Group-theoretic Approach for Symbolic Tensor Manipulation: I. Free Indices

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Abstract

We describe how Computational Group Theory provides tools for manipulating tensors in explicit index notation. In special, we present an algorithm that puts tensors with free indices obeying permutation symmetries into the canonical form. The method is based on algorithms for determining the canonical coset representative of a subgroup of the symmetric group. The complexity of our algorithm is polynomial on the number of indices and is useful for implementating general purpose tensor packages on the computer algebra systems.

Key words. Symbolic tensor manipulation, Computational Group Theory, Algorithms, Canonical coset representative, Symmetric group³ Poisson,

1 Introduction

The connection between Group Theory and Tensor Calculus was established a long time ago. For instance, Weyl [1] showed the relation of the symmetric group and group rings to tensor symmetries and tensor expressions respectively; Littlewood [2] developed tools in group representation theory to address the problem of determining the dimension of the space generated by tensor monomials. Recently, Fulling et

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al. [3] used these tools to determine the number of independent monomials up to order 12 built out of the Riemann tensor and its covariant derivative. On the other hand, these authors have not established a method to determine the independent monomials explicitly. The present work performs an important step toward this direction.

The application of Group Theory to develop algorithms for tensor manipulation is addressed in refs. [4] and [5]. Ref. [4] uses group algebra which generates an algorithm of exponential complexity that can address tensor expressions with at most 11 or 12 indices. Practical applications demand better results. Ref. [5] uses the backtrack algorithm to find the canonical form of tensor expressions built out of totally symmetric or antisymmetric tensors.

The present work addresses the problem of finding efficient algorithms for abstract tensor manipulation using Computational Group Theory. The main problem consists in simplifying tensor expressions, which can be solved if one knows an efficient algorithm that puts tensor expressions into the canonical form. Ref. [6] shows that the problem of finding the canonical form of a generic tensor expression reduces to finding the canonical forms of single tensors. At this point, the group-theoretic approach is the natural language to express the problem, since all informations about a single tensor can be represented by Group Theory, and can be efficiently processed using Computational Group Theory.

We suppose that the tensors have only free indices and obey what we now call permutation symmetries, which are a set of tensor equations of the form

$$T^{i_1 \cdots i_n} = \epsilon_{\sigma} T^{\sigma(i_1 \cdots i_n)}, \tag{1}$$

where $\sigma(i_1 \cdots i_n)$ is a permutation of $i_1 \cdots i_n$ and ϵ_{σ} is either 1 or -1. We present a polynomial-time algorithm to find the canonical forms of these tensors. This algorithm is a straightforward extension of algorithms to find the canonical coset representative of a subgroup of the symmetric group.

In section 2 we describe the representation theory for tensors. In section 3 we present the main algorithm and discuss its complexity.

2 Representation theory for tensors

In this work we use the abstract-index notation for tensor expressions such as described in Penrose and Rindler's book [7]. We take Lovelock and Rund [8] as a general reference for Tensor Calculus. Ref. [6] describes in details how a generic tensor expression can be converted into a sum of single tensors. To sum up, a generic tensor expression can be expanded so that it is a sum of tensor monomials. Each monomial is merged into a single tensor that inherits the symmetries of the original tensors. If each single tensor can be put into the canonical form, then the original tensor expression can be put also. At this point the problem consists in finding the canonical form of a single tensor obeying permutation symmetries.

In the present context, we need only three kind of informations about a tensor: sign, index configuration, and symmetries. For example, if one wants to find the canonical form of T^{cba} knowing that the rank-3 tensor T is totally antisymmetric, one starts with

$$\{+1, [c, b, a]\}$$

and ends up with

$$\{-1, [a, b, c]\}.$$

The natural canonical configuration is $-T^{abc}$.

In order to use a group-theoretical approach for this kind of manipulation we have to represent the symmetry as some group which acts on the index configuration and on the sign. This goal is achieved in the following way.

Definition 1 (Symmetry of rank-n tensor from the group-theoretic point of view.) Let S_n be the symmetric group on the set of points $\{1, 2, \dots, n\}$ and H the group $(\{+1, -1\}, \times)$ with multiplicative operation. A tensor symmetry S is a proper subgroup of the external direct product $H \otimes S_n$ such that $(-1, id) \notin S$, where id is the identity of S_n .

In order to fix notation, from now on we assume that H and S are the groups described in Def. 1. We also assume that G is the subgroup of S_n such that $H \otimes G = < (-1, id), S >$, i.e. $H \otimes G$ is the smallest subgroup of $H \otimes S_n$ which contains S and (-1, id). Therefore, the order of $H \otimes G$ is two times the order of S.

Now let us describe formally how S acts on a tensor. Each element of S is a pair consisting of a sign (± 1) and a permutation. The sign of a permutation π will be denoted by ϵ_{π} . So, an element of S has the form (ϵ_{π}, π) , where $\epsilon_{\pi} = \pm 1$ and $\pi \in G$. The action of s on a totally contravariant rank-n tensor with index configuration $T^{i_1 i_2 \cdots i_n}$ is

$$s(T^{i_1 i_2 \cdots i_n}) = \epsilon_\pi T^{i_1 \pi i_2 \pi \cdots i_n \pi}, \tag{2}$$

where the notation $i_{1^{\pi}}$ means that the subscript of i is the image of point 1 under the action of permutation π . This notation clearly shows that the permutation acts on the positions of the indices and seems to be superior to the one used in (1).

The notation $+\pi$ stands for $(1,\pi)$ and $-\pi$ for $(-1,\pi)$. For example, the group S which describes the symmetry of a totally antisymmetric rank-3 tensor is

$$S = \{+id, -(1,2), -(1,3), -(2,3), +(1,2,3), +(1,3,2)\},$$
(3)

which, in tensor notation, corresponds to

$$T^{abc} = T^{abc}, \quad T^{abc} = -T^{bac}, \quad T^{abc} = -T^{cba},$$
 $T^{abc} = -T^{acb}, \quad T^{abc} = T^{bca}, \quad T^{abc} = T^{cab}.$ (4)

We use the term "permutation" to describe the elements of S extending the syntax used for elements of S_n . The term "permutation sign" refers to ϵ_{π} . The sign ϵ_{π} has no relation to the parity of π in the general case.

With no loss of generality, we take

$$T^{i_1 i_2 \cdots i_n} \tag{5}$$

as the standard configuration. All other configurations are obtained by acting permutations of $H \otimes S_n$ on (5). A generic configuration is denoted by $T^{j_1 \cdots j_n}$. We use the sequence of j's $(j_1 \cdots j_n)$ as a generic permutation of $i_1 \cdots i_n$. The standard configuration (5) is associated with the element (+1, id), which is the minimal element of $H \otimes S_n$.

In Def. 1, the requirement that $(-1, id) \notin S$ avoids the cancelation of a tensor independently of its components. Note that if both $(+1, \pi)$ and $(-1, \pi)$ are in S, then we come to two conclusions: there are two equal index configurations such that $T^{j_1j_2\cdots j_n} = -T^{j_1j_2\cdots j_n}$ and $(-1, id) \in S$. Vice-versa, if $(-1, id) \in S$ then $(-1, \pi) \in S$ if and only if $(+1, \pi) \in S$. When implementing a tensor package in some computer language, it is useful to have an efficient method to exhibit the symmetries that cancels the tensor independently of its components. Algorithms for testing membership provide such method.

The index configuration $T^{j_1j_2\cdots j_n}$ is equivalent to $T^{i_1i_2\cdots i_n}$ if and only if there is an element in S such that

$$s(T^{i_1 i_2 \cdots i_n}) \equiv T^{j_1 j_2 \cdots j_n}. \tag{6}$$

In other words, there is an element $(+1, \pi) \in S$ such that the lists $j_1 j_2 \cdots j_n$ and $i_{1^{\pi}} i_{2^{\pi}} \cdots i_{n^{\pi}}$ are exactly the same.

Proposition 1 The set of index configurations equivalent to $T^{i_1 i_2 \cdots i_n}$ is given by the action of S over $T^{i_1 i_2 \cdots i_n}$. The cardinality of this set is the order of G (|G|).

Note that |G| = |S|.

Proposition 2 Let $T^{i_1\pi}{}^{i_2\pi\cdots i_n\pi}$ be an index configuration which is not equivalent to $\pm T^{i_1i_2\cdots i_n}$ (i.e. both $+\pi$) and $-\pi$) are not in S). The set of configurations equivalent to $T^{i_1\pi}{}^{i_2\pi\cdots i_n\pi}$ is the right coset of S in $H\otimes S_n$ which contains $(+1,\pi)$. The number of index configurations equivalent to $T^{i_1\pi}{}^{i_2\pi\cdots i_n\pi}$ is |G|.

The final part of proposition 2 follows from the fact that all cosets of S in $H \otimes S_n$ have cardinality |G|.

Proposition 3 Consider a set of independent index configurations with positive coefficients. The maximum cardinality of this set is the index of G in S_n ($|S_n:G|$).

Usually, no one describes the symmetry of a tensor in index notation by listing all equivalent index configurations. In general, one gives a few equations and skips the ones that can be obtained from the original equations. The following example illustrates this situation. Let T^{abcd} be a rank-4 tensor with the following permutation symmetries.

$$T^{abcd} = -T^{bacd}, (7a)$$

$$T^{abcd} = T^{cdab}. (7b)$$

¿From these equations we can obtain

$$T^{abcd} = -T^{abdc}. (8)$$

Note that one can describe the symmetries of T^{abcd} by using a different set of equations, for example eqs. (7b) and (8). In group-theoretic language, this is equivalent to describe a group by generators. In the example above, the generating set K for the symmetry of T^{abcd} , described by eqs. (7), is

$$K = \{-(1,2), +(1,3)(2,4)\}. \tag{9}$$

The symmetry S is the group generated by K (< K >)

$$S = \{+id, -(1,2), -(3,4), +(1,2)(3,4), +(1,3)(2,4), -(1,32,4), -(1,4,2,3), +(1,4)(2,3)\}.$$

$$(10)$$

The group G is generated by $\{(1,2), (1,3)(2,4)\}$ and is obtained from (10) by removing the permutation signs. From proposition 1, the set of configurations equivalent to the standard configuration T^{abcd} is given by the action of all elements of S on T^{abcd} , which yields

$$\{T^{abcd}, -T^{bacd}, -T^{abdc}, T^{badc}, T^{cdab}, -T^{cdba}, -T^{dcab}, T^{dcba}\}. \tag{11}$$

The number of equivalent configurations is 8, the order of S. Now consider T^{acbd} , which is not in set (11). This index configuration is obtained from T^{abcd} by the action of +(2,3). Neither +(2,3) nor -(2,3) are in S. Proposition 2 says that the set of configurations equivalent to T^{acbd} is the right coset of S in $H \otimes S_4$ which contains +(2,3). This coset is obtained by multiplying each element of S by +(2,3):

$$S \times (+(2,3)) = \{+(2,3), -(1,3,2), -(2,3,4), +(1,3,4,2), +(1,2,4,3), -(1,2,4), -(1,4,3), +(1,4)\}.$$

$$(12)$$

The action of this coset on T^{abcd} generates all index configurations equivalent to T^{acbd} . Note that $|S_4:G|=3$. From proposition 3 we know that the set of independent configurations has cardinality 3. An example of this set is

$$\{T^{abcd}, T^{acdb}, T^{adcb}\},\tag{13}$$

which is a complete right transversal for G in S_4 in tensor notation. One can easily recognize that eqs. (7) and (8) represent the symmetries of the Riemann tensor without taking into account the cyclic symmetry. The group generated by $\{(1,2), (1,3)(2,4)\}$ is the dihedral group of order 8 (D_8) . Then, the symmetry of the Riemann tensor given by (10) is the largest subgroup of $H \otimes D_8$ which does not contain (-1, id).

In order to address the problem of finding the canonical configuration equivalent to a given index configuration, we have to define an order for the permutations of S_n . Let $\mathbf{b} = [b_1, \dots, b_n]$ be a list of n distinct points of the set $\{1, \dots, n\}$. Suppose that p_k and p_l are points. We define the order " $\prec_{\mathbf{b}}$ " for points with respect to \mathbf{b} in the following way: $p_k \prec p_l$ if k < l. So, p_k is smaller that p_l if p_k comes before p_l in \mathbf{b} . We omit the index \mathbf{b} from " $\prec_{\mathbf{b}}$ " to simplify the notation. $\mathbf{b}^{\pi} = [b_1^{\pi}, \dots, b_n^{\pi}]$ is the image of \mathbf{b} under π . Define

$$\mathcal{L} = \{ \boldsymbol{b}^{\pi}, \ \pi \in S_n \}. \tag{14}$$

Now let extend the order " \prec " to the elements of \mathcal{L} . Let L_1 and L_2 be in \mathcal{L} . $L_1 \prec L_2$ if

$$L_1[1] \prec L_2[1]$$
 or $(L_1[1] = L_2[1]$ and $L_1[2..n] \prec L_2[2..n]),$ (15)

where L[i] means the *i*-th element of L and L[2..n] means $\{L[2], L[3], \dots, L[n]\}$. If π_1 and π_2 are in S_n then

$$\pi_1 \prec \pi_2 \Leftrightarrow \boldsymbol{b}^{\pi_1} \prec \boldsymbol{b}^{\pi_2}.$$
 (16)

Now we extend the order " \prec " to group S:

$$(\epsilon_{\pi_1}, \pi_1) \prec (\epsilon_{\pi_2}, \pi_2) \Leftrightarrow \pi_1 \prec \pi_2.$$
 (17)

Recall that $(+1, \pi)$ and $(-1, \pi)$ cannot be at the same time in S. So we simply disregard the sign as stated in (17). " \prec " is a well-order (total order with a minimal element) in S_n , S, and in any coset of S in $H \otimes S_n$. ¿From now on, "minimal point" refers to the order " \prec " with respect to some \boldsymbol{b} .

A canonical right transversal for G in S_n (S in $H \otimes S_n$) is a complete right transversal for G in S_n (S in $H \otimes S_n$) such that each coset representative is minimal. The set (13) is the canonical right transversal in tensor notation for group G in S_4 with respect to $\mathbf{b} = [1, 3, 2, 4]$, where G is generated by $\{(1, 2), (1, 3)(2, 4)\}$. Note that the order " \prec " allows to sort a canonical right transversal for G in S_n . This is important for addressing the simplification problem when there are side relations, such as the cyclic symmetry. This kind of symmetry is not addressed in this paper.

3 Algorithm to canonicalize tensors with free indices

Now we address the following problem. Suppose one gives a totally contravariant tensor with the symmetries described by a set of tensor equations, and a free index configuration that is not the standard one. Find the canonical index configuration with respect to the order " \prec ". For example, suppose that rank-4 tensor T has the symmetries (7), and one gives the following index configuration: T^{bcad} . What is the canonical configuration with respect to $\mathbf{b} = [1, 3, 2, 4]$?

Using the representation theory, the problem above can be solved if one knows the solution of the following problem. Given a generating set K for the group S and an element (ϵ_{π}, π) in $H \otimes S_n$, find the canonical coset representative of the coset $S \times (\epsilon_{\pi}, \pi)$ with respect to the order defined by (17).

The answer to this problem is an algorithm that can be used to put a tensor with free indices into the canonical form. Before describing the algorithm, we extend some well known definitions for permutations groups, in order to use them in connection with S, which is a direct product of groups. The extensions are straightforward.

Definition 2 Let p be a point in the set $\{1, \dots, n\}$. The *stabilizer of* p *in* S is the subgroup S_p defined by

$$S_p = \{ s \in S \,|\, p^s = p \},\tag{18}$$

where $p^s = p^{\pi}$ and $s = (\epsilon_{\pi}, \pi)$.

In other words, S_p consists of all elements of S that fix the point p. S_p is a subgroup of S. If $s = (\epsilon_{\pi}, \pi) \in S$, "s fixes p" means " π fixes p".

Definition 3 Let Q be a subset of the set of points $\{1, \dots, n\}$. The *pointwise stabilizer of* Q *in* S is the subgroup S_Q defined by

$$S_Q = \{ s \in S \mid \forall q \in Q, \ q^s = q \}. \tag{19}$$

In other words, S_Q fixes all points of the subset Q.

Definition 4 A ordered subset $\boldsymbol{b} = [b_1, \dots, b_m]$ of the set of points $\{1, \dots, n\}$ is a base for S if $S_{b_1,\dots,b_m} = (1,id)$.

This means that the only element of S that fixes all points of \mathbf{b} is the identity. A useful property of a base is that an element of S is uniquely determined by the base image. We can order the points $\{1, \dots, n\}$ such that the base points are the first m points. Let us name the remaining points l_1, \dots, l_{n-m} . They simply follow the usual increasing order. From now on, the order " \prec " defined in the previous section is based on the set $[b_1, \dots, b_m, l_1, \dots, l_{n-m}]$.

Definition 5 A strong generating set K for S relative to the base $\mathbf{b} = [b_1, \dots, b_m]$ is a generating set for S with the following property: $K \cap S_{b_1,\dots,b_j}$ is a generating set for the pointwise stabilizer S_{b_1,\dots,b_j} , for $1 \leq j \leq m-1$.

In other words, a generating set K for S is *strong* if, after selecting the permutations of K that fix the points b_1, \dots, b_j , one has a set that generates the group S_{b_1,\dots,b_j} . This must be valid for j from 1 to m-1.

The input of the algorithm is

- (a) an index configuration $T^{j_1j_2\cdots j_n}$; and
- (b) a base and a strong generating set for S.

The output is the canonical index configuration, which is obtained by the action of the canonical coset representative on the standard configuration $T^{i_1 i_2 \cdots i_n}$. If S is described by a generating set that is not strong, the first step is to obtain a strong generating set and a corresponding base. Refs. [9] and [10] present algorithms that perform this task. These algorithms must be extended in order to work within $H \otimes S_n$.

The algorithm Canonical described below uses the general structure of *chain* of stabilizers developed by Sims [11] and is an straightforward modification of the algorithm presented by Butler [12]. Following Sim's notation, let $S^{(i)}$ be the group that stabilizes the points $\{b_1, \dots, b_{i-1}\}$, i.e. $S^{(i)} = S_{b_1, \dots, b_{i-1}}$. Then $S^{(1)} = S$ and $S^{(m)} = (1, id)$. Let $\Delta^{(i)}$ be the orbit of $S^{(i)}$ that contains the point b_i , i.e. $\Delta^{(i)} = b_i^{S^{(i)}}$. Suppose that K is a strong generating set for S and define $K^{(i)} = K \cap S^{(i)}$. $K^{(i)}$ is a strong generating set for $S^{(i)}$, for $1 \leq i \leq m$. Let $\nu^{(i)}$ be the Schreier vector of $\Delta^{(i)}$ with respect to generators $K^{(i)}$. Here, the components of the Schreier vectors are elements of S. Following Butler [10], if $q \in \Delta^{(i)}$, let $trace(q, \nu^{(i)})$ be the element $(\epsilon_{\omega}, \omega)$ of $S^{(i)}$ such that $p^{\omega} = q$, where p is the minimal point of the subsets of $\Delta^{(i)}$ that contains q.

The algorithm consists of m loops. Suppose that $[q_1, \dots, q_m]$ is the base image of the canonical representative. The i-th loop finds permutation $(\epsilon_{\lambda}, \lambda)$ that determines q_i , i.e. $b_i^{\lambda} = q_i$. The permutation $(\epsilon_{\lambda}, \lambda)$ obeys the constraint

$$[(b_1)^{\lambda}, \cdots, (b_{i-1})^{\lambda}] = [q_1, \cdots, q_{i-1}].$$
 (20)

The set of all elements of S that obey (20) is given by $S^{(i)} \times (\epsilon_{\lambda}, \lambda)$, then $b_i^{S^{(i)} \times (\epsilon_{\lambda}, \lambda)}$ yields all possible images of b_i in the coset $S^{(i)} \times (\epsilon_{\lambda}, \lambda)$. q_i is the minimal point of these images. At the last loop, $(\epsilon_{\lambda}, \lambda)$ gives the complete base image $[q_1, \dots, q_m]$.

Algorithm Canonical (free indices)

Input: $T^{j_1\cdots j_n} = \epsilon_{\pi}T^{i_1\pi} i_{2^{\pi}}\cdots i_{n^{\pi}}$, where $(\epsilon_{\pi},\pi) \in S$; $\boldsymbol{b} = [b_1,\cdots,b_m]$ base for S; and K_S strong generating set for S with respect to \boldsymbol{b} . $K^{(i)}$.

Output: $\epsilon_{\lambda} T^{i_{1\lambda} i_{2\lambda} \cdots i_{n\lambda}}$, where $(\epsilon_{\lambda}, \lambda)$ is the canonical representative of the coset of S in $H \otimes S_n$ that contains the permutation (ϵ_{π}, π) .

```
begin

(* initialization of (\epsilon_{\lambda}, \lambda) and K *)

(\epsilon_{\lambda}, \lambda) := (\epsilon_{\pi}, \pi);

K := K_S;

for i from 1 to m do

(* \Delta is the basic orbit \Delta^{(i)} *)

\Delta := b_i^{< K^>};

k := position of the minimal point of \Delta^{\lambda};

p := k-th point of \Delta;

(\epsilon_{\omega}, \omega) := trace(p, \nu), where \nu is the Schreier vector of \Delta with respect to K;

(\epsilon_{\lambda}, \lambda) := (\epsilon_{\omega}, \omega) \times (\epsilon_{\lambda}, \lambda);

K := remove permutations of K that have point b_i;

end for;

return \epsilon_{\lambda} T^{i_{1\lambda}} i_{2\lambda} \cdots i_{n\lambda};
end
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Let us see an example. If one gives the index configuration T^{bcad} , where T has the symmetries (7), the element (ϵ^{π}, π) is +(1, 2, 3). A base for S is [1, 3], so the order " \prec " is based on the list $\boldsymbol{b} = [1, 3, 2, 4]$. A strong generating set with respect to base [1, 3] is

$$K = \{-(1,2), -(3,4), +(1,3)(2,4)\}.$$
(21)

First loop yields: $\Delta := \{1, 2, 3, 4\}; \ \Delta^{(1,2,3)} := \{2, 3, 1, 4\}; \ k := 3; \ p := 3; \ (\epsilon_{\omega}, \omega) := +(1,3)(2,4), \text{ since } b_1^{\omega} = p; \ (\epsilon_{\lambda}, \lambda) := +(2,4,3); \ K := \{-(3,4)\}. \ (\epsilon_{\lambda}, \lambda) \text{ applied on } T^{abcd} \text{ gives } T^{adbc}. \text{ Second loop yields: } \Delta := \{3,4\}; \ \Delta^{(2,4,3)} := \{2,3\}; \ k := 2, \text{ since } 3 \prec 2; \ p := 4; \ (\epsilon_{\omega}, \omega) := -(3,4); \ (\epsilon_{\lambda}, \lambda) := -(2,4); \ K := \{\}. \text{ The algorithm finishes and the canonical configuration is } \epsilon_{\lambda} T^{i_1 \lambda^i i_2 \lambda^i i_3 \lambda^i i_4 \lambda} = -T^{adcb}.$

The algorithms to find strong generating set, basic orbit, Schreier vector, and trace for permutation groups are described in refs. [9] and [10]. The extension of these algorithms to work within the direct product $H \otimes S_n$ is straightforward if one uses the fact that a image of a point p under the action of (ϵ_{π}, π) is p^{π} . The product of permutations in S_n is naturally extended to the product of elements of $H \otimes S_n$.

The analysis of the complexity of the algorithm Canonical is the following. Algorithms to find basic orbit, Schreier vector and trace have an $O(n^2)$ bound. Since the algorithm Canonical performs n loops in the worst case, it is bounded by $O(n^3)$. A strong generating set for symmetry S is required. It is known that Schreier-Sims algorithm has an $O(n^5)$ bound. So, if the generating set of S is not strong, the overall

bound for the algorithm to find the canonical form of tensors is $O(n^5)$, where n is the number of indices.

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