Computing Moment Polytopes of Tensors, with Applications in Algebraic Complexity and Quantum Information

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Computing Moment Polytopes of Tensors, with Applications in Algebraic Complexity and Quantum Information[*]

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Abstract

Tensors play a central role in various areas of computer science and mathematics, such as algebraic complexity theory (matrix multiplication), quantum information theory (entanglement), and additive combinatorics (slice rank). Fundamental problems about tensors are strongly tied to well-known questions in computational complexity — such as the problem of determining the matrix multiplication exponent via asymptotic rank, and the stronger Strassen asymptotic rank conjecture, which has recently been intimately linked to a whole range of computational problems.

Unlike matrices, which are often well understood through their rank, tensors have such intricate structure that understanding them (and aforementioned problems) requires information of a more subtle nature. The moment polytope, going back decades to work in symplectic geometry, invariant theory, and representation theory, is a mathematical object associated to any tensor that collects such "rank-like" information. Their relevance has become apparent in several areas: (1) through applications in geometric complexity theory (GCT), (2) in the construction of functions in Strassen's asymptotic spectrum of tensors, (3) as entanglement polytopes in quantum information theory, and (4) in optimization via scaling algorithms.

Despite their fundamental role and interest from many angles, little is known about these polytopes, and in particular for tensors beyond $\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$ and $\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$ only sporadically have they been computed. Even less is known about the polytopes' inclusions and separations (which are particularly relevant for applications).

We give a new algorithm for computing moment polytopes of tensors (and in fact moment polytopes for a natural general class of reductive algebraic groups) based on a mathematical characterization of moment polytopes by Franz. This algorithm enables us to compute moment polytopes of tensors of dimension an order of magnitude larger than previous methods, allowing us to compute with certainty, for the first time, all moment polytopes of tensors in $\mathbb{C}^3 \otimes \mathbb{C}^3 \otimes \mathbb{C}^3$, and with high probability those in $\mathbb{C}^4 \otimes \mathbb{C}^4 \otimes \mathbb{C}^4$.

Towards an open problem in geometric complexity theory, we prove (guided by moment polytopes computed with our algorithm) separations between the moment polytopes of matrix multiplication tensors and unit tensors, showing in particular that the matrix multiplication moment polytopes are not maximal (i.e., not equal to the corresponding Kronecker polytopes).

As a consequence of the above, we obtain a no-go result for a certain operational characterization of moment polytope inclusion, by proving that Strassen's asymptotic restriction on tensors does not imply moment polytope inclusion.

Finally, based on our algorithmic observations, we construct explicit (concise) non-free tensors in every format $\mathbb{C}^n \otimes \mathbb{C}^n \otimes \mathbb{C}^n$, thus solving a "hay in a haystack" problem for this generic property that plays an important role in Strassen's theory of asymptotic spectra.

CCS Concepts

• **Computing methodologies** → **Algebraic algorithms**; • **Mathematics of computing** → **Mathematical software**; • **Theory of computation** → *Algebraic complexity theory*.

Keywords

Tensors, moment polytopes, algebraic complexity theory, quantum information theory, algorithms, matrix multiplication, border subrank, tensor networks, matrix product states (MPS), Kronecker polytope, asymptotic restriction, free tensors

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1 Introduction

Tensors play a central role in various areas of computer science and mathematics, such as algebraic complexity theory, quantum information theory, and additive combinatorics [12, 16, 29, 55]. Indeed, fundamental open problems about tensors are strongly tied to questions in computational complexity. A well-known such problem is to determine the matrix multiplication exponent, which corresponds to the asymptotic rank of the matrix multiplication tensor. This problem has been studied for decades from many angles (computational, geometric, algebraic) [3, 14, 20, 53, 54, 63, 65, 77]. The theory developed for these tensors has carved out classes of tensors with special, relevant properties (e.g., tight and free tensors [29, 30, 68]). A central conjecture in this area is Strassen's asymptotic rank conjecture, which has long been known to be intimately linked to the matrix multiplication exponent, and a recent burst of results has developed a range of strong connections between this conjecture and problems in computational complexity theory [10, 11, 47, 59]. Related to this, often described as "finding hay in a haystack", it is an open problem to construct explicit tensors that have large tensor rank (despite random tensors having that property!); achieving this would have far-reaching consequences [13, 60]. In quantum information theory, tensors are the natural formalism to study multipartite entangled quantum states, their applications, and relations under local operations, leading to fundamental problems like the quantum marginal problem [25, 33, 41, 45, 51, 73, 76].

Whereas matrices are understood through simple invariants like their rank, tensors have such intricate structure and relations that understanding them (and aforementioned problems) requires information of a richer nature. The *moment polytope* is a mathematical object associated to any tensor that collects such fundamental "rank-like" information, in a precise sense that allows several different characterizations. Going back decades to fundamental work in symplectic geometry, invariant theory, and representation theory [15, 48, 56, 57], the relevance of moment polytopes has become apparent in several areas:

- in algebraic complexity theory as potential *obstructions* in geometric complexity theory (GCT) [20] (through understanding inclusions and separations between moment polytopes),
- as the basis for the construction of elements in Strassen's *asymptotic spectrum* [27, 65] (the subject of Strassen's duality theorem for asymptotic rank and the matrix multiplication exponent),
- in quantum information as *entanglement polytopes* that characterize entanglement in terms of the reachable quantum marginals [75], and
- in optimization through a class of algorithms called *scaling algorithms*, which optimize over such polytopes [17–19, 34, 38, 44].

Despite their fundamental role and the interest they have received from mathematical and computational angles, much is still unknown about moment polytopes. In particular, they are notoriously hard to compute. For tensors beyond $\mathbb{C}^2\otimes\mathbb{C}^2\otimes\mathbb{C}^2$ [42, 62, 75] and $\mathbb{C}^2\otimes\mathbb{C}^2\otimes\mathbb{C}^2\otimes\mathbb{C}^2$ [75] only sporadically have they been determined. Moreover, little is known about inclusions and separations between moment polytopes, and about their operational meaning, which is particularly relevant for aforementioned applications.

In this paper, based on a characterization of moment polytopes by Franz [36] we introduce an algorithm to compute moment polytopes of tensors and more general group representations. This algorithm computes for the first time the moment polytopes of all tensors in $\mathbb{C}^3\otimes\mathbb{C}^3\otimes\mathbb{C}^3$ with certainty (in seconds), as well as those in $\mathbb{C}^4\otimes\mathbb{C}^4\otimes\mathbb{C}^4$ with high probability. A new tool in the "moment polytope toolbox", this algorithm, and in particular the resulting concrete description of all moment polytopes in these shapes, can form a starting point for proving new structural results on moment polytopes. As one such result, we separate moment polytopes of matrix multiplication tensors from moment polytopes of unit tensors for a certain range of sizes. This is the first progress towards an open problem in geometric complexity theory [20, Problem 7.3] of determining these polytopes and their relations. In quantum information theory, this result implies that three pair-wise shared Einstein–Podolski–Rosen (EPR) pairs do not have the largest possible entanglement polytope, and thus cannot exhibit the full range of local marginals under stochastic local operations and classical communication (SLOCC). These separations moreover lead to upper bounds on border subrank (and subsequently, with more work, a different proof of the optimal border subrank result of [52]); we leave it as an open problem to determine the full power of separations obtained by moment polytopes. As a consequence we also obtain a no-go result on the operational meaning of moment polytope inclusion. Finally, we give, inspired by moment polytope data, the first construction of explicit non-free tensors (whose existence hitherto had only been established by dimension arguments [29]).

New results. Our results come in two parts: an algorithmic part and three structural results on moment polytopes.

- We give a new algorithm for computing moment polytopes of tensors based on a mathematical characterization by Franz [36], optimized for practical use and able to compute moment polytopes of tensors of dimension an order of magnitude larger than previous methods. This allows us to compute for the first time exactly all moment polytopes of tensors in $\mathbb{C}^3\otimes\mathbb{C}^3\otimes\mathbb{C}^3$ with certainty and in $\mathbb{C}^4\otimes\mathbb{C}^4\otimes\mathbb{C}^4$ with high probability. (Our algorithm is in fact much more general and applies to moment polytopes for general reductive groups acting by linear maps on finite-dimensional vector spaces.)
- Towards an open problem of Bürgisser and Ikenmeyer in geometric complexity theory [20], we prove (inspired by experimental data obtained using the above algorithm) separations between the moment polytopes of matrix multiplication tensors and unit tensors, showing in particular that the matrix multiplication moment polytopes are not maximal.
- As a consequence of the above, we obtain a no-go result for a certain operational characterization of moment polytope inclusion: we prove that Strassen's asymptotic restriction [66] on tensors does not imply moment polytope inclusion.
- Based on our algorithmic data, we construct explicit (concise) non-free tensors in every cubic format $\mathbb{C}^n\otimes\mathbb{C}^n\otimes\mathbb{C}^n$ for $n \geq 3$, thus solving a type of "hay in a haystack" problem for this generic property [29] that plays a central role in Strassen's theory of asymptotic spectra [27, 69].

2 Tensors, their Moment Polytopes, and Applications to Algebraic Complexity and Entanglement

We give here a brief overview of the context and background of this work on tensors and moment polytopes in various areas before we discuss our results in Section 3.

2.1 Tensors as Quantum States

In quantum information theory, tensors describe pure quantum states of multipartite finite-dimensional quantum systems. For example, a tensor $T \in \mathbb{C}^a \otimes \mathbb{C}^b \otimes \mathbb{C}^c$ of norm one describes a pure quantum state of a quantum system composed of three local systems (also called subsystems) $\mathbb{C}^a, \mathbb{C}^b$, and $\mathbb{C}^c$. The tensor T describes the global state, including entanglement between the local systems. The local state in each system is described by a Hermitian linear operator on the local system. These linear operators are called *marginal* density matrices (akin to marginal distributions in probability theory), and they can be defined as taking the partial trace of $TT^* \in \mathbb{C}^{a\times a} \otimes \mathbb{C}^{b\times b} \otimes \mathbb{C}^{c\times c}$ with respect to the other two systems. For example, the marginal density matrix of the first system is a Hermitian matrix of shape $a \times a$.

A central goal in quantum information theory is to establish *entanglement monotones*. These are measures that cannot increase under local operations. Examples of such operations are: acting by unitary matrices on the local systems (LU), LU operations with classical communication (LOCC), and LOCC operations with nonzero success probability (SLOCC). Mathematically, SLOCC operations correspond to applying matrices A, B, and C on the local systems, via $S = (A \otimes B \otimes C)T$.

Moment polytopes are fundamental entanglement monotones, and hence are also called entanglement polytopes [75]. They succinctly describe constraints on which states the tensor T can be transformed into by SLOCC operations and taking limits. That is, we act by invertible matrices A, B, and C on T but allow also the limits of tensors obtained in this way. We denote the set of all such tensors by $\overline{(\mathrm{GL}_a \times \mathrm{GL}_b \times \mathrm{GL}_c)T}$, where GL_n denotes the invertible $n \times n$ matrices, and the line indicates we include limit points. The eigenvalues of the three Hermitian marginal density operators are real, and when the tensor has unit norm they also sum to one (hence form a probability distribution). Because we can diagonalize using LU operations, these eigenvalues classify the operators. Denote with $\mathrm{r}_1(T)$ the eigenvalues of the first marginal density matrix, sorted from big to small. Similarly define $\mathrm{r}_2(T)$ and $\mathrm{r}_3(T)$. Then we can define the *moment polytope* $\Delta(T)$ of T as

$$\Delta(T) = \left\{ \left(\mathrm{r}_1(S), \mathrm{r}_2(S), \mathrm{r}_3(S)\right) \,\middle|\, S \in \overline{\mathrm{GL} \cdot T},\ \|S\| = 1 \right\} \subseteq \mathbb{R}^a \times \mathbb{R}^b \times \mathbb{R}^c,$$

where $\mathrm{GL} := \mathrm{GL}_a \otimes \mathrm{GL}_b \otimes \mathrm{GL}_c$. Even for tensors of a relatively small size, determining the moment polytope can be rather difficult.

One particular motivation for studying moment polytopes comes from matrix product states (MPS) [1, 22, 28, 39, 40]. Consider a system with k sites arranged on a circle, and give each pair of adjacent systems one maximally entangled pair of dimension n; call the resulting tensor T. Then the MPS on k sites with bond dimension n are exactly those tensors which can be obtained from T by SLOCC. Thus, the moment polytope of T characterizes the collections of one-body marginal density operators that can be realized (or approximated arbitrarily closely) using MPS of the given bond dimension. We show that for any $k \geq 3$ and any $n \geq 2$, matrix product states obey interesting constraints on top of those that are inherent from being the marginal density operators of a (pure) quantum state. Our techniques and results may also lead to new insights in other connectivity scenarios for tensor networks [23].

As moment polytopes characterize the one-body marginal density operators reachable from of a multi-party quantum state, they can be used to witness many-particle entanglement from single-particle data [75]. This test has been used in experiments [2, 78], and is relevant in the understanding of Pauli's principle [4]. Up to now, such experiments have been limited to qubits, since the polytopes of larger dimensional tensors were not known; with our algorithm, we have been able to extend knowledge of these polytopes to three qutrits and further. The test could readily be used experimentally in order to witness new types of entanglement.

2.2 Algebraic Complexity Theory

In algebraic complexity theory, tensors correspond to bilinear computational problems [16]. Examples include the *matrix multiplication tensor* $\mathsf{M}_n \in \mathbb{C}^{n^2} \otimes \mathbb{C}^{n^2} \otimes \mathbb{C}^{n^2}$ describing the multiplication of two $n \times n$ matrices, the *polynomial multiplication tensors* $\mathsf{P}_{a,b} \in \mathbb{C}^a \otimes \mathbb{C}^b \otimes \mathbb{C}^{a+b-1}$ describing the multiplication of two univariate polynomials of degrees $a-1$ and $b-1$, and the *unit tensor* $\mathsf{U}_r := \sum_{i=1}^r e_i \otimes e_i \otimes e_i \in \mathbb{C}^r \otimes \mathbb{C}^r \otimes \mathbb{C}^r$ describing elementwise multiplication of two vectors of length r. The complexity of these problems corresponds to the number of required multiplications between the two inputs, which is called the *rank* of the tensor. *Restrictions* apply linear transformations to the inputs and the output separately, and we write $T \leq S$ whenever $T = (A \otimes B \otimes C)S$ for some matrices A, B, and C of suitable sizes. Whenever there exists a restriction $T \leq S$, this means we can compute T using as many multiplications between inputs as is required for S. Naturally, we may define the rank $\mathrm{R}(T)$ of T as the smallest $r \in \mathbb{N}$ such that $T \leq \mathsf{U}_r$.

A central open problem is to determine the asymptotic complexity of matrix multiplication. The goal is to determine the smallest (in the sense of infimum) real number ω such that $\mathrm{R}(\mathsf{M}_n) = O(n^\omega)$. This number is called the *matrix multiplication exponent* [64]. The best known upper bound is $\omega \leq 2.3721339\ldots$ [3], and the best known lower bound is $\omega \geq 2$.

An important property of matrix multiplication is its recursive structure. Indeed, block matrices can be multiplied block-wise. This property is observed in the tensor by the fact that the Kronecker product of two matrix multiplication tensors gives another matrix multiplication tensor: $\mathsf{M}_m \otimes \mathsf{M}_\ell = \mathsf{M}_{m\ell}$. As a consequence, knowing the behaviour of $\mathrm{R}(\mathsf{M}_2^{\otimes n})$ for large n allows us to determine ω. We define the *asymptotic rank* as $\underset{\sim}{\mathrm{R}}(T) := \lim_{n\to\infty} \mathrm{R}(T^{\otimes n})^{1/n}$, where the limit can be replaced by an infimum by Fekete's lemma. It can be shown that $\underset{\sim}{\mathrm{R}}(\mathsf{M}_2) = 2^\omega$. In fact, here M_2 can be replaced with any matrix multiplication tensor of fixed shape to characterize ω.

The moment polytope of T describes representation-theoretic properties of tensor powers $T^{\otimes n}$. These come in the form of discrete data given by triples of integer vectors $(\lambda, \mu, \nu) \in \mathbb{N}^a \times \mathbb{N}^b \times \mathbb{N}^c$ with non-negative and non-increasing entries that each sum to n

(Young diagrams). There exist natural projections of $T^{\otimes n}$ to certain tensors $[T^{\otimes n}]_{\lambda,\mu,\nu}$ with strong representation-theoretic or invariant-theoretic properties. The moment polytope of T describes the (λ, μ, ν) such that this projection is non-zero, each normalized to a triple of probability distributions, that is,

$$\Delta(T) = \overline{\left\{ \left(\frac{\lambda}{n}, \frac{\mu}{n}, \frac{\nu}{n}\right) \,\middle|\, (\lambda, \mu, \nu) \ \text{s.t.} \ \left[T^{\otimes n}\right]_{\lambda,\mu,\nu} \neq 0 \right\}}, \tag{2.1}$$

where the closure is the Euclidean closure. It turns out that among all moment polytopes $\Delta(T)$ for tensors in a given space $\mathbb{C}^a \otimes \mathbb{C}^b \otimes \mathbb{C}^c$ there is a maximal one (which is also obtained for "generic" tensors). This polytope is also known as the *Kronecker polytope*, called so because it captures precisely the asymptotic support of the Kronecker coefficients in the representation theory of the symmetric group [50, 71]. An important questions is as follows: *What are the moment polytopes of important computational problems?* This question was raised by Ikenmeyer and Bürgisser concerning specifically M_n and U_r [20]. They computed a related but different kind of polytope for these tensors and showed that they are maximal. We make progress towards answering their question for the moment polytopes proper by finding explicit points that are contained in the moment polytope of $\Delta(\mathsf{U}_r)$ but *not* in $\Delta(\mathsf{M}_n)$, for certain n, r, showing in particular that the moment polytope of the matrix multiplication tensor is *not* maximal.

2.3 Strassen's Asymptotic Spectrum and the Quantum Functionals

Moment polytopes play a central role in algebraic complexity theory in the construction of *quantum functionals* [27], which combines the geometric and representation-theoretic perspectives. The quantum functionals are a family of functions from k-tensors to $\mathbb{R}_{\geq 0}$, which map U_r to r for every $r \in \mathbb{N}$ and are monotone under restriction, multiplicative under Kronecker products, and additive under direct sums. The collection of all functions with these properties form the *asymptotic spectrum* of k-tensors [67]. The landmark result by Strassen tells us that given a tensor T, its asymptotic rank is equal to the supremum of $f(T)$ for all f in the asymptotic spectrum. More generally, the asymptotic spectrum characterizes the existence of so-called asymptotic restrictions between k-tensors.

It has proven to be a challenge to describe the asymptotic spectrum explicitly. For almost 30 years the only known points were the *flattening ranks*, until the construction of the quantum functionals [27]. The flattening ranks are defined by flattening the tensor into a matrix (in one of three possible ways) and computing the matrix rank. The *quantum functionals* are defined for 3-tensors T as $2^{E_\theta(T)}$ with $E_\theta(T) \coloneqq \max_{(p_1,p_2,p_3)\in\Delta(T)} \theta_1 H(p_1) + \theta_2 H(p_2) + \theta_3 H(p_3)$, where $(\theta_1, \theta_2, \theta_3)$ is any probability vector and H denotes the Shannon entropy. Quantum functionals have been used to show barrier results for the techniques used to prove upper bounds on the matrix multiplication exponent [26]. It is unknown whether the quantum functionals make up the entire asymptotic spectrum of 3-tensors. If the answer is yes, this would in particular imply the matrix multiplication exponent equals 2. Another notion relating strongly to the moment polytope is the G-stable rank [31].

The quantum functionals are maximizations of concave functions on the moment polytope, and can hence be computed in polynomial time using standard convex optimization techniques given efficient access to the moment polytope. Scaling algorithms [17, 18] provide suitable membership oracles which are effective in practice but are not known to run in polynomial time in all parameters. However, these optimization-based techniques do not yield a description of the moment polytopes in terms of vertices or inequalities. This presents a bottleneck, and indeed finding such a description even for not too large tensor shapes seems far out of reach for known methods. The moment polytopes of tensors of shape $2 \times 2 \times 2$ and $2 \times 2 \times 2 \times 2$ were computed via Eq. (2.1) and a complete understanding of the underlying invariant theory [75]; but such an understanding is not available in higher dimensions. We advance the computational state-of-the art significantly with our algorithm. In particular, our results allow us to compute for the first time the moment polytopes (and derived quantities) for all tensors of the shape $3 \times 3 \times 3$.

In the context of quantum information, the quantum functionals are monotones for asymptotic SLOCC. There is also an analogous theory for (asymptotic) LOCC [46, 74].

2.4 Non-Free Tensors

Strassen's *support functionals* [68] are a (continuously parametrized just like the quantum functionals) family of functions for which Strassen proved that, restricted to so-called *oblique* tensors, they are in the asymptotic spectrum. That is, the support functionals satisfy the properties listed above when restricted to oblique tensors. All examples of tensors we have discussed so far (e.g. M_n, U_r) are oblique. An interesting aspect of the support functionals is that they are defined over fields of positive characteristic as well [24].

Oblique tensors are a special case of free tensors, which are defined as follows. We say a support $\{(i, j, k) \mid T_{i,j,k} \neq 0\}$ is free when any two distinct elements (i, j, k) and (i', j', k') differ in at least two coordinates. We say T is a *free tensor* when its support is free after some change of basis, that is, if $(A \otimes B \otimes C)T$ has free support for some $(A, B, C) \in \mathrm{GL}_a \times \mathrm{GL}_b \times \mathrm{GL}_c$. Free tensors are a class of tensors that play a special role in several parts of the theory of moment polytopes and asymptotic spectra [36, 69]. For instance, it is known that the support functionals and quantum functionals coincide on free tensors [27]. This begs the following question: *Are the support functionals and quantum functionals equal also on tensors that are not free?*

To approach this question, we need a better understanding of non-free tensors. Via a dimension counting argument, it can be shown that (many) non-free tensors exist [29]. Indeed, a random tensor in $\mathbb{C}^n \otimes \mathbb{C}^n \otimes \mathbb{C}^n$ for $n \geq 4$ will be non-free almost surely. However, methods for verifying this for any explicitly generated random tensor have been lacking. In fact, before this paper, no explicit examples of non-free tensors were known. Such situations are common in mathematics and computer science for "generic" properties. For instance, we do not have explicit constructions of tensors with high tensor rank [13, 29, 60]. For non-freeness we solve this "hay in a haystack" problem in this paper by constructing explicit non-free tensor for every cubic tensor shape.

2.5 Polytope Inclusion

Given two tensors, we can ask whether their moment polytopes are included in one another. The inclusion of moment polytopes defines a relation between tensors that encodes inherent asymptotic and geometric information. At the same time, moment polytopes can be succinctly described via finitely many inequalities. This makes this relations interesting to study: *What inclusions and separations can we prove and using which techniques?* We algorithmically determine the moment polytopes of all $3\times3\times3$ tensors, revealing in particular all inclusions among them. Furthermore, we prove the moment polytope of the unit tensor is not contained in that of the matrix multiplication tensor of the same size. The above separation directly implies an upper bound on the so-called border subrank of matrix multiplication. This quantity is essential for constructions of matrix multiplication algorithms [12]. The techniques we use to prove this separation we then extend to give an alternative proof of the best possible upper bound on border subrank of matrix multiplication [52], and in particular establish new connections with polynomial multiplication tensors.

The asymptotic nature of moment polytopes and previous applications via the quantum functionals [27] suggests a connection to asymptotic restriction between tensors. Using the moment polytope relations and separations that we found, we show by counterexample that an a priori natural such connection is false.

3 Results

We now present our main results in more detail. Our first result is of algorithmic and experimental nature, namely an algorithm to compute concrete moment polytopes. This algorithm, while not poly-time in the dimension, is in particular able to compute the moment polytopes of any tensor in $\mathbb{C}^3\otimes\mathbb{C}^3\otimes\mathbb{C}^3$ with certainty and in $\mathbb{C}^4\otimes\mathbb{C}^4\otimes\mathbb{C}^4$ with high probability. The resulting data then led us to prove the structural results that we discuss below. We will further discuss the algorithm itself in Section 4.

3.1 Separation of Moment Polytope of Matrix Multiplication and Unit Tensors

Bürgisser and Ikenmeyer [20, Problem 7.3], motivated by the geometric complexity theory approach to lower bounds on the matrix multiplication exponent (as part of a more general program aimed at solving the VP vs. VNP problem), posed as a central open problem to determine the moment polytopes of the matrix multiplication tensors M_n and the unit tensors U_r. While a related (but different) kind of polytope were shown to coincide for M_n and U_{n^2}, no progress was made on computing or relating these moment polytopes since. We prove the following separations.

Theorem 3.1. *For every $c,n\in\mathbb{N}$ satisfying $n^2-n+1<c\le n^2$, there exists a point p_c such that $p_c\notin\Delta(\mathsf{M}_n)$ and $p_c\in\Delta(\mathsf{U}_c)$. In particular, the moment polytope of M_n is not maximal for any $n\ge2$.*

The point p_c that we obtain in our proof of Theorem 3.1 is given by $p_c\coloneqq(u_2,u_{c-1},u_c)$, where $u_m=\sum_{i=1}^m e_i/m\in\mathbb{R}^{n^2}$ is the uniform probability vector on the first m coordinates. The first instance of this separation (which we then extended to all n,c as above) was indeed obtained from our algorithmic data, which showed that the polytope of the 2×2 matrix multiplication tensor $\mathsf{M}_{2,2,2}$ is strictly smaller than the maximal polytope in $\mathbb{C}^4\otimes\mathbb{C}^4\otimes\mathbb{C}^4$, and in particular that the point $p_4=\big((\frac12,\frac12,0,0),(\frac13,\frac13,\frac13,0),(\frac14,\frac14,\frac14,\frac14)\big)$ was not included. Indeed, we prove that a point p_c of similar shape is a general separating point.

As an important ingredient for the proof of Theorem 3.1, we prove certain degenerations between matrix multiplication tensors and polynomial multiplication tensors $\mathsf{P}_{a,b}$ are not possible. We say a tensor T degenerates to a tensor S, denoted by $T\trianglerighteq S$, whenever S is a limit of restrictions from T. We show:

Lemma 3.2. *For $b>n\big(n-\lfloor\sqrt{a-1}\rfloor\big)$ we have $\mathsf{M}_n\not\trianglerighteq\mathsf{P}_{a,b}$.*

The border subrank of a tensor T is defined as the largest r such that $T\trianglerighteq\mathsf{U}_r$. Since $\mathsf{U}_{a+b-1}\trianglerighteq\mathsf{P}_{a,b}$ [16] and degeneration is a transitive relation, Lemma 3.2 directly implies the best possible upper bound for border subrank by choosing the optimal values for a and b, recovering (with a new proof) the result of [52, Theorem 3]: The border subrank of the $n\times n$ matrix multiplication tensor is upper bounded by $\lceil\frac34 n^2\rceil$, which matches the lower bound by Strassen [66]. In fact, the moment polytope separation in Theorem 3.1 immediately implies the weaker upper bound of n^2-n+1. We leave as an open problem whether the improved bound can be obtained from moment polytope separations alone.

In the context of quantum information theory, the matrix multiplication tensor M_n describes the quantum state of three quantum systems, with each pair sharing a generalized EPR pair $\sum_{i=1}^n e_i\otimes e_i$ (or many copies of EPR pairs if n is a power of 2). Then Theorem 3.1 tells us that there exists marginals that cannot be reached using SLOCC transformations. Moreover, these marginals can be reached starting from the generalized GHZ state U_c for all $c>n^2-n+1$. This shows in particular that M_n is not "maximally entangled" in the SLOCC setting, and it follows that the same is true in the LOCC and LU settings. This is an especially interesting result as such pair-wise shared EPR pairs form the basis for many applications in tensor network theory studying entanglement [22]. We show that the same holds for the iterated matrix multiplication tensor, which corresponds to pair-wise shared EPR pairs arranged on a cycle. In other words, matrix product states with bond dimension n satisfy extra constraints that are already visible on the level of their one-body marginal density operators.

3.2 Moment Polytopes are Not an Asymptotic Restriction Monotone

Moment polytopes are monotone under degeneration (if $T\trianglerighteq S$, then $\Delta(T)\supseteq\Delta(S)$), and they also have an asymptotic nature: the representation-theoretic description in Eq. (2.1) involves large Kronecker powers of a tensor. Motivated by understanding potential operational interpretations of moment polytope inclusion, it is natural to ask if asymptotic restriction implies moment polytope inclusion. We say a tensor T asymptotically restricts to a tensor S if $T^{\boxtimes n+o(n)}\ge S^{\boxtimes n}$, which we denote by $T\gtrsim S$. It is known that $T\trianglerighteq S$ implies $T\gtrsim S$. We show that moment polytopes are *not* monotone under asymptotic restriction:

Theorem 3.3. *There exist (explicit) tensors T and S such that $T\gtrsim S$ but $\Delta(T)\not\supseteq\Delta(S)$.*

As discussed, the quantum functionals are defined via an optimization problem over the moment polytope, and hence moment polytope inclusion implies monotonicity of the quantum functionals [27]. Strassen showed that $T \gtrsim S$ if and only if $f(T) \geq f(S)$ for all functions f in the asymptotic spectrum [67]. It is an important open problem to determine whether the quantum functionals make up the entire asymptotic spectrum for 3-tensors [27]; if this is not the case, it also directly implies Theorem 3.3.

In quantum information theory, Theorem 3.3 implies that an asymptotic SLOCC transformation from T to S does not imply that T is necessarily "more entangled" than S, in the following sense: there can exist collections of marginal density operators only reachable from S and not from T.

We give two examples of such pairs T and S in Theorem 3.3: the first is $T = \mathsf{M}_n$ and $S = \mathsf{U}_{n^2}$, and the second is $T = e_1 \wedge e_2 \wedge e_3$ and $S = \mathsf{U}_3$. The fact that the first pair is an example follows from the separation between the moment polytope of M_n and U_{n^2} of Theorem 3.1, as well as the known fact that the asymptotic subrank of M_n is n^2 [52, 66]. For the second pair, we use that the asymptotic subrank of T is known to equal 3. This follows from a characterization of asymptotic subrank for a subclass of so-called tight tensors by Strassen [68]. To separate the moment polytopes, we prove a correspondence between the *maxranks* of a tensor to the inclusion of specific points in its moment polytope. This correspondence was discovered through computational observations.

3.3 Explicit Non-Free Tensors of All Cubic Dimensions

Free tensors are a class of tensors that play a special role in several parts of the theory of moment polytopes and asymptotic spectra [36, 69]. As mentioned, for free tensors it is known the support functionals and quantum functionals coincide [27], but it is not known whether they are equal in general. This motivates the search for explicit examples of non-free tensors. Non-freeness is a generic property for sufficiently large n, as follows from a dimension argument [27, Remark 4.19]. In [29] the dimension of the Zariski-closure of the set of free tensors in $\mathbb{C}^n \otimes \mathbb{C}^n \otimes \mathbb{C}^n$ was determined exactly to be $4n^2 - 3n$. This implies that for every $n \geq 4$ non-free tensors exist in $\mathbb{C}^n \otimes \mathbb{C}^n \otimes \mathbb{C}^n$. However, no explicit non-free tensors were known. We construct explicit non-free tensors in every cubic shape of size $n \geq 3$. In particular, we establish that already for $n = 3$, non-free tensors exist, even though random tensors of that shape are free.

THEOREM 3.4. *For every $n \geq 3$, the following tensor in $\mathbb{C}^n \otimes \mathbb{C}^n \otimes \mathbb{C}^n$ is non-free:*

$$T = \sum_{i=1}^{n-1} \big(e_i \otimes e_i \otimes e_i + e_i \otimes e_n \otimes e_n\big) + \sum_{j=1}^{n-1} e_n \otimes e_j \otimes e_{j+1}.$$

Moreover, a generic tensor with support in $\{(i, j, j) : i, j \in [n-1]\} \cup \{(n, j, j+1) : j \in [n-1]\}$ is equivalent to T and hence non-free.

For example, for $n = 4$ this corresponds to the tensor

$$T = \left[\begin{array}{cccc|cccc|cccc|cccc} 1&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0 \\ 0&0&0&0&0&1&0&0&0&0&0&0&0&0&1&0 \\ 0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&1 \\ 0&0&0&1&0&0&0&1&0&0&0&1&0&0&0&0 \end{array}\right].$$

The construction of this family was inspired by the analysis of two tensors in $\mathbb{C}^3 \otimes \mathbb{C}^3 \otimes \mathbb{C}^3$, T_2 and T_5 (originating from the classification by Nurmiev [32, 58]), which turned out to be non-free. Central in our proof is a new general criterion for freeness in terms of the moment polytope: for tensors whose marginals map to the minimal norm point of their moment polytope, the tensor is free if and only if its support can be made free using a unitary change of bases. We prove this result using machinery from the symplectic-geometric viewpoint on moment polytopes. Our computational results allowed us to determine exactly the points of minimal norm of the moment polytopes of T_2 and T_5, and to construct the tensors in their respective orbits that map to these minimum-norm points. Disproving freeness of the support under unitary base changes afterwards is then feasible. Using Franz' characterization of the the moment polytope [36], we were able to generalize this construction to larger cubic shapes.

We observe numerically that for small instances of the non-free tensors constructed above the support functionals and quantum functionals coincide. The question whether these two functionals coincide or not in general remains open.

3.4 All Moment Polytopes of Tensors in $\mathbb{C}^3 \otimes \mathbb{C}^3 \otimes \mathbb{C}^3$

There is a classification of all tensors of this shape by Nurmiev [32, 58]. Notably, this classification contains families with continuous parameters. We were able to use our algorithms, along with analytical proofs that certain families have the largest possible moment polytope, to compute all moment polytopes for tensors in $\mathbb{C}^3 \otimes \mathbb{C}^3 \otimes \mathbb{C}^3$. Only the largest possible moment polytope (Kronecker polytope) was previously computed for $\mathbb{C}^3 \otimes \mathbb{C}^3 \otimes \mathbb{C}^3$ in [36] (and for $\mathbb{C}^4 \otimes \mathbb{C}^4 \otimes \mathbb{C}^4$ in [71]). Our computations in particular reveal all inclusion relations between the moment polytopes in this format. The results are available at [70].

4 Algorithm for Computing Moment Polytopes

We present an algorithm for computing the moment polytope of a tensor $T \in \mathbb{C}^a \otimes \mathbb{C}^b \otimes \mathbb{C}^c$ based on the description of moment polytopes by Franz [36], which characterizes moment polytopes in terms of the support of the tensor after applying lower-triangular matrices to the three factors, which we will now discuss.

Denote by $\mathrm{supp}(T)$ the set of vectors $(e_i, e_j, e_k) \in \mathbb{R}^a \times \mathbb{R}^b \times \mathbb{R}^c$ such that $T_{i,j,k} \neq 0$ and denote by $\mathcal{D}$ the set of triples of vectors with non-increasing entries (called *dominant* vectors) in $\mathbb{R}^a \times \mathbb{R}^b \times \mathbb{R}^c$. Write $\mathrm{conv}\, Q$ for the convex hull of a set Q. Then we define the *Borel polytope* of a tensor S as

$$\Delta_{\mathrm{B}}(S) \coloneqq \bigcap_{\substack{(A,B,C) \in \mathrm{GL} \\ \text{lower triangular}}} \mathrm{conv}\,\mathrm{supp}\big((A \otimes B \otimes C)S\big) \cap \mathcal{D} \tag{4.1}$$

where $\mathrm{GL} \coloneqq \mathrm{GL}_a \times \mathrm{GL}_b \times \mathrm{GL}_c$. Borel polytopes have a geometric and representation-theoretic description as well [17, 35]. From the representation-theoretic description it is possible to deduce that for every S in a dense subset of the orbit $\mathrm{GL} \cdot T$, we have $\Delta_{\mathrm{B}}(S) = \Delta(T)$. In fact, this dense subset is exactly described by the non-vanishing of a certain set of polynomials, and hence equality holds for a nonempty Zariski-open subset of $\mathrm{GL} \cdot T$.

Franz's description leads to an algorithm for computing moment polytopes. First generate a random element $S \in \mathrm{GL} \cdot T$, and then iterate over all possible supports, for each support checking whether it is attainable by lower-triangular action on S. This last step can be achieved by solving a polynomial system, and can be done using symbolic methods such as Gröbner basis computation. The result will then equal $\Delta(T)$ with high probability. The random element may also be described symbolically; in this way $\Delta(T)$ may be computed with certainty.

However, this approach quickly becomes unfeasible due to the exponential number of possible supports, and cannot go much beyond previous methods. The crucial insight is to instead focus on the inequalities defining $\Delta(T)$. The inequalities defining $\Delta(T)$ (e.g. the inequalities that are tight on some face of $\Delta(T)$) must all be defining for at least one of the finitely many terms occuring in the intersection in Eq. (4.1). We can characterize such inequalities combinatorially. The first step of our algorithm computes all of them and stores them into a finite set $\mathcal{H}$.

We call an inequality *attainable* for S whenever there exists lower triangular matrices (A, B, C) such that all elements of the support $\mathrm{supp}((A \otimes B \otimes C)S)$ satisfy the inequality. For step two of our algorithm we iterate over $\mathcal{H}$ and keep all $h \in \mathcal{H}$ that are attainable. The resulting inequalities $\mathcal{H}_S$ will define $\Delta_{\mathrm{B}}(S)$, after the straightforward intersection with $\mathcal{D}$. This describes the basic outline of the algorithms, which we summarize here:

Algorithm 1 Computing the moment polytope $\Delta(T)$.

Determine all candidate inequalities $\mathcal{H}$ (or retrieve from storage, since this only depends on the dimensions a, b, c).
Generate random (or symbolic) $S \in (\mathrm{GL}_a \times \mathrm{GL}_b \times \mathrm{GL}_c) \cdot T$.
Determine the attainable inequalities $\mathcal{H}_S \subseteq \mathcal{H}$ with respect to S using Gröbner bases.
Determine the polytope defined by $\mathcal{H}_S$ and intersect with $\mathcal{D}$.

We also provide a verification algorithm which determines if P equals $\Delta(T)$ for some polytope P without requiring iteration over the large set $\mathcal{H}$. It makes use of the *tensor scaling algorithm* as developed in [17] (cf. [18, 19, 34, 38]). Substantial further effort was required to translate the above procedure into a practical program. We briefly list a selection of the optimizations essential for making running times tractable.

- **Exploiting symmetries.** We make use of the permutation symmetries of the set of possible supports to greatly improve the running times for determining $\mathcal{H}$.
- **Filtering via point inclusions.** If we know beforehand a point $p \in \Delta(T)$, we can remove all inequalities from $\mathcal{H}$ that exclude it. This greatly reduces the amount of the expensive symbolic computations required when determining $\mathcal{H}_S$. For example, the point (e_1, e_1, e_1) is always included. Additionally, we prove (and use) that a notion called the *maxranks* of T leads to the inclusion of certain points in $\Delta(T)$.
- **Filtering generic inequalities.** Some inequalities are true for the moment polytope of any tensor in a given shape. These inequalities describe the Kronecker polytope, which has been computed in some cases. We use the Kronecker polytopes of shapes $3 \times 3 \times 3$ and $4 \times 4 \times 4$ as computed in [36, 71]. We can include all inequalities valid for it into $\mathcal{H}_S$ by default.
- **Modular arithmetic.** As discussed, we use Gröbner bases to determine attainability of inequalities. A known problem in Gröbner basis algorithms is that of intermediate coefficient swell [5], which can make computations infeasible due to memory and runtime issues. We solve the issue by computing Gröbner basis in some finite field $\mathbb{F}_q$ for a large random prime q, and argue for the feasibility of this heuristic.
- **Heuristics for polytope construction.** We observe that inequalities defining moment polytopes have low "complexity", in the sense that they are described by vectors with relatively small integer coefficients. By sorting the candidate inequalities in $\mathcal{H}$ based on their norm, we are likely to find all defining inequalities early in the loop over $\mathcal{H}$. We can construct an intermediate outer approximation of the polytope during the loop, and filter the remaining inequalities for redundancy.
  The same idea can be applied to greatly speed up vertex enumeration. Vertex enumeration for polyhedra is NP-hard in the unbounded case [49] (although for our setting of bounded polytopes, the complexity is open), and in particular implementations can be slow in scenarios when there are many redundant inequalities, as is the case for us.
- **Derandomization.** To verify the results with certainty, it is required to run Algorithm 1 using a symbolic element in the orbit of T. This greatly increases the hardness of the Gröbner basis computations, and in many cases makes it infeasible to perform them directly. However, the Gröbner bases for randomly generated S can provide structural information about this symbolic Gröbner basis. We use this fact to derandomize our results in concrete situations. In particular, we establish the polytopes of all tensors in $\mathbb{C}^3 \otimes \mathbb{C}^3 \otimes \mathbb{C}^3$ with certainty.

5 General Theory

Moment polytopes can be defined not just for tensors but for a broad range of groups and representations. We can replace the group $\mathrm{GL}_a \times \mathrm{GL}_b \times \mathrm{GL}_c$ with any reductive algebraic group, which can be modeled concretely by a subgroup G of GL_n, defined by polynomial equations, that is closed under taking conjugate transposes. This includes for instance all the complex classical Lie groups and products between them. We can replace the representation $\mathbb{C}^a \otimes \mathbb{C}^b \otimes \mathbb{C}^c$ by any rational representation of G, that is, by any action that is given by polynomials in the matrix entries of the group element and in $\det^{-1}$. This naturally captures applications such as the well-known Horn's problem [9, 34] and algorithmic problems of quiver representations [21, 37, 72], and it enables new ones, such as symmetric tensors (polynomials) in the setting of algebraic and geometric complexity theory [20]. Scaling algorithms generalize naturally to this general setting; see [18] for a structural and algorithmic account.

Our algorithm generalizes naturally to this setting, and almost all optimizations that we develop generalize as well. For example, the permutation symmetries on the set of possible supports corresponds to symmetries of the so-called Weyl group of G. Our algorithm can exploit these symmetries in the same way as we do for tensors.

6 Outlook

We believe that our algorithm for computing moment polytopes will be of independent interest for the discovery of relevant patterns towards examples and conjectures, and that this addition to the "moment polytope toolbox", alongside scaling algorithms, will be a useful tool for future work on moment polytopes. In particular, our algorithm brings moment polytope computation "up to speed" with general methods for Kronecker polytope computation, which is currently known up to $\mathbb{C}^4 \otimes \mathbb{C}^4 \otimes \mathbb{C}^4$ [71] (however, several special cases for Kronecker polytopes of other (incomparable) shapes are known as well [43, 50]).

Moment polytopes of tensors can have an exponential number of vertices and inequalities [17, 18, 37, 61]. Our algorithm does not improve over previous methods in terms of asymptotic complexity, only in terms of practicality, with the "experimental mathematics" goal in mind: generating computationally a large set of examples from which we can extract general results.

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