathbf{A}_i) + d(\epsilon) \pmod{2} \end{aligned}$$

I.2 PERMUTATION EQUIVARIANT TENSOR FUNCTIONS

As noted in Col. 3.1.1 and in Fig. 3, the co-domain is decomposed into harmonic tensor spaces using harmonic decomposition. Upon plugging in the models of the harmonic components back into the decomposition the tensor function representations of the desired space are build by keeping the correct symmetries of the group. So, it is worthwhile to mention that the current methodology in

972 this work implicitly imposes equivariance of the permutation group through the harmonic decomposition.
 973 Extensions to groups in higher dimensions (> 3) and other general groups are out of scope
 974 for this current work.

976 J MORE MATHEMATICAL BACKGROUND

978 Some mathematical background and preliminaries used throughout this work were defined in Sec-
 979 tion. 2. Here, more prerequisites are presented with brief examples.

981 A *ring* R is a set accompanied with the addition and multiplication operations such that R is an
 982 abelian group with respect to addition ($0 \in R$, if $x \in R$, then $-x \in R$) and the multiplication is
 983 associative and distributive over addition. If a ring is *commutative*, $xy = yx, \forall x, y \in R$. An example
 984 is the *polynomial ring* which is commonly encountered this work. The set of all polynomials

$$985 \quad 986 \quad f(x) = a_0 + a_1x + \cdots + a_nx^n$$

987 for some $n > 0$ and $a_i \in R$, where x is an indeterminate, form the polynomial ring $R[x]$ with
 988 coefficients in R .

990 If R is a ring, then an *R -module* is an abelian group M equipped with a multiplication by elements
 991 of R , such that :

$$993 \quad 994 \quad a(x + y) = ax + ay \\ 995 \quad (a + b)x = ax + bx \\ 996 \quad (ab)x = a(bx) \\ 997 \quad 1x = x$$

999 for all $a, b \in R, x, y \in M$. If $u_1, u_2, \dots, u_n \in M$ are such that all elements of M can be written
 1000 as $x_1u_1 + x_2u_2 + \dots + x_nu_n$ for some $x_i \in R$, then $u_1, u_2, \dots, u_n \in M$ is called as the *generating*
 1001 *set* of M . It is called *minimal* if removing any u_i would disable the generating set from spanning
 1002 the entire module. It is called as a *basis* if the elements are R -linearly independent. It is possible to
 1003 have minimal generating sets of different dimensions. For example on \mathbb{Z} , both $\{1\}$ and $\{2, 3\}$ are
 1004 minimal generators. But only $\{1\}$ is a basis.

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