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ADVENTURES IN INVARIANT THEORY

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Abstract

We provide an introduction to enumerating and constructing invariants of group representations via character methods. The problem is contextualized via two case studies, arising from our recent work: entanglement invariants for characterizing the structure of state spaces for composite quantum systems; and Markov invariants, a robust alternative to parameter-estimation intensive methods of statistical inference in molecular phylogenetics.

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1. Introduction

What can the pursuits of (i) investigating quantum entanglement, via multicomponent wavefunctions, on the one hand, and (ii) studying frequency array data in order to infer species evolution in molecular phylogenetics, on the other – both hot topics in their respective fields – possibly have to do with one another? Quite a lot, as it turns out – as becomes clear, once the elegant connections with group representations and tensor analysis are made transparent. The following is an overview of some of the salient background, and a selection of applications of invariant theory to the respective topics, arising from our recent work in both areas (see, for example, Jarvis [15] and Sumner et al. [35]). The results which we report here provide novel instances of how group representation theory, and specifically classical invariant theory, can provide well-founded and useful tools in the realms of both quantum information and mathematical biology. In particular, the enumeration and identification of local unitary invariants, in the case of quantum systems, and Markov invariants, in the phylogenetic context, are of practical importance in characterizing general properties of the systems under study. In the quantum case, this is because they are by definition impervious to local

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unitary operations, and form the raw material for constructing interesting entanglement measures. In the phylogenetic case, the Markov invariants tend to be independent of how the specific Markov change model is parametrized, but nonetheless they can give information about the underlying tree.

Given a group G and a G-module V (a space carrying a linear G action, or representation), there is a standard construct $\mathbb{C}[V]$, the space of "polynomials in the components of the vectors in V". Natural objects of special interest in this space are the *invariants*, that is, functions $f(x)$ which are unchanged (up to scalar multiplication) under the action of G, $f(g \cdot x) = \lambda_g f(x)$. Of course, λ_g must be a one-dimensional representation, $\lambda_g \lambda_h = \lambda_{gh}$, and for the cases studied here, this will be realized by various matrix determinants.

We would like to characterize the sub-ring of invariants, $I(V) = \mathbb{C}[V]^G$. In view of the grading of $\mathbb{C}[V]$ by degree, the coarsest characterization is the associated Molien series, $h(z) = \sum_0^\infty h_n z^n$, with $h_n = \dim(\mathbb{C}[V]_n^G)$. In well-behaved cases, $I(V)$ has a regular structure (and is finitely generated), and $h(z)$ is a very pleasant rational function. For G semi-simple and compact, Molien's theorem [25] gives an integral representation of $h(z)$ via the Haar measure on G. Knowledge of $h(z)$ and of a set of generators of $I(V)$ is generally important for applications. For example, if V is the adjoint representation, with G semi-simple, Harish-Chandra's isomorphism [10] states that $I(V)$ is a polynomial ring, whose generators are nothing but the fundamental Casimir elements of the Lie algebra $\mathfrak{g} = L(G)$ of G. For a comprehensive introduction to the theory of representations and invariants of the classical groups see, for example, Goodman and Wallach [10]. We now turn to our discussion of applications.

2. Application I – quantum entanglement

In nonrelativistic quantum mechanics with continuous variable systems, we work with the Schrödinger representation, whose uniqueness is guaranteed by the celebrated Stone–von Neumann theorem (see, for example, Hall [12]). The V's are thus various complex L^2 spaces, and for multipartite systems, tensor products thereof. However, for purely "spin" systems, where the state space is spanned by a finite set of eigenstates of some selected observable quantity, the Hilbert spaces are simply finite-dimensional complex vector spaces, $V \cong \mathbb{C}^N$. Our interest here is in composite systems with K parts. In the context of quantum information, a subsystem with dimension D is referred to as a qu$D$it. Then, for K qu$D$its, $N = D^K$. The simplest example is the binary case $D = 2$ (corresponding to spin $-1/2$, for example, "up" or "down" electronic spin states in an atom), and we have K qubits, with V the K-fold tensor product $\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \cdots \mathbb{C}^2$ of dimension $N = 2^K$.

The quantum state of the system as a whole is described as usual by a vector in the total space V. In the spirit of quantum "thought experiments" we imagine experimenters Alice, Bob, Carol, . . . , and Karl who are each able to access only one subsystem. In the oft-described scenario of "spooky action at a distance", Alice, Bob, Carol, . . . , and Karl, despite remaining in their spatially separated labs, each manipulate their own subsystem independently, but observable outcomes between their measurements, and those in their colleagues' labs, are nonetheless not independent. The properties of each subsystem's quantum state in this case are correlated with those of the other $K - 1$ subsystems, and the overall state is described as *entangled*.

One strategy available to each of Alice, Bob, Carol, ... and Karl is simply to let his or her individual subsystem change under some time evolution, which can be engineered independently of the others. However, such local transformations do not affect the entanglement of the joint, K-party quantum state of the system as a whole. Hence, any proposed numerical measure of entanglement must be invariant under appropriate symmetry transformations. Since standard time evolution of quantum states is represented by unitary operators, entanglement measures should, therefore, be invariant under the Cartesian product of K unitary groups, each acting on one experimenter's qu$D$it Hilbert space. In the qubit case, then, the symmetry group is just $G = U(2) \times U(2) \times \cdots \times U(2)$ acting on the said K-fold tensor product space $V \cong \otimes^K \mathbb{C}^2$.

The invariants from $I(V)$ are perfectly suited for quantifying these local quantum effects resulting from unitary transformations, and are referred to as *local unitary invariants*. There is a great deal of interest in using these invariants to build complete entanglement measures[1] [37], and the first problem is to characterize and evaluate the invariants in different situations. A famous case in point for tripartite entanglement ($K = 3$) is the use of the Cayley hyperdeterminant, which is called the *tangle* in the physics literature [6]. See Eltschka and Siewert [7] and Horodecki et al. [14] for recent reviews on quantum entanglement.

A less well-studied case is that of so-called mixed states, where the system itself is described in a statistical sense – an ensemble of electrons, each of whose members is an electron described by a state vector which is an equal superposition of spin "up" and spin "down", is physically very different from an ensemble wherein, in 50% of instances the electron spin is "up", and in the other 50% the electron spin is "down". The state is now specified by a density operator (a self-adjoint positive semidefinite linear operator on V of unit trace[2]), and hence, transforms in the adjoint representation, equivalent to the tensor product $V \otimes V^*$ of the defining representation with its contragradient. Even just for $K = 2$ (that is, for *two* qubit mixed states), the structure of the invariant ring is quite rich, for example being considerably more complicated than the *four* qubit pure state case [36]. The Molien series [11, 19, 24]

$$h(z) = \frac{1 + z^4 + z^5 + 3z^6 + 2z^7 + 2z^8 + 3z^9 + z^{10} + z^{11} + z^{15}}{(1 - z)(1 - z^2)^3(1 - z^3)^2(1 - z^4)^3(1 - z^6)}$$

[1]More general procedures open to Alice, Bob, Carol, ... and Karl involve various types of general quantum operations (measurements). For example, under reversible operations which succeed only with some probability less than one, the transformation group on each subsystem would be extended from $U(2)$ to $\mathrm{GL}(2, \mathbb{C})$, and the group as a whole would become $\times^K \mathrm{GL}(2, \mathbb{C})$. Of course, such local transformations do modify state entanglement, although numerical measures which are bona fide *entanglement monotones* are defined to be *nonincreasing* under such changes [37].

[2]An example may be the convex sum of two orthogonal projectors, $\lambda\mathbb{P} + (1 - \lambda)\mathbb{P}^{\perp}$.

enumerates a plethora of primary and secondary invariants, whose precise role in the formulation of suitable entanglement measures, is still not completely elucidated [11, 24]. For partial results on the mixed two qutrit system ($D = 3$), see Jarvis [15].

3. Application II – phylogenetics

What of molecular phylogenetics? The simplest, so-called *general Markov model* of molecular evolution [3, 27] is given as follows. For a given set of K species (*taxonomic units*), a probabilistic description is adopted for some set of D observed characters (in the sense of quantifiable attributes, for the purpose of classifying phenotypes). Models are constructed, which describe the frequency of patterns derived from morphological features, or in molecular phylogenetics, from alignments of homologous nucleic acid sequences, with nucleotide bases $\{A, C, G, T\}$ with $D = 4$; or of homologous proteins, with amino acid residues denoted as $\{A, R, N, D, C, E, Q, G, H, I, L, K, M, F, P, S, T, W, Y, V\}$ with $D = 20$; or a variety of other molecular motifs or repeated units. These models are constructed by assuming molecular sequences evolving from a common ancestor via a Markov process, punctuated by speciation events (see, for example, Semple and Steel [27]). The data, corresponding to the observed frequencies, are taken as a sample of the probabilities on the basis that each site in the alignment independently follows an identical random process. These assumptions are contestable, but are well motivated by considerations of finding a balance between biological realism and statistical tractability.

Contained within this model is the description of the evolution of the K *extant* species and their characters. This is a process in which the K-way probability array, sampled by the pattern frequencies, evolves according to the tensor product of K independent $D \times D$ Markov transition matrices. This scenario is analogous to the set-up of quantum entanglement described above. Algebraically, it becomes an instance of the classical invariant theory problem, by extending the *set* of Markov matrices to the smallest containing matrix *group*. In the case of continuous-time models, there is no difficulty, since the matrices describing substitution *rates* between molecular units, formally belong to the relevant matrix Lie algebra [34, 35], and the Markov transition matrices are their matrix exponentials – and are, therefore, invertible. From this algebraic perspective, it also makes sense to work over $\mathbb{C}$ from the outset, and later examine stochastic parameter regions as required for applications. This will be elaborated through a specific example below.

The K-fold tensor product module $\mathbb{C}^D \otimes \mathbb{C}^D \otimes \cdots \otimes \mathbb{C}^D$ thus transforms under $G = GL_1(D) \times GL_1(D) \times \cdots \times GL_1(D)$, where the nonreductive group[1] $GL_1(D)$ is the Markov *stochastic group* of invertible $D \times D$ unit row-sum matrices [18, 26] ($GL_1(D)$ which is of course a matrix subgroup of $GL(D)$, and is isomorphic to the affine group Aff_{D-1} which is one-dimension lower; the *doubly stochastic* group is the

[1]This group is thus the workhorse of Markov models, playing a role analogous to $GL(D)$, which Weyl in his book [38] famously referred to as "her all-embracing majesty" amongst the classical groups.

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subgroup having unit row-sums *and* column-sums, and is isomorphic to $\mathrm{GL}(D-1)$ (see Appendix)). In this nonreductive case, there is no Molien theorem, and no guarantee of the invariant ring being finitely generated. However, there is no difficulty in counting one-dimensional representations degree by degree in tensor powers, and indeed, we have shown that a slightly modified version of the standard combinatorial results applies (see Appendix). In practical terms, this allows us to identify useful invariants for the purpose of phylogenetic inference. In this context, we call such objects *Markov invariants*.

One such quantity, the so-called `logDet`, has been known and used by phylogenetic practitioners for over two decades [3, 21, 23]. For the case of two taxonomic units (taxa), the determinant function of the 2-fold phylogenetic tensor array (a polynomial of degree D) is certainly a one-dimensional representation under the action of $\mathrm{GL}(D) \times \mathrm{GL}(D)$ itself, in fact transforming as $\mathrm{Det} \otimes \mathrm{Det}$, and thus necessarily an invariant of the Markov subgroup. Taking the negative logarithm, and with the usual matrix relation $\ln \mathrm{Det} = \mathrm{Tr} \ln$, we recover the negative of the sum of the diagonal rate generators, multiplied by the evolved time. With some further assumptions about the distribution of characters belonging to the presumed common ancestor of the two taxa, this can be taken as a measure of the total *evolutionary distance* between them, essentially the sum of all the individual rates changing characters into one another, multiplied by the time. The `logDet` can be recorded for all pairs of taxa, using marginalizations of the K-fold probability array, and thus leads to a robust *distance-based* method for phylogenetic inference. In fact, Buneman's theorem [4] guarantees reconstruction of a tree from a pairwise *metric* satisfying certain additional conditions.

Using our technical results, Markov invariants beyond the 2-fold case can be counted and constructed, and it is important to investigate them. Also, in data sets where the number of species K is large, and where the pairwise nature of `logDet` can lead to significant loss of evolutionary information, they may provide alternative or supplementary information to help with inference. In view of the previous discussion of quantum entanglement, it turns out that for the case of binary characters ($D = 2$), and threefold arrays ($K = 3$) or tripartite marginalizations of higher arity arrays, the Cayley hyperdeterminant (degree $n = 4$) is precisely such a candidate [30], and we have identified analogous low-degree tangles for $D = 3$ and 4 [31]. For four taxa, $K = 4$, and four characters, $D = 4$, we have found a remarkable, symmetrical set of three degree-five ($n = 5$) Markov invariants dubbed the *squangles* (stochastic quartet tangles) [13, 29, 32]. A simple least squares analysis of their values [13] allows a direct ranking of one of the three possible unrooted tree topologies for quartets[1]. The squangles provide a low-parameter and statistically powerful way of resolving quartets based on the general Markov model [13], without any special assumption on the types of rate matrices in the model, and independent of any recourse to pairwise distance measures. They are useful because many reconstruction methods for large trees build

[1] It is here that careful account of the stochastic parameter regime should be taken, since a crucial aspect of the least squares analysis requires certain inequalities to hold.

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a *consensus tree* from some kind of ranking of quartet subtrees, where robust decisions at the quartet level are absolutely crucial. Further details are given in the Appendix.

It must be noted that Markov invariants are in general distinct from the so-called *phylogenetic invariants* [5]. These are polynomials that evaluate to zero for a subset of phylogenetic trees, regardless of particular model parameters, and hence can serve in principle to discriminate trees from models. Their formal presentation can be given in terms of algebraic geometry [2, 20]. However, in contrast to Markov invariants which are one-dimensional G-modules, phylogenetic invariants, in general, belong to high-dimensional G-modules [1, 33].

Our Markov invariants are necessarily quite large objects – they are polynomials of reasonably high degree in a significant number of variables. For example, the squangles are polynomials of degree five in the components of a $4^4 = 256$-element array, and given their combinatorial origins, it is perhaps not surprising to find that they each have 66 744 terms (which is still $\ll O(256^5)$). However, once defined, there is no numerical problem with evaluations[1] – their utility is in their ability to syphon useful information out of the complexity of the data. As such, they provide a viable alternative to parameter-estimation intensive phylogenetic methods, where massive likely optimizations are required in order to make decisions about much more tightly specified models.

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Appendix. Counting invariants – some character theorems

The mathematical setting for both the study of entanglement measures for composite quantum systems, and of analogous quantities for the setting of phylogenetics, is that there is a model space V which is a K-fold tensor product, $V \cong \mathbb{C}^D \otimes \mathbb{C}^D \otimes \cdots \otimes \mathbb{C}^D$. In the case of quantum mechanics the components of V in some standard basis describe the state; for example, in standard Dirac notation a pure state is a ket $|\Psi\rangle \in V$ of the form $|\Psi\rangle = \sum_{j=1}^{K} \sum_{i_j=0}^{D-1} \Psi_{i_1 i_2 \cdots i_K} |i_1, i_2, \ldots, i_K\rangle$ in the case of qu$D$its (see, for example, Hall [12]). The case of mixed states will be treated presently. In the phylogenetic case, we simply have a K-way frequency array $\{P_{i_1 i_2 \cdots i_K}\}$ sampling the probability of a specific pattern, say $i_1 i_2 \cdots i_K$, where each $i_k \in \{A, C, G, T\}$ for nucleotide data at a particular site in a simultaneous alignment of a given homologous sequence across all K of the species under consideration.

[1]Explicit forms for the squangles, together with R code for their evaluation, are available from the authors.

We focus attention on the linear action of the appropriate matrix group $G = G_1 \times G_2 \times \cdots \times G_K$ on V. In the quantum qu$D$it case, each local group G_k is a copy of $U(D)$, but given the irreducibility of the fundamental representation, for polynomial representations the analysis can be done using the character theory of the complex group[1] $\mathrm{GL}(D, \mathbb{C})$. This group is too large for the phylogenetic case, where the pattern frequency array P evolves as $P \to P' = g \cdot P$, namely

$$P' = M_1 \otimes M_2 \otimes \cdots \otimes M_K \cdot P,$$

where each M_k belongs to the stochastic Markov group $\mathrm{GL}_1(D, \mathbb{C})$ (the group of nonsingular complex unit row-sum $D \times D$ matrices).

We compute the Molien series $h(z) = \sum_0^\infty h_n z^n$ for $\mathbb{C}[V]^G$ degree-by-degree using combinatorial methods based on classical character theory for $\mathrm{GL}(D)$, adapted slightly for the stochastic case $\mathrm{GL}_1(D)$, which we now describe. All evaluations are carried out using the group representation package ©`Schur` [39].

In terms of class parameters (eigenvalues) $x_1, x_2, \ldots, x_D$ for a nonsingular matrix $M \in \mathrm{GL}(D)$, that is, for the defining representation, the character is simply $\mathrm{Tr}(M) = x_1 + x_2 + \cdots + x_D$, and the contragradient has character $\mathrm{Tr}(M^{T\,-1}) = x_1{}^{-1} + x_2{}^{-1} + \cdots + x_D{}^{-1}$. Irreducible polynomial and rational characters of $\mathrm{GL}(D)$ are given in terms of the celebrated Schur functions [22, 38] denoted by $s_\lambda(x)$, where $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_D)$, $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_D$, is an integer partition of at most D nonzero parts. The length of the partition, $\ell(\lambda)$, is the index of the last nonzero entry, thus, $\ell(\lambda) = D$ if $\lambda_D > 0$. The weight of the partition, $|\lambda|$, is the sum $|\lambda| = \lambda_1 + \lambda_2 + \cdots + \lambda_D$, which we write as $\lambda \vdash |\lambda|$. The partition is visualized graphically as a Ferrers diagram, a left-justified array of boxes with decreasing row lengths corresponding to the parts of λ. For brevity, we write the Schur function simply as $\{\lambda\}$, when the class parameters are understood. Thus, the space V, which is a representation of G as a K-fold Cartesian product, is endowed with the corresponding product of K characters of the above defining representation of each local group, $\chi = \{1\} \cdot \{1\} \cdot \cdots \cdot \{1\}$ in the quantum mechanical pure state and stochastic cases. For the quantum mechanical mixed state case, the density operator ρ undergoes the transformation rule $\rho \to \rho' = g^{-1}\rho g$, with character $\chi = (\{1\}\{\overline{1}\}) \cdot (\{1\}\{\overline{1}\}) \cdot \cdots \cdot (\{1\}\{\overline{1}\})$ where again $\{1\}$ is the character of the defining representation, and $\{\overline{1}\}$ that of its contragradient. The space of polynomials of degree n in Ψ or P, $\mathbb{C}[V]_n$ (or $\mathbb{C}[V \otimes V^*]_n$ in the case of the density operator ρ), is a natural object of interest, and by a standard result, is isomorphic to the n-fold symmetrized tensor product $V \vee V \vee \cdots \vee V$, a specific case of a Schur functor, $\mathbb{S}_{\{n\}}(V)$ (or $\mathbb{S}_{\{n\}}(V \otimes V^*)$, in the mixed state case). Its character is determined by the corresponding Schur function *plethysm*, $\chi \underline{\otimes} \{n\}$, and the task at hand is to enumerate the one-dimensional representations occurring therein.

Before giving the relevant results it is necessary to note two further rules for combining Schur functions. The *outer* Schur function product is simply the pointwise

[1]This technical point differs from the previous comment about extending the analysis to local quantum operations and communication of these between parties, and the role of the general linear group therein.

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product of Schur functions, arising from the character of a tensor product of two representations. Of importance here is the *inner* Schur function product "$*$" defined via the Frobenius mapping between Schur functions and irreducible characters of the symmetric group. We provide here only the definitions sufficient to state the required counting theorems in technical detail. For a more comprehensive, Hopf-algebraic setting for symmetric functions and characters of classical (and some nonclassical) groups, see the papers by Fauser and Jarvis [8] and Fauser et al. [9].

We introduce structure constants for inner products in the Schur function basis as follows:

$$\{\lambda\} * \{\mu\} = \begin{cases} \sum_\nu g^\nu_{\lambda,\mu}\{\nu\}, & |\lambda| = |\mu|, \\ 0, & |\lambda| \neq |\mu|. \end{cases}$$

For partitions λ, μ of equal weight, this expresses the reduction of a tensor product of two representations of the symmetric group $\mathfrak{S}_n$ labelled by partitions λ, μ. By associativity, we can extend the definition of the structure constants to K-fold inner products,

$$\{\tau_1\} * \{\tau_2\} * \cdots * \{\tau_K\} = \sum_\nu g^\nu_{\tau_1,\tau_2,\ldots,\tau_K}\{\nu\}.$$

Theorem A.1 (Counting invariants).

(a) *Quantum pure states. Let D divide n, $n = rD$, and let τ be the partition (r^D) (that is, with Ferrers diagram a rectangular array of r columns of length D). Then*

$$h_n = g^{(n)}_{\tau,\tau,\ldots,\tau} \quad (K\text{-}\,fold\ inner\ product).$$

If D does not divide n, then $h_n = 0$.

(b) *Quantum mixed states. We have*

$$h_n = \sum_{|\tau|=n,\ell(\tau)\leq D^2} \Big(\sum_{|\sigma|=n,\ell(\sigma)\leq D} g^\tau_{\sigma,\sigma} \Big)^2.$$

(c) *Phylogenetic K-way pattern frequencies, general Markov model. We have*

$$h_n = g^{(n)}_{\tau_1,\tau_2,\ldots,\tau_K} \quad (K\text{-}fold\ inner\ product)$$

for each τ_k of the form $(r_k + s_k, r_k^{(D-1)})$ such that $n = r_k D + s_k$, $s_k \geq 0$.

(d) *Phylogenetic K-way pattern frequencies, doubly stochastic model. We have*

$$h_n = g^{(n)}_{\tau_1,\tau_2,\ldots,\tau_K} \quad (K\text{-}fold\ inner\ product)$$

for each τ_k of the form $(r_k + s_k, r_k^{(D-2)}, t_k)$ such that $n = r_k(D-1) + s_k + t_k$, $0 \leq t_k \leq r_k$, $s_k \geq 0$. □

An example of identifying invariants is the case of the three squangle quantities. We find $g^{(5)}{}_{\tau\tau\tau\tau} = 4$, where τ is the partition $(2, 1, 1, 1) \equiv (2, 1^3)$ which is of course of dimension 4 and irreducible in GL(4), but indecomposable in $\mathrm{GL}_1(4)$, as it contains a one-dimensional representation. One of the four linearly independent degree-five candidates is discounted because of algebraic dependence on lower-degree invariants. Recourse to the appropriate quartet tree isotropy group [32] reveals that one of the remaining three is not tree-informative. Further, the situation with respect to the final two objects is expressed symmetrically in terms of the *three* squangle quantities, Q_1, Q_2, Q_3, which satisfy $Q_1 + Q_2 + Q_3 = 0$, as follows. For tree one, for example, 12|34, we have on evaluation with stochastic parameters, $Q_1 = 0$, and $-Q_3 = Q_2 > 0$. This pattern recurs cyclically for the other two unrooted quartet trees: for tree 2, 13|24, $Q_2 = 0$, whereas $-Q_1 = Q_3 > 0$, and for tree 3, 14|23, $Q_3 = 0$, and $-Q_2 = Q_1 > 0$. As noted above, the strict inequalities entailed in the above evaluations are crucial for the validity of the least squares method for ranking quartet trees using squangles.

There are many more gems to be examined amongst Markov invariants for different models and subgroups [16, 17], with potential practical and theoretical interest. As one instance of as yet unexplored terrain for $K = 3$, we have evidence [28, 29] at degree eight for stochastic tangle (*stangle*) invariants with mixed weight, since it turns out that

$$g^{(8)}_{(51^3),(2^4),(2^4)} = 1 \quad (\equiv g^{(8)}_{(2^4),(51^3),(2^4)} \equiv g^{(8)}_{(2^4),(2^4),(51^3)}).$$

Thus, there are three mixed weight stangle candidates, which differ in the information they reveal about each leg of their ancestral star tree.

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