TENSOR NETWORK RANKS

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Abstract. In problems involving approximation, completion, denoising, dimension reduction, estimation, interpolation, modeling, order reduction, regression, etc, we argue that the near-universal practice of assuming that a function, matrix, or tensor (which we will see are all the same object in this context) has *low rank* may be ill-justified. There are many natural instances where the object in question has high rank with respect to the classical notions of rank: matrix rank, tensor rank, multilinear rank — the latter two being the most straightforward generalizations of the former. To remedy this, we show that one may vastly expand these classical notions of ranks: Given any undirected graph G, there is a notion of G-rank associated with G, which provides us with as many different kinds of ranks as there are undirected graphs. In particular, the popular tensor network states in physics (e.g., MPS, TTNS, PEPS) may be regarded as functions of a specific G-rank for various choices of G. Among other things, we will see that a function, matrix, or tensor may have very high matrix, tensor, or multilinear rank and yet very low G-rank for some G. In fact the difference is in the orders of magnitudes and the gaps between G-ranks and these classical ranks are arbitrarily large for some important objects in computer science, mathematics, and physics. Furthermore, we show that there is a G such that almost every tensor has G-rank exponentially lower than its rank or the dimension of its ambient space.

1. Introduction

A universal problem in science and engineering is to find a function from some given data. The function may be a solution to a PDE with given boundary/initial data or a target function to be learned from a training set of data. In modern applications, one frequently encounters situations where the function lives in some state space or hypothesis space of prohibitively high dimension — a consequence of requiring very high accuracy solutions or having very large training sets. A common remedy with newfound popularity is to assume that the function has low rank, i.e., may be expressed as a sum of a small number of separable terms. But such a low-rank assumption often has weak or no justification; rank is chosen only because there is no other standard alternative. Taking a leaf from the enormously successful idea of *tensor networks* in physics [4, 7, 13, 23, 28, 30, 31, 33, 34, 35, 36, 37, 38], we define a notion of G-rank for any undirected graph G. Like tensor rank and multilinear rank, which are extensions of matrix rank to higher order, G-ranks contain matrix rank as a special case.

Our definition of G-ranks shows that every tensor network — tensor trains, matrix product states, tree tensor network states, star tensor network states, complete graph tensor network states, projected entangled pair states, multiscale entanglement renormalization ansatz, etc — is nothing more than a set of functions/tensors of some G-rank for some undirected graph G. It becomes straightforward to explain the effectiveness of tensor networks: They serve as a set of 'low G-rank functions' that can be used for various purposes (as an ansatz, a regression function, etc). The flexibility of choosing G based on the underlying problem can provide a substantial computational advantage — a function with high rank or high H-rank for a graph H can have much lower G-rank for another suitably chosen graph G. We will elaborate on these in the rest of this introduction, starting with an informal discussion of tensor networks and G-ranks, followed by an outline of our main results.

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The best known low-rank decomposition is the *matrix rank decomposition*

$$f(x,y) = \sum_{i=1}^{r} \varphi_i(x)\psi_i(y) \tag{1}$$

that arises in common matrix decompositions such as LU, QR, EVD, SVD, Cholesky, Jordan, Schur, etc — each differing in the choice of additional structures on the factors φ_i and ψ_i. In higher order, say, order three for notational simplicity, (1) generalizes as *tensor rank decomposition*,

$$f(x,y,z) = \sum_{i=1}^{r} \varphi_i(x)\psi_i(y)\theta_i(z), \tag{2}$$

or as *multilinear rank decomposition*

$$f(x,y,z) = \sum_{i,j,k=1}^{r_1,r_2,r_3} \varphi_i(x)\psi_j(y)\theta_k(z). \tag{3}$$

Like (1), (2) and (3) decompose a function f into a sum of products of factors φ_i, ψ_j, θ_k, simpler functions that depend on fewer variables than f. This simple idea is ubiquitous, underlying the separation-of-variables technique in partial differential equations [3] and special functions [26], fast Fourier transforms [24], tensor product splines [5] in approximation theory, mean field approximations [14] in statistical physics, naïve Bayes model [22] and tensor product kernels [12] in machine learning, blind multilinear identification [21] in signal processing.

The decompositions (2) and (3) can be inadequate when modeling more complicated interactions, calling for *tensor network decompositions*. Some of the most popular ones include *matrix product states* (MPS) [44],

$$f(x,y,z) = \sum_{i,j,k=1}^{r_1,r_2,r_3} \varphi_{ij}(x)\psi_{jk}(y)\theta_{ki}(z),$$

tree tensor network states (TTNS) [31],

$$f(x,y,z,w) = \sum_{i,j,k=1}^{r_1,r_2,r_3} \varphi_{ijk}(x)\psi_i(y)\theta_j(z)\pi_k(w),$$

tensor train[1] (TT) [45],

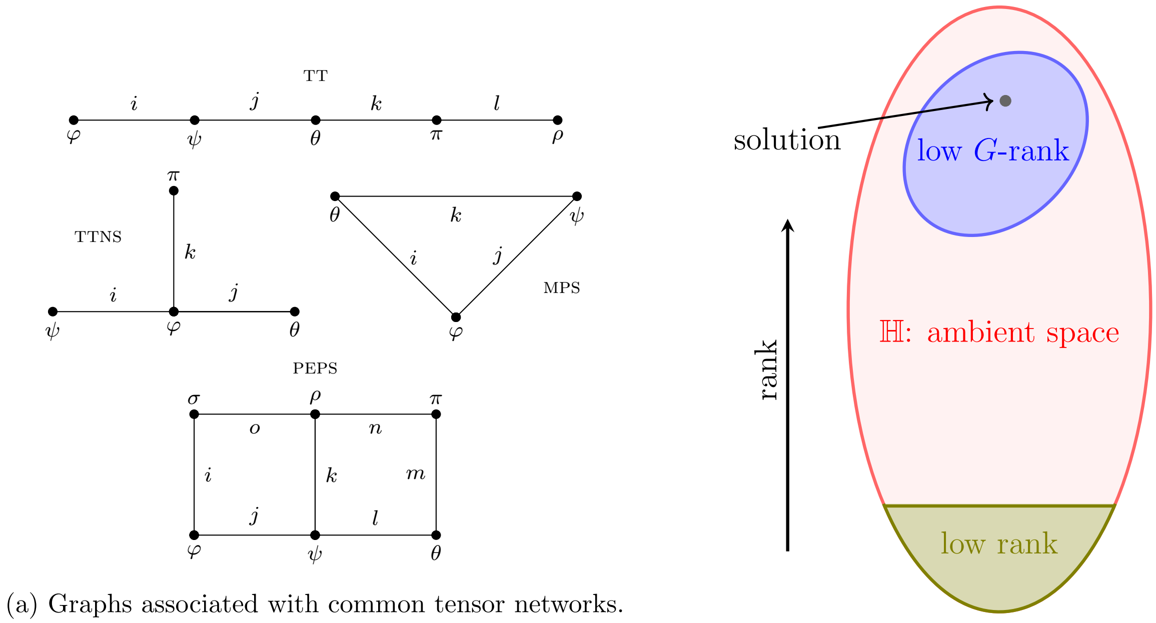
$$f(x,y,z,u,v) = \sum_{i,j,k,l=1}^{r_1,r_2,r_3,r_4} \varphi_i(x)\psi_{ij}(y)\theta_{jk}(z)\pi_{kl}(u)\rho_l(v),$$

and *projected entangled pair states* (PEPS) [33],

$$f(x,y,z,u,v,w) = \sum_{i,j,k,l,m,n,o=1}^{r_1,r_2,r_3,r_4,r_5,r_6,r_7} \varphi_{ij}(x)\psi_{jkl}(y)\theta_{lm}(z)\pi_{mn}(u)\rho_{nko}(v)\sigma_{oi}(w),$$

among many others. Note that all these decompositions, including those in (1), (2), (3), are of the same nature — they decompose a function into a sum of *separable functions*. Just as (2) and (3) differ in how the factors are indexed, tensor network decompositions differ from each other and from (2) and (3) in how the factors are indexed. Every tensor network decomposition is defined by an undirected graph G that determines the indexing of the factors. The graphs associated with MPS, TTNS, TT, and PEPS are shown in Figure 1a. The decompositions above represent the simplest non-trivial instance for each tensor network — they can become arbitrarily complicated with increasing *order*, i.e., the number of arguments of the function f or, equivalently, the number of vertices in the corresponding graphs. In Section 2, we will formally define tensor network states in a mathematically rigorous and, more importantly, coordinate-free manner — the importance of the latter stems from the avoidance of a complicated mess of indices, evident even in the simplest instance of PEPS above. For now, a *tensor network state* is an f that has a tensor network decomposition corresponding to a given graph G, and a *tensor network* corresponding to G is the set of all such functions.

[1]We are aware that tensor trains [29] have long been known in physics [45, 38, 37] and are often called matrix product states *with open boundary conditions* [28]. What we called matrix product states are known more precisely as matrix product states *with periodic boundary conditions* [28]. We thank our colleagues in physics for pointing this out to us on many occasions. In our article, we use the terms TT and MPS merely for the convenience of easy distinction between the two types of MPS. We will say more about our nomenclature after Definition 2.2.



(a) Graphs associated with common tensor networks.

(b) G-rank versus rank.

FIGURE 1. Every undirected graph G defines a G-rank. Solution that we seek may have high rank but low G-rank.

The minimum r in (1) gives us the matrix rank of f; the minimum r in (2) and the minimum (r_1, r_2, r_3) in (3) give us the *tensor rank* and *multilinear rank* of f respectively. Informally, the tensor network rank or G-rank of f may be similarly defined by requiring some form of minimality for $(r_1, \dots, r_c)$ in the other decompositions for MPS, TT, TTNS, PEPS (with an appropriate graph G in each case). Note that this is no longer so straightforward since (i) $\mathbb{N}^c$ is not an ordered set when $c > 1$; (ii) it is not clear that any function would have such a decomposition for an arbitrary G.

We will show in Section 4 that any d-variate function or d-tensor has a G-rank for any undirected connected graph G with d vertices. While this has been defined in special cases, particularly when G is a path graph (TT-rank [10]) or more generally when G is a tree (hierarchical rank [9, Chapter 11] or tree rank [2]), we show that the notion is well-defined for *any* undirected connected graph G: Given any d vector spaces $\mathbb{V}_1, \dots, \mathbb{V}_d$ of arbitrary dimensions, there is a class of tensor network states associated with G, as well as a G-rank for any $T \in \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$; or equivalently, for any function $f \in L^2(X_1 \times \cdots \times X_d)$; or, for those accustomed to working in terms of coordinates, for any hypermatrix $A \in \mathbb{C}^{n_1 \times \cdots \times n_d}$. See Section 2 for a discussion on the relations between these objects (d-tensors, d-variate functions, d-hypermatrices).

Formalizing the notions of tensor networks and G-ranks provides several advantages, the most important of which is that it allows one to develop a rich calculus for working with tensor networks: deleting vertices, removing edges, restricting to subgraphs, taking unions of graphs, restricting to subspaces, taking intersections of tensor network states, etc. We develop some of these basic techniques and properties in Sections 3 and 6, deferring to [39] the more involved properties that are not needed for the rest of this article. Among other advantages, the notion of G-rank also sheds light on existing methods in scientific computing: In hindsight, the algorithm in [41] is one that approximates a given tensor network state by those of low G-rank.

The results in Section 5 may be viewed as the main impetus for tensor networks (as we pointed out earlier, these are 'low G-rank tensors' for various choices of G):

- a tensor may have very high matrix, tensor, or multilinear rank and yet very low G-rank;
- a tensor may have very high H-rank and very low G-rank for $G \neq H$;

We will exhibit an explicit example where tensor rank, multilinear rank, matrix rank, and TT-rank are all $O(n^2)$ but whose MPS-rank is $O(n)$. In Section 6, we will see that there is a choice of G such that in a space of dimension $O(n^d)$, *almost every* tensor has G-rank $O\big(n(d-1)\big)$ and tensor rank $O\big(n^d/(nd-d+1)\big)$, i.e., for that particular G, almost every tensor has G-rank that is exponentially lower than its tensor rank or the dimension of its ambient space.

We will study in detail the simplest and most common G-ranks: TT-rank (G is a path graph) in Section 7, TTNS-rank (G is a tree) in Section 8, MPS-rank (G is a cyclic graph) in Section 9, paying particular attention to questions of uniqueness, existence of best low G-rank approximations, polynomial-time computability, dimensions, generic and maximal G-ranks, etc.

Some other insights that may be worth highlighting include:

- Any tensor network state is the contraction of a rank-one tensor (Section 2).
- G-rank is polynomial-time computable when G is acyclic (Section 8).
- A best low G-rank approximation always exists if G is acyclic (Section 8) but may not necessarily exist if G contains a cycle[2] (Section 9).
- G-ranks are distinct from tensor rank and multilinear rank in that neither is a special case of the other (Section 11) but G-ranks may be regarded as an 'interpolant' between tensor rank and multilinear rank (Section 4).

In Section 10, we determine G-ranks of decomposable tensors, decomposable symmetric and skew-symmetric tensors, monomials, W state, GKZ state, and the structure tensor of matrix-matrix product for various choices of G.

2. Tensor network states

We have left the function spaces in the decompositions in Section 1 unspecified. In physics applications where tensor networks were first studied [28], they are often assumed to be Hilbert spaces. For concreteness we may assume that they are all L^2-spaces, e.g., in MPS we have $\varphi_{ij} \in L^2(X)$, $\psi_{jk} \in L^2(Y)$, $\theta_{ki} \in L^2(Z)$ for all i, j, k and $f \in L^2(X \times Y \times Z) = L^2(X) \otimes L^2(Y) \otimes L^2(Z)$, although we may also allow for other function spaces that admit tensor product.

The reason we are not concern with the precise type of function space is that in this article we limit ourselves to finite-dimensional spaces, i.e., $X, Y, Z, \dots$ are finite sets and $x, y, z, \dots$ are discrete variables that take a finite number of values. In this case, it is customary[3] to identify $L^2(X) \cong \mathbb{C}^m$, $L^2(Y) \cong \mathbb{C}^n$, $L^2(Z) \cong \mathbb{C}^p$, $L^2(X \times Y \times Z) \cong \mathbb{C}^{m \times n \times p}$, where $m = \#X$, $n = \#Y$, $p = \#Z$, and write an MPS decomposition as a decomposition

$$A_{\text{MPS}} = \sum\nolimits_{i,j,k=1}^{r_1,r_2,r_3} a_{ij} \otimes b_{jk} \otimes c_{ki}, \tag{4}$$

where $A \in \mathbb{C}^{m \times n \times p}$, $a_{ij} \in \mathbb{C}^m$, $b_{jk} \in \mathbb{C}^n$, $c_{kl} \in \mathbb{C}^p$ for all i, j, k. In order words, in finite dimension, the function f is represented by a hypermatrix A and the factor functions φ_{ij}, ψ_{jk}, θ_{ki} are represented by factor vectors a_{ij}, b_{jk}, c_{kl} respectively. Henceforth we will use the word *factor* regardless of whether it is a function or a vector.

The same applies to other tensor networks when the spaces are finite-dimensional — they may all be regarded as decompositions of hypermatrices into sums of tensor products of vectors. For easy reference, we list the TTNS, TT, PEPS decompositions below:

$$A_{\text{TTNS}} = \sum\nolimits_{i,j,k=1}^{r_1,r_2,r_3} a_{ijk} \otimes b_i \otimes c_j \otimes d_k, \tag{5}$$

$$A_{\text{TT}} = \sum\nolimits_{i,j,k,l=1}^{r_1,r_2,r_3,r_4} a_i \otimes b_{ij} \otimes c_{jk} \otimes d_{kl} \otimes e_l, \tag{6}$$

$$A_{\text{PEPS}} = \sum\nolimits_{i,j,k,l,m,n,o=1}^{r_1,r_2,r_3,r_4,r_5,r_6,r_7} a_{ij} \otimes b_{jkl} \otimes c_{lm} \otimes d_{mn} \otimes e_{nko} \otimes f_{oi}, \tag{7}$$

[2] This was established in [17] for $G = C_3$, a 3-cycle; we show that it holds for any G that contains a d-cycle, $d \geq 3$.

[3] A vector $a \in \mathbb{C}^n$ is a function $f : \{1, \dots, n\} \to \mathbb{C}$ with $f(i) = a_i$; and a matrix/hypermatrix $A \in \mathbb{C}^{n_1 \times \cdots \times n_d}$ is a function $f : \{1, \dots, n_1\} \times \cdots \times \{1, \dots, n_d\} \to \mathbb{C}$ with $f(i_1, \dots, i_d) = a_{i_1 \cdots i_d}$ [20].

Note that A_{TTNS}, A_{TT}, A_{PEPS} are hypermatrices of orders 4, 5, 7 respectively. In particular we observe that the simplest nontrivial instance of PEPS already involve a tensor of order 7, which is a reason tensor network decompositions are more difficult than the well-studied decompositions associated with tensor rank and multilinear rank, where order-3 tensors already capture most of their essence.

From these examples, it is not difficult to infer the general definition of a tensor network decomposition *in coordinates*. Take any undirected graph $G = (V, E)$ and assign a positive integer weight to each edge. Then a tensor network decomposition associated with G may be constructed from the correspondence in Table 1.

Graph	*Tensor* (function/hypermatrix)	*Notation*
vertices	factors	$\varphi, \psi, \theta, \dots / a, b, c, \dots$
edges	contraction indices	$i, j, k, \dots$
degree of vertex	number of indices in each factor	$n_1, \dots, n_d$
weight of edge	upper limit of summation	$r_1, \dots, r_c$
number of vertices	order of tensor	d
number of edges	number of indices contracted	c

TABLE 1. How a graph determines a tensor network decomposition.

As we can see from even the simplest instance of PEPS above, a coordinate-dependent approach quickly run up against an impenetrable wall of indices. Aside from having to keep track of a large number of indices and their summation limits, we also run out of characters for labeling them (e.g., the functional form of the simplest instance of PEPS on p. 2 already uses up 20 Roman and Greek alphabets), requiring even messier sub-indices. We may observe that the label of a factor, i.e., $\varphi, \psi, \theta, \dots$ in the case of functions and $a, b, c, \dots$ in the case of vectors, plays no role in the decompositions — only its indices matter. This is the impetus behind physicists' Dirac notation, in which MPS, TTNS, TT, PEPS are expressed as

$$\begin{aligned}
A_{\text{MPS}} &= \sum\nolimits_{i,j,k=1}^{r_1,r_2,r_3} |i,j\rangle|j,k\rangle|k,i\rangle, \\
A_{\text{TTNS}} &= \sum\nolimits_{i,j,k=1}^{r_1,r_2,r_3} |i,j,k\rangle|i\rangle|j\rangle|k\rangle, \\
A_{\text{TT}} &= \sum\nolimits_{i,j,k,l=1}^{r_1,r_2,r_3,r_4} |i\rangle|i,j\rangle|j,k\rangle|k,l\rangle|l\rangle, \\
A_{\text{PEPS}} &= \sum\nolimits_{i,j,k,l,m,n,o=1}^{r_1,r_2,r_3,r_4,r_5,r_6,r_7} |i,j\rangle|j,k,l\rangle|l,m\rangle|m,n\rangle|n,k,o\rangle|o,i\rangle,
\end{aligned}$$

respectively. While this notation is slightly more economical, it does not circumvent the problem of indices. With this in mind, we will adopt a modern *coordinate-free* definition of tensor networks similar to the one in [17] that by and large avoids the issue of indices.

Let $G = (V, E)$ be an undirected graph where the set of d vertices and the set of c edges are labeled respectively by

$$V = \{1, \dots, d\} \quad \text{and} \quad E = \bigl\{\{i_1, j_1\}, \dots, \{i_c, j_c\}\bigr\} \subseteq \binom{V}{2}. \tag{8}$$

We will assign arbitrary directions to the edges:

$$\underline{E} = \bigl\{(i_1, j_1), \dots, (i_c, j_c)\bigr\} \subseteq V \times V$$

but still denote the resulting directed graph G for the following reason: Tensor network states depend only on the undirected graph structure of G — two directed graphs with the same underlying undirected graph give isomorphic tensor network states [17]. For each $i \in V$, let

$$\text{IN}(i) = \bigl\{j \in \{1, \dots, c\} : (j, i) \in \underline{E}\bigr\}, \qquad \text{OUT}(i) = \bigl\{j \in \{1, \dots, c\} : (i, j) \in \underline{E}\bigr\},$$

i.e., the sets of vertices pointing into and out of i respectively. As usual, for a directed edge (i, j), we will call i its head and j its tail.

The recipe for constructing tensor network states is easy to describe informally: Given any graph $G = (V, E)$, assign arbitrary directions to the edges to obtain $\underline{E}$; attach a vector space $\mathbb{V}_i$ to each vertex i; attach a covector space $\mathbb{E}_j^*$ to the head and a vector space $\mathbb{E}_k$ to the tail of each directed edge (j, k); do this for all vertices in V and all directed edges in $\underline{E}$; contract along all edges to obtain a tensor in $\mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$. The set of all tensors obtained this way form the tensor network states associated with G. We make this recipe precise in the following.

We will work over $\mathbb{C}$ for convenience although the discussions in this article will also apply to $\mathbb{R}$. We will also restrict ourselves mostly to finite-dimensional vector spaces as our study here is undertaken with a view towards computations and in computational applications of tensor networks, infinite-dimensional spaces are invariably approximated by finite-dimensional ones.

Let $\mathbb{V}_1, \dots, \mathbb{V}_d$ be complex vector spaces with $\dim \mathbb{V}_i = n_i$, $i = 1, \dots, d$. Let $\mathbb{E}_1, \dots, \mathbb{E}_c$ be complex vector spaces with $\dim \mathbb{E}_j = r_j$, $j = 1, \dots, c$. We denote the dual space of $\mathbb{V}_i$ by $\mathbb{V}_i^*$ (and that of $\mathbb{E}_j$ by $\mathbb{E}_j^*$). For each $i \in V$, consider the tensor product space

$$\Bigl(\bigotimes\nolimits_{j\in\textsc{in}(i)} \mathbb{E}_j\Bigr) \otimes \mathbb{V}_i \otimes \Bigl(\bigotimes\nolimits_{j\in\textsc{out}(i)} \mathbb{E}_j^*\Bigr) \tag{9}$$

and the contraction map

$$\kappa_G : \bigotimes\nolimits_{i=1}^{d} \Bigl[\Bigl(\bigotimes\nolimits_{j\in\textsc{in}(i)} \mathbb{E}_j\Bigr) \otimes \mathbb{V}_i \otimes \Bigl(\bigotimes\nolimits_{j\in\textsc{out}(i)} \mathbb{E}_j^*\Bigr)\Bigr] \to \bigotimes\nolimits_{i=1}^{d} \mathbb{V}_i, \tag{10}$$

defined by contracting factors in $\mathbb{E}_j$ with factors in $\mathbb{E}_j^*$. Since any directed edge (i, j) must point out of a vertex i and into a vertex j, each copy of $\mathbb{E}_j^*$ is paired with one and only one copy of $\mathbb{E}_j$, i.e., the contraction is well-defined.

Definition 2.1. A tensor in $\mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$ that can be written as $\kappa_G(T_1 \otimes \cdots \otimes T_d)$ where

$$T_i \in \Bigl(\bigotimes\nolimits_{j\in\textsc{in}(i)} \mathbb{E}_j\Bigr) \otimes \mathbb{V}_i \otimes \Bigl(\bigotimes\nolimits_{j\in\textsc{out}(i)} \mathbb{E}_j^*\Bigr), \qquad i = 1, \dots, d,$$

and κ_G as in (10), is called a *tensor network state* associated to the undirected graph G and vector spaces $\mathbb{V}_1, \dots, \mathbb{V}_d$, $\mathbb{E}_1, \dots, \mathbb{E}_c$. The set of all such tensor network states is called the *tensor network* and denoted

$$\begin{aligned}\textsc{tns}(G; \mathbb{E}_1, \dots, \mathbb{E}_c; \mathbb{V}_1, \dots, \mathbb{V}_d) \coloneqq \Bigl\{&\kappa_G(T_1 \otimes \cdots \otimes T_d) \in \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d : \\ &T_i \in \Bigl(\bigotimes\nolimits_{j\in\textsc{in}(i)} \mathbb{E}_j\Bigr) \otimes \mathbb{V}_i \otimes \Bigl(\bigotimes\nolimits_{j\in\textsc{out}(i)} \mathbb{E}_j^*\Bigr),\ i = 1, \dots, d\Bigr\}.\end{aligned}$$

We will always require that $\mathbb{E}_1, \dots, \mathbb{E}_c$ be finite-dimensional but $\mathbb{V}_1, \dots, \mathbb{V}_d$ may be of any dimensions, finite or infinite. Since a vector space is determined up to isomorphism by its dimension, when the vector spaces $\mathbb{E}_1, \dots, \mathbb{E}_c$ are unimportant (these play the role of contraction indices), we will simply denote the tensor network by $\textsc{tns}(G; r_1, \dots, r_c; \mathbb{V}_1, \dots, \mathbb{V}_d)$; or, if the vector spaces $\mathbb{V}_1, \dots, \mathbb{V}_d$ are also unimportant and finite-dimensional, we will denote it by $\textsc{tns}(G; r_1, \dots, r_c; n_1, \dots, n_d)$. As before, $n_i = \dim \mathbb{V}_i$ and $r_j = \dim \mathbb{E}_j$.

While we have restricted Definition 2.1 to tensor products of vector spaces $\mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$ for the purpose of this article, the definition works with any types of mathematical objects with a notion of tensor product: $\mathbb{V}_1, \dots, \mathbb{V}_d$ may be modules or algebras, Hilbert or Banach spaces, von Neumann or C^*-algebras, Hilbert C^*-modules, etc. In fact we will need to use Definition 2.1 in the form where $\mathbb{V}_1, \dots, \mathbb{V}_d$ are vector bundles in Section 3.

Since they will be appearing with some frequency, we will introduce abbreviated notations for the *inspace* and *outspace* appearing in (9): For each vertex $i = 1, \dots, d$, set

$$\mathbb{I}_i \coloneqq \bigotimes\nolimits_{j\in\textsc{in}(i)} \mathbb{E}_j \qquad \text{and} \qquad \mathbb{O}_i \coloneqq \bigotimes\nolimits_{j\in\textsc{out}(i)} \mathbb{E}_j^*. \tag{11}$$

Note that the image of every contraction map $\kappa_G(T_1 \otimes \cdots \otimes T_d)$ gives a decomposition like the ones we saw in (4)–(7). We call such a decomposition a *tensor network decomposition* associated with G. A tensor $T \in \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$ is said to be *G-decomposable* if it can be expressed as $T = \kappa_G(T_1 \otimes \ldots T_d)$ for some $r_1, \ldots, r_c \in \mathbb{N}$; a fundamental result here (see Theorem 4.1) is that:

> *Given any G and any $\mathbb{V}_1, \ldots, \mathbb{V}_d$, every tensor in $\mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$ is G-decomposable when $r_1, \ldots, r_c$ are sufficiently large.*

The tensor network $\operatorname{TNS}(G; r_1, \ldots, r_c; \mathbb{V}_1, \ldots, \mathbb{V}_d)$ is simply the set of all G-decomposable tensors for a fixed choice of $r_1, \ldots, r_c$. A second fundamental result (see Definition 4.3 and discussions thereafter) is that:

> *Given any G and any $T \in \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$, there is minimum choice of $r_1, \ldots, r_c$ such that $T \in \operatorname{TNS}(G; r_1, \ldots, r_c; \mathbb{V}_1, \ldots, \mathbb{V}_d)$.*

The undirected graph G can be extremely general. We impose no restriction on G — self-loops, multiple edges, disconnected graphs, etc — are all permitted. However, we highlight the following:

Self-loops: Suppose a vertex i has a self-loop, i.e., an edge e from i to itself. Let $\mathbb{E}_e$ be the vector space attached to e. Then by definition $\mathbb{E}_e$ and $\mathbb{E}_e^*$ must both appear in the inspace and outspace of i and upon contraction they serve no role in the tensor network state; e.g., for C_1, the single vertex graph with one self-loop, $\kappa_{C_1}(\mathbb{E}_e \otimes \mathbb{V}_i \otimes \mathbb{E}_e^*) = \mathbb{V}_i$. Hence self-loops in G have no effect on the tensor network states defined by G.

Multiple edges: Multiple edges $e_1, \ldots, e_m$ with vector spaces $\mathbb{E}_1, \ldots, \mathbb{E}_m$ attached have the same effect as a single edge e with the vector space $\mathbb{E}_1 \otimes \cdots \otimes \mathbb{E}_m$ attached, or equivalently, multiple edges $e_1, \ldots, e_m$ with edge weights $r_1, \ldots, r_m$ have the same effect as a single edge with edge weight $r_1 \cdots r_m$.

Degree-zero vertices: If G contains a vertex of degree zero, i.e., an isolated vertex not connected to the rest of the graph, then by Definition 2.1,

$$\operatorname{TNS}(G; r_1, \ldots, r_c; n_1, \ldots, n_d) = \{0\}. \tag{12}$$

Weight-one edges: If G contains an edge of weight one, i.e., a one-dimensional vector space is attached to that edge, then by Definition 2.1, that edge may be dropped. See Proposition 3.5 for details.

In particular, allowing for a multigraph adds nothing to the definition of tensor network states and we may assume that G is always a simple graph, i.e., no self-loops or multiple edges. However degree-zero vertices and weight-one edges will be permitted since they are convenient in proofs.

Definition 2.2. Tensor network states associated to specific types of graphs are given special names. The most common ones are as follows:

(i) if G is a path graph, then tensor network states associated to G are variously called *tensor trains* (TT) [29], *linear tensor network* [32], *concatenated tensor network states* [13], *Heisenberg chains* [37, 38], or *matrix product states with open boundary conditions*;
(ii) if G is a star graph, then they are called *star tensor network states* (STNS) [4];
(iii) if G is a tree graph, then they are called *tree tensor network states* (TTNS) [31] or *hierarchical tensors* [9, 10, 2];
(iv) if G is a cycle graph, then they are called *matrix product states* (MPS) [7, 30] or, more precisely, *matrix product states with periodic boundary conditions*;
(v) if G is a product of $d \geq 2$ path graphs, then they are called d-dimensional *projected entangled pair states* (PEPS) [33, 34];
(vi) if G is a complete graph, then they are called *complete graph tensor network states* (CTNS) [23].

We will use the term tensor trains as its acronym TT reminds us that they are a special case of tree tensor network states TTNS. This is a matter of nomenclature convenience. As we can see from the references in (i), the notion has been rediscovered many times. The original sources for what we call tensor trains are [37, 38] where they are called Heisenberg chains. In fact, as we have seen, tensor trains are also special cases of matrix product states. In some sources [28], the tensor trains in (i) are called "matrix product states with open boundary conditions" and the matrix product states in (iv) are called "matrix product states with periodic conditions."

FIGURE 2. Path graphs P_2, P_3, P_4, P_5. Each gives a TT decomposition.

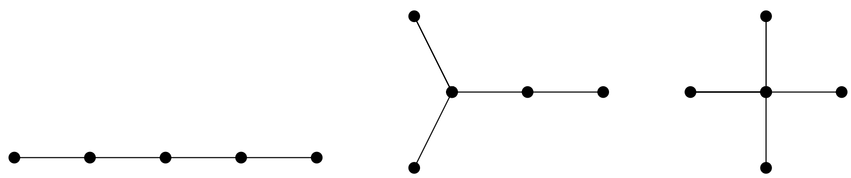


FIGURE 3. All five-vertex trees, including P_5 and S_5. Each gives a TTNS decomposition.

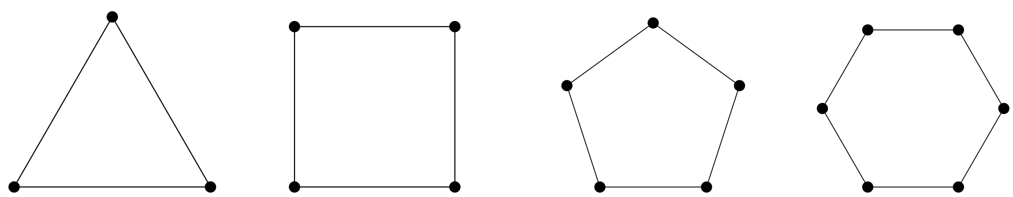


FIGURE 4. Cycle graphs C_3, C_4, C_5, C_6. Each gives an MPS decomposition.

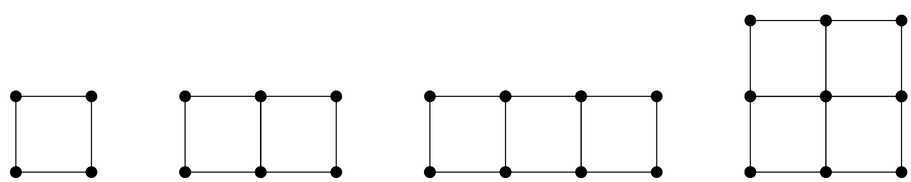


FIGURE 5. Four products of path graphs. Each gives a PEPS decomposition.

To illustrate Definition 2.1 for readers unfamiliar with multilinear algebraic manipulations, we will work out the MPS decomposition for the 3-vertex graph in Figure 1a and the PEPS decomposition from the 6-vertex graph in Figure 1a in full details.

Example 2.3 (MPS)**.** Let C_3 be the 3-vertex cycle graph for MPS in Figure 1a. We attach vector spaces $\mathbb{A}, \mathbb{B}, \mathbb{C}$ to the vertices labeled x, y, z respectively and vector spaces $\mathbb{D}, \mathbb{E}, \mathbb{F}$ to the edges labeled i, j, k respectively. $\operatorname{TNS}(C_3; \mathbb{D}, \mathbb{E}, \mathbb{F}; \mathbb{A}, \mathbb{B}, \mathbb{C})$, the set of MPS tensor network states corresponding to C_3, is obtained as follows. First, assign arbitrary directions to the edges, say, $x \xrightarrow{j} y \xrightarrow{k} z \xrightarrow{i} x$. Next, consider tensors

$$T_1 \in \mathbb{D} \otimes \mathbb{A} \otimes \mathbb{E}^*, \qquad T_2 \in \mathbb{E} \otimes \mathbb{B} \otimes \mathbb{F}^*, \qquad T_3 \in \mathbb{F} \otimes \mathbb{C} \otimes \mathbb{D}^*.$$

An MPS tensor network state is obtained by contracting factors in $\mathbb{D}$, $\mathbb{E}$, $\mathbb{F}$ with those in $\mathbb{D}^*$, $\mathbb{E}^*$, $\mathbb{F}^*$ respectively, giving us $\kappa_{C_3}(T_1 \otimes T_2 \otimes T_3) \in \mathbb{A} \otimes \mathbb{B} \otimes \mathbb{C}$. Let

$$\dim \mathbb{A} = n_1, \quad \dim \mathbb{B} = n_2, \quad \dim \mathbb{C} = n_3, \quad \dim \mathbb{D} = r_1, \quad \dim \mathbb{E} = r_2, \quad \dim \mathbb{F} = r_3.$$

Let $\{d_1, \dots, d_{r_1}\}$, $\{e_1, \dots, e_{r_2}\}$, $\{f_1, \dots, f_{r_3}\}$ be bases on $\mathbb{D}$, $\mathbb{E}$, $\mathbb{F}$; and $\{d_1^*, \dots, d_{r_1}^*\}$, $\{e_1^*, \dots, e_{r_2}^*\}$, $\{f_1^*, \dots, f_{r_3}^*\}$ be the corresponding dual bases on $\mathbb{D}^*$, $\mathbb{E}^*$, $\mathbb{F}^*$. Then

$$T_1 = \sum\nolimits_{i,j=1}^{r_1, r_2} d_i \otimes a_{ij} \otimes e_j^*, \quad T_2 = \sum\nolimits_{j,k=1}^{r_2, r_3} e_j \otimes b_{jk} \otimes f_k^*, \quad T_3 = \sum\nolimits_{k,i=1}^{r_3, r_1} f_k \otimes c_{ki} \otimes d_i^*.$$

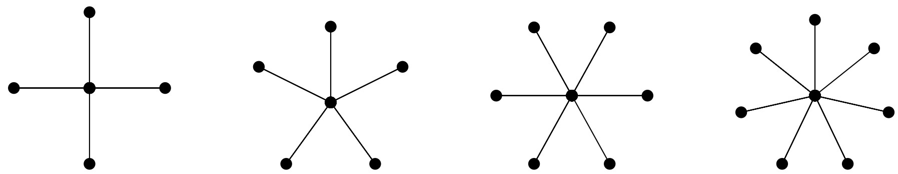


FIGURE 6. Star graphs S_5, S_6, S_7, S_8. Each gives a STNS decomposition.

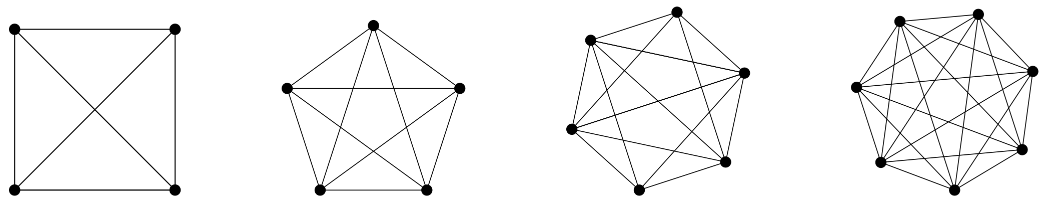


FIGURE 7. Complete graphs K_4, K_5, K_6, K_7. Each gives a CTNS decomposition.

We will derive the expression for T_1 for illustration: Let $a_1, \dots, a_{n_1}$ be a basis of $\mathbb{A}$. Then a tensor in $\mathbb{D} \otimes \mathbb{A} \otimes \mathbb{E}^*$ has the form

$$T_1 = \sum\nolimits_{i,k,j=1}^{r_1,n_1,r_2} \alpha_{ikj} d_i \otimes a_k \otimes e_j^*,$$

for some coefficients $\alpha_{ikj} \in \mathbb{C}$. We may then express T_1 as

$$T_1 = \sum\nolimits_{i,j=1}^{r_1,r_2} d_i \otimes \Bigl(\sum\nolimits_{k=1}^{n_1} \alpha_{ikj} a_k\Bigr) \otimes e_j^* = \sum\nolimits_{i,j=1}^{r_1,r_2} d_i \otimes a_{ij} \otimes e_j^*,$$

where $a_{ij} \coloneqq \sum_{k=1}^{n_1} \alpha_{ikj} a_k$. Finally we obtain the MPS decomposition as

$$\begin{aligned}
\kappa_{C_3}(T_1 \otimes T_2 \otimes T_3) &= \sum\nolimits_{i,i',j,j',k,k'=1}^{r_1,r_1,r_2,r_2,r_3,r_3} \kappa\bigl((d_i \otimes a_{ij} \otimes e_j^*) \otimes (e_{j'} \otimes b_{j'k} \otimes f_k^*) \otimes (f_{k'} \otimes c_{k'i'} \otimes d_{i'}^*)\bigr)\\
&= \sum\nolimits_{i,i',j,j',k,k'=1}^{r_1,r_1,r_2,r_2,r_3,r_3} d_{i'}^*(d_i)\, e_j^*(e_{j'})\, f_k^*(f_{k'}) \cdot a_{ij} \otimes b_{j'k} \otimes c_{k'i'}\\
&= \sum\nolimits_{i,i',j,j',k,k'=1}^{r_1,r_1,r_2,r_2,r_3,r_3} (\delta_{i,i'}\delta_{j,j'}\delta_{k,k'}) \cdot a_{ij} \otimes b_{j'k} \otimes c_{k'i'} = \sum\nolimits_{i,j,k=1}^{r_1,r_2,r_3} a_{ij} \otimes b_{jk} \otimes c_{ki},
\end{aligned}$$

where $\delta_{i,i'}$ denotes the Kronecker delta.

Example 2.4 (PEPS)**.** Let G be the 6-vertex graph for PEPS in Figure 1a. We attach vector spaces $\mathbb{V}_1, \dots, \mathbb{V}_6$ to the vertices labeled x, y, z, u, v, w and vector spaces $\mathbb{E}_1, \dots, \mathbb{E}_7$ to the edges labeled i, j, k, l, m, n, o respectively. $\operatorname{TNS}(G; \mathbb{E}_1, \dots, \mathbb{E}_7; \mathbb{V}_1, \dots, \mathbb{V}_6)$, the set of PEPS tensor network states, is obtained as follows. First, assign arbitrary directions to the edges, say, $x \xrightarrow{j} y \xrightarrow{l} z \xrightarrow{m} u \xrightarrow{n} v \xrightarrow{k} y$ and $v \xrightarrow{o} w \xrightarrow{i} x$. Next, consider tensors $T_i \in \bigl(\bigotimes_{j\in\operatorname{IN}(i)} \mathbb{E}_j\bigr) \otimes \mathbb{V}_i \otimes \bigl(\bigotimes_{j\in\operatorname{OUT}(i)} \mathbb{E}_j^*\bigr)$, i.e.,

$$\begin{aligned}
&T_1 \in \mathbb{E}_1 \otimes \mathbb{V}_1 \otimes \mathbb{E}_2^*, && T_2 \in (\mathbb{E}_2 \otimes \mathbb{E}_3) \otimes \mathbb{V}_2 \otimes \mathbb{E}_4^*, && T_3 \in \mathbb{E}_4 \otimes \mathbb{V}_3 \otimes \mathbb{E}_5^*,\\
&T_4 \in \mathbb{E}_5 \otimes \mathbb{V}_4 \otimes \mathbb{E}_6^*, && T_5 \in \mathbb{E}_6 \otimes \mathbb{V}_5 \otimes (\mathbb{E}_3^* \otimes \mathbb{E}_7^*), && T_6 \in \mathbb{E}_7 \otimes \mathbb{V}_6 \otimes \mathbb{E}_1^*.
\end{aligned}$$

Finally, we contract factors in $\mathbb{E}_j$ with those in $\mathbb{E}_j^*$, $j = 1, \dots, 6$, giving us $\kappa_G(T_1 \otimes \cdots \otimes T_6) \in \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_6$. If we choose bases on $\mathbb{E}_1, \dots, \mathbb{E}_7$, then we obtain the expression for a PEPS tensor network state in coordinates,

$$\kappa_G(T_1 \otimes \cdots \otimes T_6) = \sum\nolimits_{i,j,k,l,m,n,o=1}^{r_1,r_2,r_3,r_4,r_5,r_6,r_7} a_{ij} \otimes b_{jkl} \otimes c_{lm} \otimes d_{mn} \otimes e_{nko} \otimes f_{oi},$$

as in Example 2.3; here $r_j = \dim \mathbb{E}_j$.

We end this section with a simple observation.

Proposition 2.5. *For any undirected graph G with d vertices and c edges, $\operatorname{TNS}(G; r_1, \dots, r_c; \mathbb{V}_1, \dots, \mathbb{V}_d)$ is an irreducible constructible subset of $\mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$.*

Proof. Let $\mathbb{U}_i = \mathbb{I}_i \otimes \mathbb{V}_i \otimes \mathbb{O}_i$ for $i = 1, \dots, d$. Let X be the irreducible variety of decomposable tensors in $\mathbb{U}_1 \otimes \dots \otimes \mathbb{U}_d$, i.e., $X = \{T_1 \otimes \dots \otimes T_d \in \mathbb{U}_1 \otimes \dots \otimes \mathbb{U}_d : T_i \in \mathbb{U}_i,\ i = 1, \dots, d\}$. Since X is irreducible and κ_G is a morphism between two varieties, the image $\kappa_G(X) = \textsc{tns}(G; r_1, \dots, r_c; \mathbb{V}_1, \dots, \mathbb{V}_d)$ must be irreducible and constructible. □

The proof of this proposition also reveals the following illuminating insight, which in retrospect should have been obvious from (10) and Definition 2.1.

Corollary 2.6. *Every tensor network state is a tensor contraction of a rank-one tensor.*

3. Calculus of tensor networks

Let $\mathbb{N}$ and $\mathbb{N}_0$ denote the set of positive and nonnegative integers respectively. We will introduce some basic tools for manipulating tensor network states. We begin by introducing the notion of criticality, which will allow for various reductions of tensor network states.

Definition 3.1. Let $\textsc{tns}(G; r_1, \dots, r_c; n_1, \dots, n_d)$ be a tensor network and the notations be as in Definition 2.1. Set

$$m_i := \prod_{j \in \textsc{in}(i) \cup \textsc{out}(i)} r_j, \qquad i = 1, \dots, d.$$

A vertex $i \in V$ is called *subcritical* if $n_i < m_i$, *critical* if $n_i = m_i$, and *supercritical* if $n_i > m_i$. We say that $\textsc{tns}(G; r_1, \dots, r_c; n_1, \dots, n_d)$ is

(i) *subcritical* if $n_i \le m_i$ for all $i = 1, \dots, d$, and at least one inequality is strict;
(ii) *critical* if $n_i = m_i$ for all $i = 1, \dots, d$;
(iii) *supercritical* if $n_i \ge m_i$ for all $i = 1, \dots, d$, and at least one inequality is strict.

Let $\mathbb{V}$ be a n-dimensional vector space. For $k = 1, \dots, n$, we let $\operatorname{Gr}(k, \mathbb{V})$ denote the Grassmannian of k-dimensional subspaces of $\mathbb{V}$. For the special case, $\mathbb{V} = \mathbb{C}^n$, we write $\operatorname{Gr}(k, n)$ for the Grassmannian of k-planes in $\mathbb{C}^n$.

Let $(r_1, \dots, r_c) \in \mathbb{N}^c$ and other notations be as in Definition 2.1. The *tautological vector bundle* on $\operatorname{Gr}(k, \mathbb{V})$, denoted $\mathcal{S}$, is the vector bundle whose base space is $\operatorname{Gr}(k, \mathbb{V})$ and whose fiber over $[\mathbb{W}] \in \operatorname{Gr}(k, \mathbb{V})$ is simply the k-dimensional linear subspace $\mathbb{W} \subseteq \mathbb{V}$. For any $k_1, \dots, k_c \in \mathbb{N}$, the *tensor network bundle*, denoted

$$\textsc{tns}(G; r_1, \dots, r_c; \mathcal{S}_1, \dots, \mathcal{S}_d),$$

is the fiber bundle over the base space $\operatorname{Gr}(k_1, \mathbb{V}_1) \times \dots \times \operatorname{Gr}(k_d, \mathbb{V}_d)$ whose fiber over a point $([\mathbb{W}_1], \dots, [\mathbb{W}_d]) \in \operatorname{Gr}(k_1, \mathbb{V}_1) \times \dots \times \operatorname{Gr}(k_d, \mathbb{V}_d)$ is $\textsc{tns}(G; r_1, \dots, r_c; \mathbb{W}_1, \dots, \mathbb{W}_d)$.

We will need the following results from [17, Propositions 3 and 4], reproduced here for easy reference.

Proposition 3.2 (Reduction of degree-one subcritical vertices)**.** *Let $(r_1, \dots, r_c) \in \mathbb{N}^c$ and $G = (V, E)$ be a graph. Let $i \in V$ be a vertex of degree one adjacent to the vertex $j \in V$. If i is subcritical or critical, then we have the following reduction:*

$$\textsc{tns}(G; r_1, r_2, \dots, r_c; \mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3, \dots, \mathbb{V}_d) = \textsc{tns}(G'; r_2, \dots, r_c; \mathbb{V}_1 \otimes \mathbb{V}_2, \mathbb{V}_3, \dots, \mathbb{V}_d),$$

where $G' = (V \setminus \{i\}, E \setminus \{i, j\})$, i.e., the graph obtained by removing the vertex i and edge $\{i, j\}$ from G, and $(r_2, \dots, r_c) \in \mathbb{N}^{c-1}$. Alternatively, we may write

$$\textsc{tns}(G; r_1, r_2, \dots, r_c; n_1, n_2, n_3, \dots, n_d) = \textsc{tns}(G'; r_2, \dots, r_c; n_1 n_2, n_3, \dots, n_d).$$

Proposition 3.3 (Reduction of supercritical vertices)**.** *Let $n_i = \dim \mathbb{V}_i$, $p_i = \min\{n_i, m_i\}$, and $\mathcal{S}_i$ be the tautological vector bundle on $\operatorname{Gr}(p_i, \mathbb{V}_i)$ for $i = 1, \dots, d$. Then the map*

$$\pi : \textsc{tns}(G; r_1, \dots, r_c; \mathcal{S}_1, \dots, \mathcal{S}_d) \to \textsc{tns}(G; r_1, \dots, r_c; \mathbb{V}_1, \dots, \mathbb{V}_d), \quad ([\mathbb{W}_1], \dots, [\mathbb{W}_d], T) \mapsto T,$$

is a surjective birational map.

Immediate consequences of Proposition 3.3 are a bound on the multilinear rank of tensor network states and a reduction formula for the dimension of a tensor network.

Corollary 3.4. *Let the notations be as above. Then for any* $(r_1, \dots, r_c) \in \mathbb{N}^c$*, we have*

$$\textsc{tns}(G; r_1, \dots, r_c; \mathbb{V}_1, \dots, \mathbb{V}_d) \subseteq \operatorname{Sub}_{p_1,\dots,p_d}(\mathbb{V}_1, \dots, \mathbb{V}_d)$$

and

$$\dim \textsc{tns}(G; r_1, \dots, r_c; n_1, \dots, n_d) = \dim \textsc{tns}(G; r_1, \dots, r_c; p_1, \dots, p_d) + \sum\nolimits_{i=1}^{d} p_i(n_i - p_i).$$

Note that by Proposition 3.3, all tensor network states can be reduced to one that is either critical or subcritical.

The next proposition is useful for describing when we are allowed to remove an edge from the graph while keeping the tensor network unchanged. The reader may notice a resemblance to Proposition 3.2, which is about collapsing two vertices into one and thus results in a reduction in the total number of vertices, but the goal of Proposition 3.5 is to remove an edge while leaving the total number of vertices unchanged.

Proposition 3.5 (Edge removal)**.** *Let $G = (V, E)$ be a graph with d vertices and c edges. Let $(r_1, \dots, r_c) \in \mathbb{N}^c$ and $(n_1, \dots, n_d) \in \mathbb{N}^d$. Suppose that the edge $e \in E$ has weight $r_1 = 1$ and $G' = (V, E \setminus \{e\})$ is the graph obtained by removing the edge e from G and suppose G' has no isolated vertices. Then*

$$\textsc{tns}(G; 1, r_2, \dots, r_d; \mathbb{V}_1, \dots, \mathbb{V}_d) \simeq \textsc{tns}(G'; r_2, \dots, r_d; \mathbb{V}_1, \dots, \mathbb{V}_d).$$

Proof. Assume without loss of generality that $e = \{1, 2\}$. By definition,

$$\begin{aligned} \textsc{tns}(G; 1, r_2, \dots, r_d; \mathbb{V}_1, \dots, \mathbb{V}_d) &= \{\kappa_G(T_1 \otimes \dots \otimes T_d) : T_i \in \mathbb{I}_i \otimes \mathbb{V}_i \otimes \mathbb{O}_i,\ i = 1, \dots, d\}, \\ \textsc{tns}(G'; r_2, \dots, r_d; \mathbb{V}_1, \dots, \mathbb{V}_d) &= \{\kappa_{G'}(T_1' \otimes \dots \otimes T_d') : T_i' \in \mathbb{I}_i' \otimes \mathbb{V}_i \otimes \mathbb{O}_i',\ i = 1, \dots, d\}, \end{aligned}$$

where $\mathbb{I}_i$, $\mathbb{I}_i'$ are inspaces, $\mathbb{O}_i$, $\mathbb{O}_i'$ are outspaces, as defined in (11), and κ_G, $\kappa_{G'}$ are contraction maps, as defined in (10), associated to G and G' respectively. Since $r_1 = 1$, $\mathbb{E}_1 \simeq \mathbb{C}$ and so contributes nothing[4] to the factors $\mathbb{I}_1 \otimes \mathbb{V}_1 \otimes \mathbb{O}_1$, $\mathbb{I}_2 \otimes \mathbb{V}_2 \otimes \mathbb{O}_2$, and thus $\mathbb{I}_i \otimes \mathbb{V}_i \otimes \mathbb{O}_i \simeq \mathbb{I}_i' \otimes \mathbb{V}_i \otimes \mathbb{O}_i'$ for $i = 1, 2$. On the other hand, $\mathbb{I}_i \otimes \mathbb{V}_i \otimes \mathbb{O}_i = \mathbb{I}_i' \otimes \mathbb{V}_i \otimes \mathbb{O}_i'$ for $i = 3, \dots, d$. Therefore the images of the contraction map must be isomorphic, as required. □

The assumption that an isolated vertex does not arise in G' upon removing the edge e is necessary because of (12). An immediate consequence of Proposition 3.5 is that tensor trains are a special case of matrix product states since

$$\textsc{tns}(C_d; r_1, r_2, \dots, r_{d-1}, 1; n_1, \dots, n_d) = \textsc{tns}(P_d; r_1, \dots, r_{d-1}; n_1, \dots, n_d), \tag{13}$$

where C_d is the cycle graph with d vertices, the edge with weight 1 is adjacent to the vertex 1 and d, and P_d is the path graph with d vertices.

We end the section with a result about restriction of tensor network states to subspaces of tensors, which will be crucial for an important property of tensor network rank established in Theorem 6.1.

Lemma 3.6 (Restriction lemma)**.** *Let G be a graph with d vertices and c edges. Let $\mathbb{V}_1, \dots, \mathbb{V}_d$ be vector spaces and $\mathbb{W}_i \subseteq \mathbb{V}_i$ be subspaces, $i = 1, \dots, d$. Then for any $(r_1, \dots, r_c) \in \mathbb{N}^c$,*

$$\textsc{tns}(G; r_1, \dots, r_c; \mathbb{V}_1, \dots, \mathbb{V}_d) \cap \mathbb{W}_1 \otimes \dots \otimes \mathbb{W}_d = \textsc{tns}(G; r_1, \dots, r_c; \mathbb{W}_1, \dots, \mathbb{W}_d). \tag{14}$$

In particular, we always have

$$\textsc{tns}(G; r_1, \dots, r_c; \mathbb{W}_1, \dots, \mathbb{W}_d) \subseteq \textsc{tns}(G; r_1, \dots, r_c; \mathbb{V}_1, \dots, \mathbb{V}_d). \tag{15}$$

[4] A one-dimensional vector space is isomorphic to the field of scalars $\mathbb{C}$ and $\mathbb{C} \otimes \mathbb{E} = \mathbb{E}$ for any complex vector space $\mathbb{E}$.

Proof. It is obvious that '$\supseteq$' holds in (44) and it remains to show '$\subseteq$'. Let $\mathbb{E}_j$ be a vector space of dimension r_j, $j = 1, \dots, c$. Orient G arbitrarily and let the inspace $\mathbb{I}_i$ and outspace $\mathbb{O}_i$ be as defined in (11) for vertices $i = 1, \dots, d$. We obtain two commutative diagrams:

$$\begin{tikzcd} \prod_{i=1}^d \mathbb{I}_i \otimes \mathbb{W}_i \otimes \mathbb{O}_i \arrow[r, "\Psi'"] \arrow[d, "\kappa''"'] & \bigotimes_{i=1}^d \mathbb{I}_i \otimes \mathbb{W}_i \otimes \mathbb{O}_i \arrow[r, "\Phi"] \arrow[d, "\kappa'"'] & \bigotimes_{i=1}^d \mathbb{I}_i \otimes \mathbb{V}_i \otimes \mathbb{O}_i \arrow[d, "\kappa"] \\ \operatorname{TNS}(G; r_1, \dots, r_c; \mathbb{W}_1, \dots, \mathbb{W}_d) \arrow[r, "\psi'"] & \mathbb{W}_1 \otimes \dots \otimes \mathbb{W}_d \arrow[r, "\phi"] & \mathbb{V}_1 \otimes \dots \otimes \mathbb{V}_d \end{tikzcd}$$

and

$$\begin{tikzcd} \prod_{i=1}^d \mathbb{I}_i \otimes \mathbb{V}_i \otimes \mathbb{O}_i \arrow[r, "\Psi"] \arrow[d, "\kappa'''"'] & \bigotimes_{i=1}^d \mathbb{I}_i \otimes \mathbb{V}_i \otimes \mathbb{O}_i \arrow[d, "\kappa"'] \\ \operatorname{TNS}(G; r_1, \dots, r_c; \mathbb{V}_1, \dots, \mathbb{V}_d) \arrow[r, "\psi"] & \mathbb{V}_1 \otimes \dots \otimes \mathbb{V}_d, \end{tikzcd}$$

where Ψ' sends $(x_1, \dots, x_d)$, $x_i \in \mathbb{I}_i \otimes \mathbb{W}_i \otimes \mathbb{O}_i, i = 1, \dots, d$, to $x_1 \otimes \dots \otimes x_d$ and Ψ is defined similarly; ψ', ψ are inclusions of tensor network states into their respective ambient spaces; Φ, ϕ are inclusions induced by $\mathbb{W}_i \subseteq \mathbb{V}_i$, $i = 1, \dots, d$; κ' is the restriction of $\kappa \coloneqq \kappa_G$; κ'' the composition of κ' and Ψ'; and κ''' the composition of κ and Ψ.

For each $i = 1, \dots, d$, write $\mathbb{V}_i^+ = \mathbb{W}_i$ and decompose $\mathbb{V}_i$ into a direct sum

$$\mathbb{V}_i = \mathbb{V}_i^- \oplus \mathbb{V}_i^+$$

for some linear subspace $\mathbb{V}_i^- \subseteq \mathbb{V}_i$. These give us the decomposition

$$\prod_{i=1}^d \mathbb{I}_i \otimes \mathbb{V}_i \otimes \mathbb{O}_i = \prod_{i=1}^d \mathbb{I}_i \otimes (\mathbb{V}_i^- \oplus \mathbb{V}_i^+) \otimes \mathbb{O}_i = \prod_{i=1}^d (\mathbb{I}_i \otimes \mathbb{V}_i^- \otimes \mathbb{O}_i) \oplus (\mathbb{I}_i \otimes \mathbb{V}_i^+ \otimes \mathbb{O}_i).$$

Now we may write an element $T_1 \otimes \dots \otimes T_d \in \Psi\bigl(\prod_{i=1}^d \mathbb{I}_i \otimes \mathbb{V}_i \otimes \mathbb{O}_i\bigr)$ as

$$T_1 \otimes \dots \otimes T_d = (T_1^- + T_1^+) \otimes \dots \otimes (T_d^- + T_d^+) = \sum\nolimits_{\pm} T_1^{\pm} \otimes \dots \otimes T_d^{\pm},$$

where $T_i^- \in \mathbb{I}_i \otimes \mathbb{V}_i^- \otimes \mathbb{O}_i$ and $T_i^+ \in \mathbb{I}_i \otimes \mathbb{V}_i^+ \otimes \mathbb{O}_i$. Since $T_1^{\pm} \otimes \dots \otimes T_d^{\pm} \in \Psi\bigl(\prod_{i=1}^d \mathbb{I}_i \otimes \mathbb{V}_i^{\pm} \otimes \mathbb{O}_i\bigr)$,

$$\kappa(T_1 \otimes \dots \otimes T_d) \in \sum\nolimits_{\pm} \kappa\Bigl(\Psi\Bigl(\prod_{i=1}^d \mathbb{I}_i \otimes \mathbb{V}_i^{\pm} \otimes \mathbb{O}_i\Bigr)\Bigr) = \sum\nolimits_{\pm} \operatorname{TNS}(G; r_1, \dots, r_c; \mathbb{V}_1^{\pm}, \dots, \mathbb{V}_d^{\pm}).$$

Therefore $\kappa(T_1 \otimes \dots \otimes T_d) \in \mathbb{V}_1^+ \otimes \dots \otimes \mathbb{V}_d^+$ implies that $T_i \in \mathbb{V}_i^+ = \mathbb{W}_i$ for all $i = 1, \dots, d$ and hence $\kappa(T_1 \otimes \dots \otimes T_d) \in \operatorname{TNS}(G; r_1, \dots, r_c; \mathbb{W}_1, \dots, \mathbb{W}_d)$. $\square$

4. G-ranks of tensors

The main goal of this article is to show that there is a natural notion of rank for tensor network with respect to any connected graph G. We start by reminding our readers of the classical notions of tensor rank and multilinear rank, with a small twist — instead of first defining tensor and multilinear ranks and then defining the respective sets they cut out, i.e., secant quasiprojective variety and subspace variety, we will reverse the order of these definitions. This approach will be consistent with how we define tensor network ranks later. The results in this and subsequent sections require that the vector spaces $\mathbb{V}_1, \dots, \mathbb{V}_d$ be finite-dimensional.

The *Segre variety* is the set of all decomposable tensors,

$$\operatorname{Seg}(\mathbb{V}_1, \dots, \mathbb{V}_d) \coloneqq \{T \in \mathbb{V}_1 \otimes \dots \otimes \mathbb{V}_d : T = v_1 \otimes \dots \otimes v_d,\ v_i \in \mathbb{V}_i\}.$$

The *r-secant quasiprojective variety* of the Segre variety is

$$s_r\bigl(\operatorname{Seg}(\mathbb{V}_1, \dots, \mathbb{V}_d)\bigr) \coloneqq \Bigl\{T \in \mathbb{V}_1 \otimes \dots \otimes \mathbb{V}_d : T = \sum\nolimits_{i=1}^r T_i,\ T_i \in \operatorname{Seg}(\mathbb{V}_1, \dots, \mathbb{V}_d)\Bigr\},$$

and its closure is the *r-secant variety* of the Segre variety,

$$\sigma_r\bigl(\operatorname{Seg}(\mathbb{V}_1, \dots, \mathbb{V}_d)\bigr) \coloneqq \overline{s_r\bigl(\operatorname{Seg}(\mathbb{V}_1, \dots, \mathbb{V}_d)\bigr)}.$$

The $(r_1,\dots,r_d)$-*subspace variety* [15] is the set

$$\operatorname{Sub}_{r_1,\dots,r_d}(\mathbb{V}_1,\dots,\mathbb{V}_d) \coloneqq \{T \in \mathbb{V}_1\otimes\cdots\otimes\mathbb{V}_d : T \in \mathbb{W}_1\otimes\cdots\otimes\mathbb{W}_d,\ \mathbb{W}_i\subseteq\mathbb{V}_i,\ \dim\mathbb{W}_i = r_i\}.$$

The *tensor rank* or just rank [11] of a tensor $T \in \mathbb{V}_1\otimes\cdots\otimes\mathbb{V}_d$ is

$$\operatorname{rank}(T) \coloneqq \min\bigl\{r\in\mathbb{N}_0 : T \in s_r\bigl(\operatorname{Seg}(\mathbb{V}_1,\dots,\mathbb{V}_d)\bigr)\bigr\},$$

its *border rank* [15] is

$$\overline{\operatorname{rank}}(T) \coloneqq \min\bigl\{r\in\mathbb{N}_0 : T \in \sigma_r\bigl(\operatorname{Seg}(\mathbb{V}_1,\dots,\mathbb{V}_d)\bigr)\bigr\},$$

and its *multilinear rank* [11, 6, 15] is

$$\mu\operatorname{rank}(T) \coloneqq \min\bigl\{(r_1,\dots,r_d)\in\mathbb{N}_0^d : T\in \operatorname{Sub}_{r_1,\dots,r_d}(\mathbb{V}_1,\dots,\mathbb{V}_d)\bigr\}.$$

Note that $\operatorname{rank}(T) = 0$ iff $\mu\operatorname{rank}(T) = (0,\dots,0)$ iff $T = 0$ and that $\operatorname{rank}(T) = 1$ iff $\mu\operatorname{rank}(T) = (1,\dots,1)$. Thus

$$\begin{aligned}
\operatorname{Seg}(\mathbb{V}_1,\dots,\mathbb{V}_d) &= \{T\in\mathbb{V}_1\otimes\cdots\otimes\mathbb{V}_d : \operatorname{rank}(T)\le 1\} = \operatorname{Sub}_{1,\dots,1}(\mathbb{V}_1,\dots,\mathbb{V}_d),\\
s_r\bigl(\operatorname{Seg}(\mathbb{V}_1,\dots,\mathbb{V}_d)\bigr) &= \{T\in\mathbb{V}_1\otimes\cdots\otimes\mathbb{V}_d : \operatorname{rank}(T)\le r\},\\
\operatorname{Sub}_{r_1,\dots,r_d}(\mathbb{V}_1,\dots,\mathbb{V}_d) &= \{T\in\mathbb{V}_1\otimes\cdots\otimes\mathbb{V}_d : \mu\operatorname{rank}(T)\le (r_1,\dots,r_d)\}.
\end{aligned}$$

When the vector spaces are unimportant or when we choose coordinates and represent tensors as hypermatrices, we write

$$\begin{aligned}
\operatorname{Seg}(n_1,\dots,n_d) &= \{T\in\mathbb{C}^{n_1\times\cdots\times n_d} : \operatorname{rank}(T)\le 1\},\\
s_r(n_1,\dots,n_d)\bigr) &= \{T\in\mathbb{C}^{n_1\times\cdots\times n_d} : \operatorname{rank}(T)\le r\},\\
\operatorname{Sub}_{r_1,\dots,r_d}(n_1,\dots,n_d) &= \{T\in\mathbb{C}^{n_1\times\cdots\times n_d} : \mu\operatorname{rank}(T)\le (r_1,\dots,r_d)\}.
\end{aligned}$$

The dimension of a subspace variety is given by

$$\dim\operatorname{Sub}_{r_1,\dots,r_d}(n_1,\dots,n_d) = \sum\nolimits_{i=1}^d r_i(n_i-r_i) + \prod\nolimits_{j=1}^d r_j. \tag{16}$$

Unlike tensor rank and multilinear rank, the existence of a tensor network rank is not obvious and will be established in the following. A tensor network $\textsc{tns}(G; r_1,\dots,r_c; \mathbb{V}_1,\dots,\mathbb{V}_d)$ is defined for any graph G although it is trivial when G contains an isolated vertex (see (12)). However, tensor network ranks or G-ranks will require the stronger condition that G be *connected.*

Theorem 4.1 (Every tensor is a tensor network state)**.** *Let $T\in\mathbb{V}_1\otimes\cdots\otimes\mathbb{V}_d$ and let G be a connected graph with d vertices and c edges. Then there exists $(r_1,\dots,r_c)\in\mathbb{N}^c$ such that*

$$T\in\textsc{tns}(G; r_1,\dots,r_c; \mathbb{V}_1,\dots,\mathbb{V}_d).$$

In fact, we may choose $r_1=\cdots=r_c=\operatorname{rank}(T)$, the tensor rank of T.

Proof. Let $r = \operatorname{rank}(T)$. Then there exist $v_1^{(i)},\dots,v_r^{(i)}\in\mathbb{V}_i$, $i=1,\dots,d$, such that

$$T = \sum\nolimits_{p=1}^r v_p^{(1)}\otimes\cdots\otimes v_p^{(d)}.$$

Let us take $r_1=\cdots=r_c=r$ and for each $i=1,\dots,d$, let

$$T_i = \sum\nolimits_{p=1}^r\Bigl(\bigotimes\nolimits_{j\in\textsc{in}(i)} e_p^{(j)}\Bigr)\otimes v_p^{(i)}\otimes\Bigl(\bigotimes\nolimits_{j\in\textsc{out}(i)} e_p^{(j)*}\Bigr),$$

where $e_1^{(j)},\dots,e_r^{(j)}\in\mathbb{E}_j$ are a basis with dual basis $e_1^{(j)*},\dots,e_r^{(j)*}\in\mathbb{E}_j^*$, i.e., $e_p^{(j)*}(e_q^{(j)}) = \delta_{pq}$ for $p,q=1,\dots,r$ and $j=1,\dots,d$. In addition, we set $e_p^{(0)} = e_p^{(d+1)} = 1\in\mathbb{C}$ to be one-dimensional vectors (i.e., scalars), $p=1,\dots,r$. We claim that upon contraction,

$$\kappa_G(T_1\otimes\cdots\otimes T_d) = T.$$

To see this, observe that for each $i=1,\dots,d$, there exists a unique h such that whenever $j\in\textsc{in}(i)\cap\textsc{out}(h)$, $e_p^{(j)}$ and $e_q^{(j)*}$ contract to give δ_{pq}; so the summand vanishes except when $p=q$.

This together with the assumption that G is connected implies that $\kappa_G(T_1 \otimes \cdots \otimes T_d)$ reduces to a sum of terms of the form $v_p^{(1)} \otimes \cdots \otimes v_p^{(d)}$ for $p = 1, \dots, r$, which is of course is just T. $\square$

As an example to illustrate the above proof, let $d = 3$ and $G = P_3$, the path graph with three vertices. Let $e_1, \dots, e_r$ be a basis of $\mathbb{E}_1$ and let $e_1^*, \dots, e_r^*$ be the dual basis. Let $f_1, \dots, f_r$ be a basis of $\mathbb{E}_2$ and let $f_1^*, \dots, f_r^*$ be the dual basis. Given a tensor

$$T = \sum\nolimits_{p=1}^{r} u_p \otimes v_p \otimes w_p \in \mathbb{V}_1 \otimes \mathbb{V}_2 \otimes \mathbb{V}_3,$$

consider

$$T_1 = \sum\nolimits_{p=1}^{r} u_p \otimes e_p^* \in \mathbb{V}_1 \otimes \mathbb{E}_1^*, \;\; T_2 = \sum\nolimits_{p=1}^{r} e_p \otimes v_p \otimes f_p^* \in \mathbb{E}_1 \otimes \mathbb{V}_2 \otimes \mathbb{E}_2^*, \;\; T_3 = \sum\nolimits_{p=1}^{r} f_p \otimes w_p \in \mathbb{E}_2 \otimes \mathbb{V}_3.$$

Now observe that a nonzero term in $\kappa_G(T_1 \otimes T_2 \otimes T_3)$ must come from contracting e_p^* with e_p and f_p^* with f_p, showing that $T = \kappa_G(T_1 \otimes T_2 \otimes T_2) \in \textsc{tns}(G; r, r; \mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3)$.

By Theorem 4.1 and Corollary 3.4, we obtain the following general inclusion relations (independent of G) between a tensor network and the sets of rank-r tensors and multilinear rank-$(r_1, \dots, r_d)$ tensors.

Corollary 4.2. *Let G be a connected graph with d vertices and c edges. Let $\mathbb{V}_1, \dots, \mathbb{V}_d$ be vector spaces of dimensions $n_1, \dots, n_d$. Then*

$$s_r := \{T \in \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d : \operatorname{rank}(T) \le r\} \subseteq \textsc{tns}(G; \underbrace{r, \dots, r}_{c}; \mathbb{V}_1, \dots, \mathbb{V}_d).$$

Let $(r_1, \dots, r_c) \in \mathbb{N}^c$ and let $(p_1, \dots, p_d) \in \mathbb{N}^d$ be given by

$$p_i := \min\Bigl\{\prod\nolimits_{j \in \textsc{in}(i) \cup \textsc{out}(i)} r_j, n_i\Bigr\}, \qquad i = 1, \dots, d.$$

Then

$$\textsc{tns}(G; r_1, \dots, r_c; \mathbb{V}_1, \dots, \mathbb{V}_d) \subseteq \operatorname{Sub}_{p_1, \dots, p_d}(\mathbb{V}_1, \dots, \mathbb{V}_d)$$

In particular, if we let $(p_1, \dots, p_d) \in \mathbb{N}^d$ where $p_i := \min\{r^{b_i}, n_i\}$ and $b_i := \# \textsc{in}(i) \cup \textsc{out}(i)$, then

$$s_r \subseteq \textsc{tns}(G; r, \dots, r; \mathbb{V}_1, \dots, \mathbb{V}_d) \subseteq \operatorname{Sub}_{p_1, \dots, p_d}(\mathbb{V}_1, \dots, \mathbb{V}_d).$$

Since $\mathbb{N}^c$ is a partially ordered set, in fact, a *lattice* [8], with respect to the usual partial order

$$(r_1, \dots, r_c) \le (s_1, \dots, s_c) \qquad \text{iff} \qquad r_1 \le s_1, \dots, r_c \le s_c.$$

For a non-empty subset $S \subset L$, a partially ordered set, we denote the set of *minimal elements* of S by $\min(S)$. For example, if $S = \{(1,2), (2,1), (2,2)\} \subset \mathbb{N}^2$, then $\min(S) = \{(1,2), (2,1)\}$. By Theorem 4.1, for any graph G, any vector spaces $\mathbb{V}_1, \dots, \mathbb{V}_d$, and any tensor $T \in \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$,

$$\{(r_1, \dots, r_c) \in \mathbb{N}^c : T \in \textsc{tns}(G; r_1, \dots, r_c; \mathbb{V}_1, \dots, \mathbb{V}_d)\} \neq \varnothing.$$

Hence we may define tensor network rank with respect to a given graph G, called G-rank for short, as the set-valued function

$$\begin{aligned} &\operatorname{rank}_G : \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d \to 2^{\mathbb{N}^c}, \\ &\qquad\qquad T \mapsto \min\{(r_1, \dots, r_c) \in \mathbb{N}^c : T \in \textsc{tns}(G; r_1, \dots, r_c; \mathbb{V}_1, \dots, \mathbb{V}_d)\}, \end{aligned}$$

where $2^{\mathbb{N}^c}$ is the power set of all subsets of $\mathbb{N}^c$. Note that by Theorem 4.1, $\operatorname{rank}_G(T)$ will always be a finite subset of $\mathbb{N}^c$.

Nevertheless, following convention, we prefer to have $\operatorname{rank}_G(T)$ be an element as opposed to a subset of $\mathbb{N}^c$. So we will define G-rank to be any minimal element as opposed to the set of all minimal elements.

Definition 4.3 (Tensor network rank and maximal rank)**.** Let G be a graph with d vertices and c edges. We say that $(r_1, \dots, r_c) \in \mathbb{N}^c$ is a *G-rank* of $T \in \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$, denoted by

$$\operatorname{rank}_G(T) = (r_1, \dots, r_c),$$

if $(r_1, \dots, r_c)$ is minimal such that $T \in \textsc{tns}(G; r_1, \dots, r_c; \mathbb{V}_1, \dots, \mathbb{V}_d)$, i.e.,

$$T \in \textsc{tns}(G; r_1', \dots, r_c'; \mathbb{V}_1, \dots, \mathbb{V}_d) \text{ and } r_1 \ge r_1', \dots, r_c \ge r_c' \quad \Longrightarrow \quad r_1' = r_1, \dots, r_c' = r_c.$$

A *G-rank decomposition* of T is its expression as element of $\textsc{tns}(G; r_1, \dots, r_c; \mathbb{V}_1, \dots, \mathbb{V}_d)$ where $\operatorname{rank}_G(T) = (r_1, \dots, r_c)$. We say that $(m_1, \dots, m_c) \in \mathbb{N}^c$ is a *maximal G-rank* of $\mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$ if $(m_1, \dots, m_c)$ is minimal such that every $T \in \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$ has rank not more than $(m_1, \dots, m_c)$.

Definition 4.3 says nothing about the uniqueness of a minimal $(r_1, \dots, r_c) \in \mathbb{N}^c$. We will see later that for an acyclic graph G, the minimal $(r_1, \dots, r_c)$ is unique. We will see an extensive list of examples in Section 10 where we compute, for various G's, the G-ranks of a number of special tensors: decomposable tensors, monomials (viewed as a symmetric tensor and thus a tensor), the noncommutative determinant and permanent, the W and GHS states, and the structure tensor of matrix-matrix product.

It follows from Definition 4.3 that

$$\textsc{tns}(G; r_1, \dots, r_c; \mathbb{V}_1, \dots, \mathbb{V}_d) = \{T \in \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d : \operatorname{rank}_G(T) \le (r_1, \dots, r_c)\}. \tag{17}$$

By Corollary 4.2, G-rank may be viewed as an 'interpolant' between tensor rank and multilinear rank; although in Section 11, we will see that they are strictly distinct notions — tensor and multilinear ranks are not special cases of G-ranks for specific choices of G. Since the set in (17) is in general not closed [17], we let

$$\overline{\textsc{tns}}(G; r; \mathbb{V}_1, \dots, \mathbb{V}_d) := \overline{\textsc{tns}(G; r; \mathbb{V}_1, \dots, \mathbb{V}_d)}$$

denote its Zariski closure. With this, we obtain G-rank analogues of border rank and generic rank.

Definition 4.4 (Tensor network border rank and generic rank)**.** Let G be a graph with d vertices and c edges. We say that $(r_1, \dots, r_c) \in \mathbb{N}^c$ is a *border G-rank* of $T \in \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$, denoted by

$$\overline{\operatorname{rank}}_G(T) = (r_1, \dots, r_c),$$

if $(r_1, \dots, r_c)$ is minimal such that $T \in \overline{\textsc{tns}}(G; r_1, \dots, r_c; \mathbb{V}_1, \dots, \mathbb{V}_d)$. We say that $(r_1, \dots, r_c) \in \mathbb{N}^c$ is a *generic G-rank* of $\mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$ if $(g_1, \dots, g_c)$ is minimal such that every $T \in \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$ has border rank not more than $(g_1, \dots, g_c)$.

Observe that by Definitions 4.3 and 4.4, we have

$$\begin{aligned}
\textsc{tns}(G; r_1, \dots, r_c; \mathbb{V}_1, \dots, \mathbb{V}_d) &= \{T \in \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d : \operatorname{rank}_G(T) \le (r_1, \dots, r_c)\}, \\
\overline{\textsc{tns}}(G; r_1, \dots, r_c; \mathbb{V}_1, \dots, \mathbb{V}_d) &= \{T \in \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d : \overline{\operatorname{rank}}_G(T) \le (r_1, \dots, r_c)\}, \\
\overline{\textsc{tns}}(G; g_1, \dots, g_c; \mathbb{V}_1, \dots, \mathbb{V}_d) &= \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d = \textsc{tns}(G; m_1, \dots, m_c; \mathbb{V}_1, \dots, \mathbb{V}_d),
\end{aligned}$$

for any $(r_1, \dots, r_c) \in \mathbb{N}^c$ and where $(m_1, \dots, m_c)$ and $(g_1, \dots, g_c)$ are respectively a maximal and a generic G-rank of $\mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$. Note also our use of the indefinite article — *a* border/generic/maximal G-rank — since these are not in general unique if G is not acyclic. A more pedantic definition would be in terms of set-valued functions as in the discussion before Definition 4.3.

Following Definition 2.2, when G is a path graph, tree, cycle graph, product of path graphs, or a graph obtained from gluing trees and cycle graphs along edges, then we may also use the terms TT-rank, TTNS-rank, MPS-rank, PEPS-rank, or CTNS-rank to describe the respective G-ranks, and likewise for their respective generic G-rank and border G-rank. The terms *hierarchical rank* [9, Chapter 11] and *tree rank* [2] have also been used for TTNS-rank. Discussions of TT-rank, TTNS-rank, MPS-rank will be deferred to Sections 7, 8, and 9 respectively. We will also compute many examples of G-ranks and border G-ranks for important tensors arising from algebraic computational complexity and quatum mechanics in Section 10.

5. Tensor network ranks can be much smaller than matrix, tensor, and multilinear ranks

Our first result regarding tensor network ranks may be viewed as the main impetus for tensor networks — we show that a tensor may have arbitrarily high tensor rank or multilinear rank and yet arbitrarily low G-rank for some graph G, in the sense that there is an arbitrarily large gap between the two ranks. The same applies to tensor network ranks corresponding to two different graphs. For all our comparisons in this section, a single example — the structure tensor for matrix-matrix product — suffices to demonstrate the gaps in various ranks. We will see more examples in Section 10. In Theorem 6.5, we will exhibit a graph G such that *almost every* tensor has exponentially small G-rank compared to its tensor rank or the dimension of its ambient space.

5.1. **Comparison with tensor and multilinear ranks.** In this and the next subsection, we will compare different ranks $(r_1, \dots, r_c) \in \mathbb{N}^c$ and $(s_1, \dots, s_{c'}) \in \mathbb{N}^{c'}$ by a simple comparison of their 1-norms $r_1 + \cdots + r_c$ and $s_1 + \cdots + s_{c'}$. In Section 5.3, we will compare the actual dimensions of the sets of tensors with these ranks.

Theorem 5.1. *For any $d \ge 3$, there exists a tensor $T \in \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$ such that for some connected graph G with d vertices and c edges,*

(i) *the tensor rank* $\operatorname{rank}(T) = r$ *is much larger than the G-rank* $\operatorname{rank}_G(T) = (r_1, \dots, r_c)$ *in the sense that*
$$r \gg r_1 + \cdots + r_c;$$
(ii) *the multilinear rank* $\mu\operatorname{rank}(T) = (s_1, \dots, s_d)$ *is much larger than the G-rank* $\operatorname{rank}_G(T) = (r_1, \dots, r_c)$ *in the sense that*
$$s_1 + \cdots + s_d \gg r_1 + \cdots + r_c;$$
(iii) *for some graph H with d vertices and c' edges, the H-rank* $\operatorname{rank}_H(T) = (s_1, \dots, s_{c'})$ *is much larger than the G-rank* $\operatorname{rank}_G(T) = (r_1, \dots, r_c)$ *in the sense that*
$$s_1 + \cdots + s_{c'} \gg r_1 + \cdots + r_c.$$

Here "$\gg$" indicates a difference in the order of magnitude. In particular, the gap between the ranks can be arbitrarily large.

Proof. We first let $d = 3$ and later extend our construction to arbitrary $d > 3$. Set $\mathbb{V}_3 = \mathbb{C}^{n \times n}$, the n^2-dimensional vector space of complex $n \times n$ matrices and $\mathbb{V}_1 = \mathbb{V}_2 = \mathbb{V}_3^*$, its dual space. Let $T = \mu_n \in (\mathbb{C}^{n\times n})^* \otimes (\mathbb{C}^{n\times n})^* \otimes \mathbb{C}^{n\times n} \cong \mathbb{C}^{n^2 \times n^2 \times n^2}$ be the structure tensor of matrix-matrix product [40], i.e.,
$$\mu_n = \sum\nolimits_{i,j,k=1}^{n} E_{ik}^* \otimes E_{kj}^* \otimes E_{ij} \tag{18}$$
where $E_{ij} = e_i e_j^{\mathsf{T}} \in \mathbb{C}^{n \times n}$, $i, j = 1, \dots, n$, is the standard basis with dual basis $E_{ij}^* : \mathbb{C}^{n\times n} \to \mathbb{C}$, $A \mapsto a_{ij}$, $i, j = 1, \dots, n$. It is well-known that $\operatorname{rank}(\mu_n) \ge n^2$ as it is not possible to multiply two $n \times n$ matrices with fewer than n^2 multiplications. It is trivial to see that
$$\mu\operatorname{rank}(\mu_n) = (n^2, n^2, n^2). \tag{19}$$
Let P_3 and C_3 be the path graph and cycle graph on three vertices in Figures 2 and 4 respectively. Attach vector spaces $\mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3$ to the vertices of both graphs. Then $\mu_n \in \textsc{tns}(C_3; n, n, n; \mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3)$ and it is clear that $\mu_n \notin \textsc{tns}(C_3; r_1, r_2, r_3; \mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3)$ if at least one of $r_1 \le n$, $r_2 \le n$, $r_3 \le n$ holds strictly. Hence
$$\operatorname{rank}_{C_3}(\mu_n) = (n, n, n).$$
On the other hand, we also have
$$\operatorname{rank}_{P_3}(\mu_n) = (n^2, n^2).$$

See Theorems 10.10 and 10.9 for more details on computing $\operatorname{rank}_{C_3}(\mu_n)$ and $\operatorname{rank}_{P_3}(\mu_n)$. The required conclusions follow from

$$\begin{aligned}
\|\operatorname{rank}_{C_3}(\mu_n)\|_1 &= 3n \ll n^2 \le \operatorname{rank}(\mu_n),\\
\|\operatorname{rank}_{C_3}(\mu_n)\|_1 &= 3n \ll 3n^2 = \|\mu\mathrm{rank}(\mu_n)\|_1,\\
\|\operatorname{rank}_{C_3}(\mu_n)\|_1 &= 3n \ll 2n^2 = \|\operatorname{rank}_{P_3}(\mu_n)\|_1.
\end{aligned}$$

To extend the above to $d > 3$, let $0 \ne v_i \in \mathbb{V}_i$, $i = 4, \dots, d$, and set

$$T_d = \mu_n \otimes v_4 \otimes \cdots \otimes v_d \in \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d.$$

Clearly, its tensor rank and multilinear rank are

$$\operatorname{rank}(T_d) = \operatorname{rank}(\mu_n) \ge n^2, \qquad \mu\mathrm{rank}(T_d) = (n^2, n^2, n^2, \overbrace{1, \dots, 1}^{d-3}).$$

Next we compute $\operatorname{rank}_{P_d}(T_d)$ and $\operatorname{rank}_{C_d}(T_d)$. Relabeling $v_{ij1} = E_{ij}$ and $v_{11}^{(k)} = v_k$, we get

$$T_d = \Bigl(\sum\nolimits_{i,j,k=1}^{n} E_{ik}^* \otimes E_{kj}^* \otimes E_{ij}\Bigr) \otimes v_4 \otimes \cdots \otimes v_d = \Bigl(\sum\nolimits_{i,j,k=1}^{n} E_{ik}^* \otimes E_{kj}^* \otimes v_{ij1}\Bigr) \otimes v_{11}^{(4)} \otimes \cdots \otimes v_{11}^{(d)},$$

where it follows immediately that

$$T_d \in \textsc{tns}(P_d; n^2, n^2, \overbrace{1, \dots, 1}^{d-2}; \mathbb{V}_1, \dots, \mathbb{V}_d).$$

Since $\operatorname{rank}_{P_3}(\mu_n) = (n^2, n^2)$, by Theorem 10.9,

$$\operatorname{rank}_{P_d}(T_d) = (n^2, n^2, \underbrace{1, \dots, 1}_{d-2}).$$

Now rewrite T_d as

$$\begin{aligned}
T_d &= \Bigl(\sum\nolimits_{i,j,k=1}^{n} E_{ik}^* \otimes E_{kj}^* \otimes E_{ij}\Bigr) \otimes v_4 \otimes \cdots \otimes v_d\\
&= \Bigl(\sum\nolimits_{i,j,k,l=1}^{n} E_{ik}^* \otimes E_{kj}^* \otimes v_{lj}\Bigr) \otimes v_{l1}^{(4)} \otimes v_{11}^{(5)} \otimes \cdots \otimes v_{11}^{(d-1)} \otimes v_{1i}^{(d)},
\end{aligned}$$

where

$$v_{lj} = \begin{cases} E_{ij} & l = i,\\ 0 & l \ne i, \end{cases} \quad v_{l1}^{(4)} = \begin{cases} v_4 & l = i,\\ 0 & l \ne i, \end{cases} \quad v_{11}^{(5)} = v_5, \dots, v_{11}^{(d-1)} = v_{d-1}; \quad v_{1i}^{(d)} = v_d,\ i = 1, \dots, n.$$

It follows that $T_d \in \textsc{tns}(C_d; n, n, n, n, \underbrace{1, \dots, 1}_{d-4}; \mathbb{V}_1, \dots, \mathbb{V}_d)$ and so $\operatorname{rank}_{C_d}(T_d) \le (n, n, n, n, \underbrace{1, \dots, 1}_{d-4})$. Hence we obtain

$$\begin{aligned}
\|\operatorname{rank}_{C_d}(T_d)\|_1 &\le 4n + d - 4 \ll n^2 \le \operatorname{rank}(T_d),\\
\|\operatorname{rank}_{C_d}(T_d)\|_1 &\le 4n + d - 4 \ll 3n^2 + d - 3 = \|\mu\mathrm{rank}(T_d)\|_1,\\
\|\operatorname{rank}_{C_d}(T_d)\|_1 &\le 4n + d - 4 \ll 2n^2 + d - 2 = \|\operatorname{rank}_{P_d}(T_d)\|_1.
\end{aligned}$$ □

5.2. **Comparison with matrix rank.** The matrix rank of a matrix can also be arbitrarily higher than its G-rank when regarded as a 3-tensor. We will make this precise below.

Every d-tensor may be regarded as a d'-tensor for any $d' \le d$ via *flattening* [15, 20]. The most common case is when $d' = 2$ and in which case the flattening map

$$\flat_k : \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d \to (\mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_k) \otimes (\mathbb{V}_{k+1} \otimes \cdots \otimes \mathbb{V}_d), \qquad k = 2, \dots, d-1,$$

takes a d-tensor and sends it to a 2-tensor by 'forgetting' the tensor product structures in $\mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_k$ and $\mathbb{V}_{k+1} \otimes \cdots \otimes \mathbb{V}_d$. The converse of this operation also holds in the following sense. Suppose the dimensions of the vector spaces $\mathbb{V}$ and $\mathbb{W}$ factor as

$$\dim(\mathbb{V}) = n_1 \cdots n_k, \qquad \dim(\mathbb{W}) = n_{k+1} \cdots n_d$$

for integers $n_1, \dots, n_d \in \mathbb{N}$. Then we may impose tensor product structures on $\mathbb{V}$ and $\mathbb{W}$ so that

$$\mathbb{V} \cong \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_k, \qquad \mathbb{W} \cong \mathbb{V}_{k+1} \otimes \cdots \otimes \mathbb{V}_d, \tag{20}$$

where $\dim \mathbb{V}_i = n_i$, $i = 1, \dots, d$, and where $\cong$ denotes vector space isomorphism. In which case the *sharpening* map

$$\sharp_k : \mathbb{V} \otimes \mathbb{W} \to \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_k \otimes \mathbb{V}_{k+1} \otimes \cdots \otimes \mathbb{V}_d, \qquad k = 2, \dots, d-1,$$

takes a 2-tensor and sends it to a d-tensor by imposing the tensor product structures chosen in (20). Note that both $\flat_k$ and $\sharp_k$ are vector space isomorphisms. Applying this to matrices,

$$\mathbb{C}^{n_1 \cdots n_{k-1} \times n_k \cdots n_d} \cong \mathbb{C}^{n_1 \cdots n_{k-1}} \otimes \mathbb{C}^{n_k \cdots n_d} \xrightarrow{\sharp_k} \mathbb{C}^{n_1} \otimes \cdots \otimes \mathbb{C}^{n_d} \cong \mathbb{C}^{n_1 \times \cdots \times n_d},$$

and we see that any $n_1 \cdots n_{k-1} \times n_k \cdots n_d$ matrix may be regarded as an $n_1 \times \cdots \times n_d$ hypermatrix. Theorem 5.1 applies to matrices (i.e., $d = 2$) in the sense of the following corollary.

Corollary 5.2. *There exists a matrix in $\mathbb{C}^{mn \times p}$ whose matrix rank is arbitrarily larger than its C_3-rank when regarded as a hypermatrix in $\mathbb{C}^{m \times n \times p}$.*

Proof. Let $\mu_n \in \mathbb{C}^{n^2 \times n^2 \times n^2}$ be a hypermatrix representing the structure tensor in Theorem 5.1. Consider any flattening [20] of μ_n, say, $\beta_1(\mu_n) \in \mathbb{C}^{n^4 \times n^2}$. Then by (19), its matrix rank is

$$\operatorname{rank}\bigl(\beta_1(\mu_n)\bigr) = n^2 \gg 3n = \|\operatorname{rank}_{C_3}(\mu_n)\|_1. \qquad \square$$

5.3. **Comparing number of parameters.** One might argue that the comparisons in Theorem 5.1 and Corollary 5.2 are not completely fair as, for instance, a rank-r decomposition of T may still require as many parameters as a G-rank-$(r_1, \dots, r_c)$ decomposition of T, even if $r \gg r_1 + \cdots + r_c$. We will show that this is not the case: if we measure the complexities of these decompositions by a strict count of parameters, the conclusion that G-rank can be much smaller than matrix, tensor, or multilinear ranks remain unchanged.

Let μ_n be the structure tensor for matrix-matrix product as in the proof of Theorem 5.1, which also shows that

$$\operatorname{rank}_{C_3}(\mu_n) = (n, n, n), \qquad \operatorname{rank}_{P_3}(\mu_n) = (n^2, n^2), \qquad \mu\operatorname{rank}(\mu_n) = (n^2, n^2, n^2).$$

Let $r \coloneqq \operatorname{rank}(\mu_n)$, the exact value of which is open but its current best known lower bound [25] is

$$r \geq 3n^2 - 2\sqrt{2} n^{3/2} - 3n, \tag{21}$$

which will suffice for our purpose.

Geometrically, the number of parameters is the dimension. So the number of parameters required to decompose μ_n as a point in $\textsc{tns}(C_3; n, n, n; \mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3)$, $\textsc{tns}(P_3; n^2, n^2; \mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3)$, $\operatorname{Sub}_{n^2,n^2,n^2}(\mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3)$, and $\sigma_r(\operatorname{Seg}(\mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3))$ are given by their respective dimensions:

$$\dim \textsc{tns}(C_3; n, n, n; \mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3) = 3n^4 - 3n^2, \tag{22}$$

$$\dim \textsc{tns}(P_3; n^2, n^2; \mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3) = n^6, \tag{23}$$

$$\dim \operatorname{Sub}_{n^2,n^2,n^2}(\mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3) = n^6, \tag{24}$$

$$\dim \sigma_r(\operatorname{Seg}(\mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3)) \geq 9n^4 - 6\sqrt{2} n^{7/2} - 9n^3 - 6n^2 + 4\sqrt{2} n^{3/2} + 6n - 1. \tag{25}$$

The dimensions in (22) and (23) follow from [39, Theorem 5.3] and that in (24) follows from (16). The lower bound on the tensor rank in (21) gives us the lower bound on the dimension in (25) by [1, Theorem 5.2].

In conclusion, a C_3-rank decomposition of μ_n requires fewer parameters than its P_3-rank decomposition, its multilinear rank decomposition, and its tensor rank decomposition.

6. Properties of tensor network rank

We will establish some fundamental properties of G-rank in this section. We begin by showing that like tensor rank and multilinear rank, G-ranks are independent of the choice of the ambient space, i.e., for a fixed G and any vector spaces $\mathbb{W}_i \subseteq \mathbb{V}_i$, $i = 1, \dots, d$, a tensor in $\mathbb{W}_1 \otimes \cdots \otimes \mathbb{W}_d$ has the same G-rank whether it is regarded as an element of $\mathbb{W}_1 \otimes \cdots \otimes \mathbb{W}_d$ or of $\mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$. The proof is less obvious and more involved than for tensor rank or multilinear rank, a consequence of Lemma 3.6.

Theorem 6.1 (Inheritance property)**.** *Let G be a connected graph with d vertices and c edges. Let $\mathbb{W}_i \subseteq \mathbb{V}_i$ be a linear subspace, $i = 1, \dots, d$, such that $T \in \mathbb{W}_1 \otimes \cdots \otimes \mathbb{W}_d$. Then $(r_1, \dots, r_c) \in \mathbb{N}^c$ is a G-rank of T as an element in $\mathbb{W}_1 \otimes \cdots \otimes \mathbb{W}_d$ if and only if it is a G-rank of T as an element in $\mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$.*

Proof. Let $\operatorname{rank}_G(T) = (r_1, \dots, r_c)$ as an element in $\mathbb{W}_1 \otimes \cdots \otimes \mathbb{W}_d$ and $\operatorname{rank}_G(T) = (s_1, \dots, s_c)$ as an element in $\mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$. Then $(s_1, \dots, s_c) \le (r_1, \dots, r_c)$. Suppose they are not equal, then $s_i < r_i$ for at least one $i \in \{1, \dots, c\}$. Since $T \in \textsc{tns}(G; s_1, \dots, s_c; \mathbb{V}_1, \dots, \mathbb{V}_d)$ and $T \in \mathbb{W}_1 \otimes \cdots \otimes \mathbb{W}_d$, we must have $T \in \textsc{tns}(G; s_1, \dots, s_c; \mathbb{W}_1, \dots, \mathbb{W}_d)$ by Lemma 3.6, contradicting our assumption that $\operatorname{rank}_G(T) = (r_1, \dots, r_c)$ as an element in $\mathbb{W}_1 \otimes \cdots \otimes \mathbb{W}_d$. ☐

It is well-known that Theorem 6.1 holds true for tensor rank and multilinear rank [6, Proposition 3.1]; so this is yet another way G-ranks resemble the usual notions of ranks. This inheritance property has often been exploited in the calculation of tensor rank and similarly Theorem 6.1 provides a useful simplification in the calculation of G-ranks: Given $T \in \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$, we may find linear subspaces $\mathbb{W}_i \subseteq \mathbb{V}_i$, $i = 1, \dots, d$, such that $T \in \mathbb{W}_1 \otimes \cdots \otimes \mathbb{W}_d$ and determine the G-rank of T as a tensor in the smaller space $\mathbb{W}_1 \otimes \cdots \otimes \mathbb{W}_d$. With this in mind, we introduce the following terminology.

Definition 6.2. $T \in \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$ is *degenerate* if there exist subspaces $\mathbb{W}_i \subseteq \mathbb{V}_i$, $i = 1, \dots, d$, with at least one strict inclusion, such that $T \in \mathbb{W}_1 \otimes \cdots \otimes \mathbb{W}_d$. Otherwise T is *nondegenerate*.

Theorem 6.1 tells us the behavior of G-ranks with respect to subspaces. The next result tells us about the behavior of G-ranks with respect to subgraphs.

Proposition 6.3 (Subgraph)**.** *Let G be a connected graph with d vertices and c edges. Let H be a connected subgraph of G with d vertices and c' edges.*

- (i) *Let $(s_1, \dots, s_{c'}) \in \mathbb{N}^{c'}$ be a generic H-rank of $\mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$. Then there exists $(r_1, \dots, r_c) \in \mathbb{N}^c$ with $r_i \le s_i$, $i = 1, \dots, c'$, such that $(r_1, \dots, r_c)$ is a generic G-rank of $\mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$.*
- (ii) *Let $T \in \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$ and $\operatorname{rank}_H(T) = (s_1, \dots, s_{c'})$. Then there exists $(r_1, \dots, r_c) \in \mathbb{N}^c$ with $r_i \le s_i, i = 1, \dots, c'$, such that $\operatorname{rank}_G(T) = (r_1, \dots, r_c)$.*

Proof. By Proposition 3.5, we have

$$\textsc{tns}(H; s_1, \dots, s_{c'}; \mathbb{V}_1, \dots, \mathbb{V}_d) = \textsc{tns}(G; s_1, \dots, s_{c'}, \overbrace{1, \dots, 1}^{c-c'}; \mathbb{V}_1, \dots, \mathbb{V}_d). \tag{26}$$

Since $(s_1, \dots, s_{c'})$ is a generic H-rank of $\mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$,

$$\overline{\textsc{tns}}(G; s_1, \dots, s_{c'}, 1, \dots, 1; \mathbb{V}_1, \dots, \mathbb{V}_d) = \overline{\textsc{tns}}(H; s_1, \dots, s_{c'}; \mathbb{V}_1, \dots, \mathbb{V}_d) = \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d,$$

implying that $\mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$ has a generic G-rank with $r_i \le s_i$, $i = 1, \dots, c'$. The same argument and (26) show that $\operatorname{rank}_G(T) = (s_1, \dots, s_{c'}, 1, \dots, 1) \in \mathbb{N}^c$. ☐

Corollary 6.4. *Let $T \in \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$. Then among all graphs G with d vertices T has the smallest G-rank when $G = K_d$, the complete graph on d vertices.*

Theorem 5.1 tells us that some tensors have much lower G-ranks relative to their tensor rank, multilinear rank, or H-rank for some other graph H. We now prove a striking result that essentially says that for some G, almost all tensors have much lower G-ranks relative to the dimension of the tensor space. In fact, the gap is exponential in this case: For a tensor space of dimension $O(n^d)$, the G-rank of almost every tensor in it would only be $O\big(n(d-1)\big)$; to see the significance, note that almost all tensors in such a space would have tensor rank $O\big(n^d/(nd-d+1)\big)$.

Theorem 6.5 (Almost all tensors have exponentially low G-rank)**.** *There exists a connected graph G such that $\|\operatorname{rank}_G(T)\|_1 \ll \dim(\mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d)$ for all T in a Zariski dense subset of $\mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$.*

Proof. Let $G = S_d$, the star graph on d vertices in Figure 6. Let $\dim \mathbb{V}_i = n_i$, $i = 1, \dots, d$. Without loss of generality, we let the center vertex of S_d be vertex 1 and associate $\mathbb{V}_1$ to it. Clearly, any $T \in \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$ has $\operatorname{rank}_{S_d}(T) = (r_1, \dots, r_{d-1})$ where $r_i \le n_{i+1}$, $i = 1, \dots, d-1$. Moreover,

$$\{T \in \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d : \operatorname{rank}_{S_d}(T) = (n_2, \dots, n_d)\}$$

is a Zariski open dense subset of $\mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$. Now observe that

$$\|\operatorname{rank}_{S_d}(T)\|_1 = r_1 + \cdots + r_{d-1} \le n_2 + \cdots + n_d \ll n_1 \cdots n_d = \dim(\mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d).$$

In particular, if $n_i = n$, $i = 1, \dots, d$, then the exponential gap becomes evident:

$$\|\operatorname{rank}_{S_d}(T)\|_1 \le n(d-1) \ll n^d = \dim(\mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d). \qquad \square$$

Proposition 6.6 (Bound for G-ranks)**.** *Let G be a connected graph with d vertices and c edges. If $T \in \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$ is nondegenerate and $\operatorname{rank}_G(T) = (r_1, \dots, r_c) \in \mathbb{N}^c$, then we must have*

$$\prod\nolimits_{j \in \textsc{in}(i) \cup \textsc{out}(i)} r_j \ge \dim \mathbb{V}_i, \qquad i = 1, \dots, d.$$

Proof. Suppose there exists some $i \in \{1, \dots, d\}$ such that

$$\prod\nolimits_{j \in \textsc{in}(i) \cup \textsc{out}(i)} r_j < \dim \mathbb{V}_i.$$

By Proposition 3.3, $\mathbb{V}_i$ may be replaced by a subspace of dimension $\prod_{j \in \textsc{in}(i) \cup \textsc{out}(i)} r_j$, showing that T is degenerate, a contradiction. $\square$

While we have formulated our discussions in a coordinate-free manner, the notion of G-rank applies to hypermatrices by making a choice of bases so that $\mathbb{V}_i = \mathbb{C}^{n_i}$, $i = 1, \dots, d$. In which case $\mathbb{C}^{n_1} \otimes \cdots \otimes \mathbb{C}^{n_d} \cong \mathbb{C}^{n_1 \times \cdots \times n_d}$ is the space of $n_1 \times \cdots \times n_d$ hypermatrices.

Corollary 6.7. *Let $A \in \mathbb{C}^{n_1 \times \cdots \times n_d}$ and G be a d-vertex graph.*

(i) *Let $(M_1, \dots, M_d) \in \mathrm{GL}_{n_1}(\mathbb{C}) \times \cdots \times \mathrm{GL}_{n_d}(\mathbb{C})$. Then*
$$\operatorname{rank}_G\bigl((M_1, \dots, M_d) \cdot A\bigr) = \operatorname{rank}_G(A). \tag{27}$$
(ii) *Let $n_1' \ge n_1, \dots, n_d' \ge n_d$. Then $\operatorname{rank}_G(A)$ is the same whether we regard A as an element of $\mathbb{C}^{n_1 \times \cdots \times n_d}$ or as an element of $\mathbb{C}^{n_1' \times \cdots \times n_d'}$.*

Proof. The operation $\cdot$ denotes multilinear matrix multiplication [20], which is exactly the change-of-basis transformation for d-hypermatrices. (i) follows from the fact that the definition of G-rank is basis-free and (ii) follows from Theorem 6.1. $\square$

7. Tensor trains

Tensor trains and TT-rank (i.e., P_d-rank) are the simplest instances of tensor networks and tensor network ranks. They are a special case of both TTNS in Section 8 (since P_d is a tree) and MPS in Section 9 (see (13)). However, we single them out as TT-rank generalizes matrix rank and may be related to multilinear rank and tensor rank in certain cases; furthermore, we may determine the dimension of the set of tensor trains and, in some cases, the generic and maximal TT-ranks. We begin with two examples.

Example 7.1 (Matrix rank)**.** Let $G = P_2$, the path graph on two vertices 1 and 2 (see Figure 2). This yields the simplest tensor network states: $\textsc{tns}(P_2; r; m, n)$ is simply the set rank-r matrices, or more precisely,

$$\textsc{tns}(P_2; r; m, n) = \{T \in \mathbb{C}^{m \times n} : \operatorname{rank}(T) \le r\}, \tag{28}$$

and so matrix rank is just P_2-rank. Moreover, observe that

$$\textsc{tns}(P_2; r; m, n) \cap \textsc{tns}(P_2; s; m, n) = \textsc{tns}(P_2; \min\{r, s\}; m, n),$$

a property that we will generalize in Lemma 8.1 to arbitrary G-ranks for acyclic G's.

Example 7.2 (Multilinear rank)**.** Let $G = P_3$ with vertices $1, 2, 3$, which is the next simplest case. Orient P_3 by $1 \to 2 \to 3$. Let $(r_1, r_2) \in \mathbb{N}^2$ satisfy $r_1 \le m$, $r_1 r_2 \le n$, $r_2 \le p$. In this case

$$\operatorname{TNS}(P_3; r_1, r_2; m, n, p) = \{T \in \mathbb{C}^{m\times n\times p} : \mu\mathrm{rank}(T) \le (r_1, r_1 r_2, r_2)\}, \tag{29}$$

and so

$$\operatorname{rank}_{P_3}(T) = (r_1, r_2) \quad \text{iff} \quad \mu\mathrm{rank}(T) = (r_1, r_1 r_2, r_3).$$

The P_3-rank of any $T \in \mathbb{C}^{m\times n\times p}$ is unique, a consequence of Theorem 8.3. But this may be deduced directly: Suppose T has two P_3-ranks (r_1, r_2) and (s_1, s_2). Then $T \in \operatorname{TNS}(P_3; r_1, r_2; m, n, p) \cap \operatorname{TNS}(P_3; s_1, s_2; m, n, p)$. We claim that there exists $(t_1, t_2) \in \mathbb{N}^2$ such that

$$T \in \operatorname{TNS}(P_3; t_1, t_2; m, n, p) \subseteq \operatorname{TNS}(P_3; r_1, r_2; m, n, p) \cap \operatorname{TNS}(P_3; s_1, s_2; m, n, p)$$

Without loss of generality, we may assume[5] that $r_1 \le s_1$, $r_2 \ge s_2$, and that $r_1 r_2 \le s_1 s_2$. By (29) and the observation that

$$\operatorname{Sub}_{r_1, r_1 r_2, r_2}(m, n, p) \cap \operatorname{Sub}_{s_1, s_1 s_2, s_2}(m, n, p) = \operatorname{Sub}_{r_1, r_1 r_2, s_2}(m, n, p),$$

the assumption that $r_2 \ge s_2$ allows us to conclude that

$$\operatorname{Sub}_{r_1, r_1 r_2, s_2}(m, n, p) = \operatorname{Sub}_{r_1, r_1 s_2, s_2}(m, n, p) = \operatorname{TNS}(P_3; r_1, s_2; m, n, p)$$

and therefore we may take $(t_1, t_2) = (r_1, s_2)$. So $(r_1, r_2) = \operatorname{rank}_{P_3}(T) \le (r_1, s_2)$ and we must have $r_2 = s_2$; similarly $(s_1, s_2) = \operatorname{rank}_{P_3}(T) \le (r_1, s_2)$ and we must have $r_1 = s_1$.

Example 7.3 (Rank-one tensors)**.** The set of decomposable tensors of order d, i.e., rank-1 or multilinear rank-$(1, \dots, 1)$ tensors (or the zero tensor), are exactly tensor trains of P_d-rank $(1, \dots, 1)$.

$$\operatorname{TNS}(P_d; 1, \dots, 1; n_1, \dots, n_d) = \{T \in \mathbb{C}^{n_1\times\cdots\times n_d} : \operatorname{rank}(T) \le 1\}. \tag{30}$$

The equalities (28), (29), (30) are obvious from definition and may also be deduced from the respective dimensions given in [39, Theorem 4.8].

Theorem 7.4 (Dimension of tensor trains)**.** *Let P_d be the path graph with $d \ge 2$ vertices and $d-1$ edges. Let $(r_1, \dots, r_{d-1}) \in \mathbb{N}^{d-1}$ be such that $\operatorname{TNS}(P_d; r_1, \dots, r_{d-1}; n_1, \dots, n_d)$ is supercritical or critical. Then*

$$\begin{aligned}\dim \operatorname{TNS}(P_d; r_1, \dots, r_{d-1}; n_1, \dots, n_d) = r_{d/2}^2 + \sum\nolimits_{i=1}^{d} r_{i-1} r_i (n_i - r_{i-1} r_i) \\ + \sum\nolimits_{j=1}^{\lfloor d/2\rfloor - 1} r_{j+1}^2 (r_j^2 - 1) + r_{d-j-1}^2 (r_{d-j}^2 - 1),\end{aligned} \tag{31}$$

where $r_0 = r_d := 1$ and

$$r_{d/2} := \begin{cases} r_{d/2} & \text{for } d \text{ even}, \\ r_{(d-1)/2} r_{(d+1)/2} & \text{for } d \text{ odd}. \end{cases}$$

If we set $k_i = m_i = r_{i-1} r_i$, $i = 1, \dots, d$, in (16), then

$$\dim \operatorname{Sub}_{k_1, \dots, k_d}(\mathbb{V}_1, \dots, \mathbb{V}_d) = \sum\nolimits_{i=1}^{d} r_{i-1} r_i (n_i - r_{i-1} r_i) + \prod\nolimits_{j=1}^{d-1} r_j^2,$$

and with this, we have the following corollary of (31).

Corollary 7.5. *Let P_d be the path graph of $d \ge 2$ vertices and $d-1$ edges. Let $(r_1, \dots, r_{d-1}) \in \mathbb{N}^{d-1}$ be such that $\operatorname{TNS}(P_d; r_1, \dots, r_{d-1}; \mathbb{V}_1, \dots, \mathbb{V}_d)$ is supercritical or critical and $m_i = r_{i-1} r_i$, $i = 1, \dots, d$. Then*

$$\operatorname{TNS}(P_d; r_1, \dots, r_{d-1}; \mathbb{V}_1, \dots, \mathbb{V}_d) \subseteq \operatorname{Sub}_{m_1, \dots, m_d}(\mathbb{V}_1, \dots, \mathbb{V}_d)$$

[5] We cannot have $(r_1, r_2) \le (s_1, s_2)$ or $(s_1, s_2) \le (r_1, r_2)$ since both are assumed to be P_3-ranks of T. So that leaves either (i) $r_1 \le s_1$, $r_2 \ge s_2$ or (ii) $r_1 \ge s_1$, $r_2 \le s_2$ — we pick (i) if $r_1 r_2 \le s_1 s_2$ and (ii) if $s_1 s_2 \le r_1 r_2$. By symmetry the subsequent arguments are identical.

is a subvariety of codimension

$$\prod_{j=1}^{d-1} r_j^2 - \Bigl(\sum_{j=1}^{\lfloor d/2\rfloor -1} r_{j+1}^2(r_j^2-1) + r_{d-j-1}^2(r_{d-j}^2-1) + m_{d/2}^2\Bigr).$$

In particular, we have

$$\begin{aligned}\textsc{tns}(P_2; r; \mathbb{V}_1, \mathbb{V}_2) &= \sigma_r\bigl(\operatorname{Seg}(\mathbb{V}_1, \mathbb{V}_2)\bigr),\\ \textsc{tns}(P_3; r_1, r_2; \mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3) &= \operatorname{Sub}_{r_1, r_1 r_2, r_2}(\mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3),\\ \textsc{tns}(P_d; \underbrace{1, \dots, 1}_{d-1}; \mathbb{V}_1, \dots, \mathbb{V}_d) &= \operatorname{Seg}(\mathbb{V}_1, \dots, \mathbb{V}_d),\end{aligned}$$

where $r, r_1, r_2 \in \mathbb{N}$. For all other d and r, we have a strict inclusion

$$\textsc{tns}(P_d; r_1, \dots, r_{d-1}; \mathbb{V}_1, \dots, \mathbb{V}_d) \subsetneq \operatorname{Sub}_{m_1, \dots, m_d}(\mathbb{V}_1, \dots, \mathbb{V}_d).$$

We now provide a few examples of generic and maximal TT-ranks, in which G is the path graph P_2, P_3, or P_4 in Figure 2. Again, these represent the simplest instances of more general results for tree tensor networks in Section 8 and are intended to be instructive. In the following let $\mathbb{V}_i$ be a vector space of dimension n_i, $i = 1, 2, 3, 4$.

Example 7.6 (Generic/maximal TT-rank of $\mathbb{C}^{n_1 \times n_2}$)**.** In this case maximal and generic G-ranks are equivalent since G-rank and border G-rank are equal for acyclic graphs (see Corollary 8.6). By (28), the generic P_2-rank of $\mathbb{V}_1 \otimes \mathbb{V}_2 \cong \mathbb{C}^{n_1 \times n_2}$ is $\min\{n_1, n_2\}$, i.e., the generic matrix rank.

Example 7.7 (Generic/maximal TT-rank of $\mathbb{C}^{n_1 \times n_2 \times n_3}$)**.** Assume for simplicity that $n_1 n_2 \geq n_3$, we will show that the generic P_3-rank of $\mathbb{V}_1 \otimes \mathbb{V}_2 \otimes \mathbb{V}_3 \cong \mathbb{C}^{n_1 \times n_2 \times n_3}$ is (n_1, n_3). Let $(g_1, g_2) \in \mathbb{N}^2$. By Corollary 3.4, if $\textsc{tns}(P_3; g_1, g_2; \mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3)$ is supercritical at vertices 1 and 3, then

$$\textsc{tns}(P_3; g_1, g_2; \mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3) \subsetneq \mathbb{V}_1 \otimes \mathbb{V}_2 \otimes \mathbb{V}_3.$$

So we may assume that g_1 and g_2 are large enough so that $\textsc{tns}(P_3; g_1, g_2; \mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3)$ is critical or subcritical at vertex 1 or vertex 3. Thus we must have $g_1 \geq n_1$ or $g_2 \geq n_3$. By Proposition 3.2,

$$\textsc{tns}(P_3; n_1, n_2; \mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3) = \mathbb{V}_1 \otimes \mathbb{V}_2 \otimes \mathbb{V}_3$$

and hence the generic P_3-rank of $\mathbb{V}_1 \otimes \mathbb{V}_2 \otimes \mathbb{V}_3$ is (n_1, n_3).

Example 7.8 (Generic/maximal TT-rank of $\mathbb{C}^{2\times 2\times 2\times 2}$)**.** Let $n_1 = n_2 = n_3 = n_4 = 2$. Let $(g_1, g_2, g_3) \in \mathbb{N}^3$ be the generic P_4-rank of $\mathbb{V}_1 \otimes \mathbb{V}_2 \otimes \mathbb{V}_3 \otimes \mathbb{V}_4 \cong \mathbb{C}^{2\times 2\times 2\times 2}$. By the definition of P_4-rank we must have

$$(g_1, g_2, g_3) \leq (2, 4, 2).$$

Suppose that either $g_1 = 1$ or $g_3 = 1$ — by symmetry, suppose $g_1 = 1$. In this case a 4-tensor in $\textsc{tns}(P_4; 1, g_2, g_3; \mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3, \mathbb{V}_4)$ has rank at most one when regarded as a matrix in $\mathbb{V}_1 \otimes (\mathbb{V}_2 \otimes \mathbb{V}_3 \otimes \mathbb{V}_4)$. However, a generic element in $\mathbb{V}_1 \otimes \mathbb{V}_2 \otimes \mathbb{V}_3 \otimes \mathbb{V}_4$ has rank two when regarded as a matrix in $\mathbb{V}_1 \otimes (\mathbb{V}_2 \otimes \mathbb{V}_3 \otimes \mathbb{V}_4)$, a contradiction. Thus $g_1 = g_3 = 2$. Now by Proposition 3.2, if $g_2 \leq 3$, then

$$\textsc{tns}(P_4; 2, g_2, 2; \mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3, \mathbb{V}_4) = \textsc{tns}(P_2; g_2; \mathbb{V}_1 \otimes \mathbb{V}_2, \mathbb{V}_3 \otimes \mathbb{V}_4) \subsetneq \mathbb{V}_1 \otimes \mathbb{V}_2 \otimes \mathbb{V}_3 \otimes \mathbb{V}_4,$$

since $\textsc{tns}(P_2; g_2; 4, 4)$ is the set of all 4×4 matrices of rank at most three. Hence the generic P_4-rank of $\mathbb{V}_1 \otimes \mathbb{V}_2 \otimes \mathbb{V}_3 \otimes \mathbb{V}_4$ must be $(2, 4, 2)$.

8. Tree tensor networks

We will now discuss TTNS-ranks, i.e., G-ranks where G is a tree (see Figure 3). Since G is assumed to be connected and every connected acyclic graph is a tree, this includes all acyclic G with tensor trains ($G = P_d$) and star tensor network states ($G = S_d$) as special cases. A particularly important result in this case is that TTNS-rank is always *unique* and is easily computable as matrix ranks of various flattenings of tensors.

We first establish the intersection property that we saw in Examples 7.1 and 7.2 more generally.

Lemma 8.1. *Let G be a tree with d vertices and c edges. Let $(r_1,\dots,r_c)$ and $(s_1,\dots,s_c)\in\mathbb{N}^c$ be such that $\operatorname{TNS}(G;r_1,\dots,r_c;\mathbb{V}_1,\dots,\mathbb{V}_d)$ and $\operatorname{TNS}(G;s_1,\dots,s_c;\mathbb{V}_1,\dots,\mathbb{V}_d)$ are subcritical. Then*

$$\operatorname{TNS}(G;r_1,\dots,r_c;\mathbb{V}_1,\dots,\mathbb{V}_d)\cap\operatorname{TNS}(G;s_1,\dots,s_c;\mathbb{V}_1,\dots,\mathbb{V}_d)=\operatorname{TNS}(G;t_1,\dots,t_c;\mathbb{V}_1,\dots,\mathbb{V}_d),$$

where $(t_1,\dots,t_c)\in\mathbb{N}^c$ is given by $t_j=\min\{r_j,s_j\}$, $j=1,\dots,c$.

Proof. Without loss of generality, let the vertex 1 be a degree-one vertex (which must exist in a tree) and let the edge e_1 be adjacent to the vertex 1. It is straightforward to see that

$$\operatorname{TNS}(G;t_1,\dots,t_c;\mathbb{V}_1,\dots,\mathbb{V}_d)\subseteq\operatorname{TNS}(G;r_1,\dots,r_c;\mathbb{V}_1,\dots,\mathbb{V}_d)\cap\operatorname{TNS}(G;s_1,\dots,s_c;\mathbb{V}_1,\dots,\mathbb{V}_d).$$

To prove the opposite inclusion, we proceed by induction on d. The required inclusion holds for $d\le 3$ by our calculations in Examples 7.1 and 7.2. Assume that it holds for $d-1$. Now observe that by Proposition 3.2,

$$\operatorname{TNS}(G;r_1,r_2,\dots,r_c;\mathbb{V}_1,\dots,\mathbb{V}_d)=\operatorname{TNS}(G';r_2,\dots,r_c;\mathbb{V}_1\otimes\mathbb{V}_2,\mathbb{V}_3,\dots,\mathbb{V}_d),$$

where G' is the graph obtained by removing vertex 1 and its only edge e_1. Similarly,

$$\operatorname{TNS}(G;s_1,s_2,\dots,s_c;\mathbb{V}_1,\dots,\mathbb{V}_d)=\operatorname{TNS}(G';s_2,\dots,s_c;\mathbb{V}_1\otimes\mathbb{V}_2,\mathbb{V}_3,\dots,\mathbb{V}_d).$$

Therefore,

$$\begin{aligned}\operatorname{TNS}(G;r_1,r_2,\dots,r_c;\mathbb{V}_1,\dots,\mathbb{V}_d)\cap\operatorname{TNS}(G;s_1,s_2,\dots,s_c;\mathbb{V}_1,\dots,\mathbb{V}_d)=&\\ \operatorname{TNS}(G';r_2,\dots,r_c;\mathbb{V}_1\otimes\mathbb{V}_2,\dots,\mathbb{V}_d)\cap\operatorname{TNS}(G';s_2,\dots,s_c;\mathbb{V}_1\otimes\mathbb{V}_2,\dots,\mathbb{V}_d).&\end{aligned}$$

Given $T\in\operatorname{TNS}(G';r_2,\dots,r_c;\mathbb{V}_1\otimes\mathbb{V}_2,\dots,\mathbb{V}_d)\cap\operatorname{TNS}(G';s_2,\dots,s_c;\mathbb{V}_1\otimes\mathbb{V}_2,\dots,\mathbb{V}_d)$, there must be some subspace $\mathbb{W}\subseteq\mathbb{V}_1\otimes\mathbb{V}_2$ such that $\dim\mathbb{W}\le\min\{r_2,s_2\}$ and thus

$$T\in\operatorname{TNS}(G';r_2,\dots,r_c;\mathbb{W},\mathbb{V}_3,\dots,\mathbb{V}_d)\cap\operatorname{TNS}(G';s_2,\dots,s_c;\mathbb{W},\mathbb{V}_3,\dots,\mathbb{V}_d).$$

By the induction hypothesis, we have

$$\begin{aligned}\operatorname{TNS}(G';r_2,\dots,r_c;\mathbb{W},\mathbb{V}_3,\dots,\mathbb{V}_d)\cap\operatorname{TNS}(G';s_2,\dots,s_c;\mathbb{W},\mathbb{V}_3,\dots,\mathbb{V}_d)&\\ =\operatorname{TNS}(G';t_2,\dots,t_c;\mathbb{W},\mathbb{V}_3,\dots,\mathbb{V}_d).&\end{aligned}$$

Since both $\operatorname{TNS}(G;r_1,r_2,\dots,r_c;\mathbb{V}_1,\dots,\mathbb{V}_d)$ and $\operatorname{TNS}(G;s_1,s_2,\dots,s_c;\mathbb{V}_1,\dots,\mathbb{V}_d)$ are subcritical, $\operatorname{TNS}(G;t_1,t_2,\dots,t_c;\mathbb{V}_1,\dots,\mathbb{V}_d)$ is also subcritical. By (15) and Proposition 3.2,

$$\begin{aligned}T\in\operatorname{TNS}(G';t_2,\dots,t_c;\mathbb{W},\mathbb{V}_3,\dots,\mathbb{V}_d)&\subseteq\operatorname{TNS}(G';t_2,\dots,t_c;\mathbb{V}_1\otimes\mathbb{V}_2,\dots,\mathbb{V}_d)\\&=\operatorname{TNS}(G;t_1,t_2,\dots,t_c;\mathbb{V}_1,\dots,\mathbb{V}_d),\end{aligned}$$

showing that the inclusion also holds for d, completing our induction proof. □

We are now ready to prove a more general version of Lemma 8.1, removing the subcriticality requirement. Note that Lemma 8.1 is inevitable since our next proof relies on it.

Theorem 8.2 (Intersection of TTNS). *Let G be a tree with d vertices and c edges. Let $(r_1,\dots,r_c)$ and $(s_1,\dots,s_c)\in\mathbb{N}^c$. Then*

$$\operatorname{TNS}(G;r_1,\dots,r_c;\mathbb{V}_1,\dots,\mathbb{V}_d)\cap\operatorname{TNS}(G;s_1,\dots,s_c;\mathbb{V}_1,\dots,\mathbb{V}_d)=\operatorname{TNS}(G;t_1,\dots,t_c;\mathbb{V}_1,\dots,\mathbb{V}_d),$$

where $(t_1,\dots,t_c)\in\mathbb{N}^c$ is given by $t_j=\min\{r_j,s_j\}$, $j=1,\dots,c$.

Proof. We just need to establish '$\subseteq$' as '$\supseteq$' is obvious. Let $T\in\operatorname{TNS}(G;r_1,\dots,r_c;\mathbb{V}_1,\dots,\mathbb{V}_d)\cap\operatorname{TNS}(G;s_1,\dots,s_c;\mathbb{V}_1,\dots,\mathbb{V}_d)$. Then there exist subspaces $\mathbb{W}_1\subseteq\mathbb{V}_1,\dots,\mathbb{W}_c\subseteq\mathbb{V}_c$ such that both $\operatorname{TNS}(G;r_1,\dots,r_c;\mathbb{W}_1,\dots,\mathbb{W}_d)$ and $\operatorname{TNS}(G;s_1,\dots,s_c;\mathbb{W}_1,\dots,\mathbb{W}_d)$ are subcritical and

$$\begin{aligned}T\in\operatorname{TNS}(G;r_1,\dots,r_c;\mathbb{W}_1,\dots,\mathbb{W}_d)\cap\operatorname{TNS}(G;s_1,\dots,s_c;\mathbb{W}_1,\dots,\mathbb{W}_d)&\\ =\operatorname{TNS}(G;t_1,\dots,t_c;\mathbb{W}_1,\dots,\mathbb{W}_d)\subseteq\operatorname{TNS}(G;t_1,\dots,t_c;\mathbb{V}_1,\dots,\mathbb{V}_d),&\end{aligned}$$

where the equality follows from Lemma 8.1 and the inclusion from (15). □

Note that subspace varieties also satisfy the intersection property in Theorem 8.2, i.e.,

$$\mathrm{Sub}_{r_1,\dots,r_d}(\mathbb{V}_1,\dots,\mathbb{V}_d)\cap\mathrm{Sub}_{s_1,\dots,s_d}(\mathbb{V}_1,\dots,\mathbb{V}_d)=\mathrm{Sub}_{t_1,\dots,t_d}(\mathbb{V}_1,\dots,\mathbb{V}_d).$$

However neither Lemma 8.1 nor Theorem 8.2 holds for graphs containing cycles, as we will see in Example 9.7 and Proposition 9.8.

We now establish the uniqueness of G-rank for any acyclic G, i.e., for a given d-tensor T, the G-rank of T is a unique d-tuple in $\mathbb{N}^d$, as opposed to a subset of a few d-tuples in $\mathbb{N}^d$. In particular, the TT-rank and STNS-rank of a tensor are both unique.

Theorem 8.3 (Uniqueness of TTNS-rank)**.** *The G-rank of a tensor $T\in\mathbb{V}_1\otimes\cdots\otimes\mathbb{V}_d$ is unique if G is a d-vertex tree.*

Proof. We may assume that T is nondegenerate; if not, we may replace $\mathbb{V}_1,\dots,\mathbb{V}_d$ by appropriate subspaces without affecting the G-rank of T, by Theorem 6.1. Let $(r_1,\dots,r_d)$ and $(s_1,\dots,s_d)\in\mathbb{N}^d$ be two G-ranks of T. By Proposition 6.6, T lies in the intersection of $\mathrm{TNS}(G;r_1,\dots,r_d;\mathbb{V}_1,\dots,\mathbb{V}_d)$ and $\mathrm{TNS}(G;s_1,\dots,s_d;\mathbb{V}_1,\dots,\mathbb{V}_d)$, and both of them are subcritical since T is nondegnerate. By Lemma 8.1, T lies in $\mathrm{TNS}(G;t_1,\dots,t_d;\mathbb{V}_1,\dots,\mathbb{V}_d)$ where $t_i\le r_i$ and $t_i\le s_i$, $i=1,\dots,d$. By the minimality in the definition of G-rank, we must have $r_i=s_i=t_i$, $i=1,\dots,d$, as required. ☐

Corollary 8.4 (Uniqueness of generic TTNS-rank)**.** *Let G be a tree with d vertices. For any vector spaces $\mathbb{V}_1,\dots,\mathbb{V}_d$, there is a unique generic G-rank for $\mathbb{V}_1\otimes\cdots\otimes\mathbb{V}_d$.*

As we saw in Examples 7.7 and 7.8, the unique generic P_3-rank of $\mathbb{C}^{m\times mn\times n}$ is (m,n) while the unique generic P_4-rank of $\mathbb{C}^{2\times2\times2\times2}$ is $(2,4,2)$. There will be many examples in Sections 9 and 10 showing that neither Theorem 8.3 nor Corollary 8.4 holds for graphs containing cycles.

The next result is an important one. It guarantees that whenever G is acyclic, G-rank is upper semicontinuous and thus the kind of illposedness issues in [6] where a tensor may lack a best low-rank approximation do not happen.

Theorem 8.5 (TTNS are closed)**.** *Let G be a tree with d vertices. For any vector spaces $\mathbb{V}_1,\dots,\mathbb{V}_d$ and any $(r_1,\dots,r_c)\in\mathbb{N}^c$, the set $\mathrm{TNS}(G;r_1,\dots,r_d;\mathbb{V}_1,\dots,\mathbb{V}_d)$ is Zariski closed in $\mathbb{V}_1\otimes\cdots\otimes\mathbb{V}_d$.*

Proof. We proceed by induction on d. The statement holds trivially when $d=1$ by (12). Suppose it holds for all trees with at most $d-1$ vertices. Let G be a d-vertex tree. Applying Proposition 3.3 to $\mathrm{TNS}(G;r_1,\dots,r_c;\mathbb{V}_1,\dots,\mathbb{V}_d)$, there is a subbundle $\mathcal{E}$ of the bundle $\mathcal{S}_1\times\cdots\times\mathcal{S}_d$ on $\mathrm{Gr}(k_1,n_1)\times\cdots\times\mathrm{Gr}(k_d,n_d)$ whose fiber over a point $([\mathbb{W}_1],\dots,[\mathbb{W}_d])$ is

$$F:=\mathrm{TNS}(G;r_1,\dots,r_c;\mathbb{W}_1,\dots,\mathbb{W}_d),$$

with the surjective birational map $\pi:\mathcal{E}\to\mathrm{TNS}(G;r;\mathbb{V}_1,\dots,\mathbb{V}_d)$ induced by the projection map

$$\mathrm{pr}_2:\bigl[\mathrm{Gr}(k_1,n_1)\times\cdots\times\mathrm{Gr}(k_d,n_d)\bigr]\times\bigl[\mathbb{V}_1\times\cdots\times\mathbb{V}_d\bigr]\to\mathbb{V}_1\times\cdots\times\mathbb{V}_d.$$

pr_2 is a closed map since Grassmannian varieties are projective. Thus π is also a closed map. To show that $\mathrm{TNS}(G;r_1,\dots,r_c;\mathbb{V}_1,\dots,\mathbb{V}_d)$ is Zariski closed, it suffices to show that $\mathcal{E}$ is Zariski closed in $\bigl[\mathrm{Gr}(k_1,n_1)\times\cdots\times\mathrm{Gr}(k_d,n_d)\bigr]\times\bigl[\mathbb{V}_1\times\cdots\times\mathbb{V}_d\bigr]$. As $\mathcal{E}$ is a fiber bundle on $\mathrm{Gr}(k_1,n_1)\times\cdots\times\mathrm{Gr}(k_d,n_d)$ with fiber F, it in turn suffices to show that F is Zariski closed in $\mathbb{V}_1\otimes\cdots\otimes\mathbb{V}_d$. Since $F=\mathrm{TNS}(G;r_1,\dots,r_c;\mathbb{W}_1,\dots,\mathbb{W}_d)$ is critical, we may apply Proposition 3.2 to F and regard F as the tensor network of a tree with $d-1$ vertices. Therefore F is Zariski closed by the induction hypothesis. ☐

Theorems 8.3 and 8.5 together yield the following corollary, which is in general false when G is not acyclic (see Theorem 9.12).

Corollary 8.6 (Border TTNS-rank)**.** *For any tree G, border G-rank equals G-rank and is unique.*

It is well-known that tensor rank is NP-hard but multilinear rank is polynomial-time computable. We will next see that like multilinear rank, G-rank is polynomial-time computable whenever G is acyclic. We begin with some additional notations. Let $G=(V,E)$ be a connected tree with

d vertices and c edges. Since G is a connected tree, removing any edge $\{i,j\} \in E$ results in a disconnected graph with two components.[6] Let $V(i)$ denote the set of vertices in the component connected to the vertex i. Then we have a disjoint union $V = V(i) \sqcup V(j)$. Now for any vector spaces $\mathbb{V}_1, \dots, \mathbb{V}_d$, we may define a *flattening map* associated with each edge $\{i,j\} \in E$,

$$\flat_{ij} : \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d \to \Bigl(\bigotimes\nolimits_{h \in V(i)} \mathbb{V}_h\Bigr) \otimes \Bigl(\bigotimes\nolimits_{h \in V(j)} \mathbb{V}_h\Bigr). \tag{32}$$

Note that $\operatorname{rank}\bigl(\flat_{ij}(T)\bigr)$ is polynomial-time computable as matrix rank for any $T \in \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$.

Lemma 8.7. *Let $\mathbb{V}_1, \mathbb{V}_2, \mathbb{E}$ be vector spaces and let $\kappa : (\mathbb{V}_1 \otimes \mathbb{E}) \times (\mathbb{E}^* \otimes \mathbb{V}_2) \to \mathbb{V}_1 \otimes \mathbb{V}_2$ defined by contracting factors in $\mathbb{E}$ with factors in $\mathbb{E}^*$. For any $T_1 \in \mathbb{V}_1 \otimes \mathbb{E}$ and $T_2 \in \mathbb{E}^* \otimes \mathbb{V}_2$, the rank of $\kappa((T_1, T_2))$ is at most $\dim \mathbb{E}$.*

Proof. We denote by r the dimension of $\mathbb{E}$ and we take a basis $e_1, \dots, e_r$ of $\mathbb{E}$ with dual basis $e_1^*, \dots, e_r^*$. By definition, we may write

$$T_1 = \sum\nolimits_{i=1}^{r} e_i \otimes x_i, \quad T_2 = \sum\nolimits_{i=1}^{r} e_i^* \otimes y_i,$$

for some $x_i \in \mathbb{V}_1, y_i \in \mathbb{V}_2, i = 1, \dots, r$. Hence we have

$$\kappa((T_1, T_2)) = \sum\nolimits_{i=1}^{r} x_i \otimes y_i,$$

and this shows that the rank of $\kappa((T_1, T_2))$ is at most r. $\square$

Theorem 8.8 (TTNS-rank is polynomial-time computable)**.** *Let G be a tree with d vertices and c edges labeled as in (8), i.e., $V = \{1, \dots, d\}$ and $E = \bigl\{\{i_1, j_1\}, \dots, \{i_c, j_c\}\bigr\}$. Then for any $T \in \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$, the G-rank of T is given by*

$$\operatorname{rank}_G(T) = (r_1, \dots, r_c), \qquad r_p = \operatorname{rank}\bigl(\flat_{i_p j_p}(T)\bigr), \qquad p = 1, \dots, c. \tag{33}$$

Proof. We will show that for $(r_1, \dots, r_c)$ as defined in (33), (i) $T \in \operatorname{TNS}(G; r_1, \dots, r_c; \mathbb{V}_1, \dots, \mathbb{V}_d)$, i.e., $\operatorname{rank}_G(T) \le (r_1, \dots, r_c)$; and (ii) it is minimal in $\mathbb{N}_0^c$ such that (i) holds. Together, (i) and (ii) imply that $\operatorname{rank}_G(T) = (r_1, \dots, r_c)$.

Let p be an integer such that $1 \le p \le c$. Since $r_p = \operatorname{rank}\bigl(\flat_{i_p j_p}(T)\bigr)$, we may write

$$T = \sum\nolimits_{i=1}^{r_p} R_i \otimes S_i, \quad R_i \in \bigotimes\nolimits_{h \in V(i_p)} \mathbb{V}_h, \quad S_i \in \bigotimes\nolimits_{h \in V(j_p)} \mathbb{V}_h, \quad i = 1, \dots, r_p.$$

Let $\mathbb{E}_p$ be a vector space of dimension r_p attached to the edge $\{i_p, j_p\}$. Let $e_1, \dots, e_{r_p}$ be a basis of $\mathbb{E}_p$ and $e_1^*, \dots, e_{r_p}^*$ be the corresponding dual basis of $\mathbb{E}_p^*$. Then

$$T = \kappa_G\Bigl(\Bigl[\sum\nolimits_{i=1}^{r_p} R_i \otimes e_i\Bigr] \otimes \Bigl[\sum\nolimits_{j=1}^{r_p} e_j^* \otimes S_j\Bigr]\Bigr).$$

We let R_i (resp. S_j) take the role of T and repeat the argument. Let $\{i_q, j_q\} \in E$ be such that i_q, j_q are both in $V(i_p)$. Then $V(i_p)$ is the disjoint union $V(i_p, i_q) \sqcup V(i_p, j_q)$ where $V(i_p, *)$ denotes the subset of $V(i_p)$ comprising all vertices in the component of vertex $*$ upon removal of $\{i_q, j_q\}$ (see Footnote 6). Since $R_i \in \bigotimes_{h \in V(i_p)} \mathbb{V}_h$, we may write

$$R_i = \sum\nolimits_{k=1}^{r} P_{ik} \otimes Q_{ki}, \quad P_{ik} \in \bigotimes\nolimits_{h \in V(i_p, i_q)} \mathbb{V}_h, \quad Q_{kj} \in \bigotimes\nolimits_{h \in V(i_p, j_q)} \mathbb{V}_h, \quad k = 1, \dots, r, \tag{34}$$

for some $r \in \mathbb{N}$. We claim that we may choose $r \le r_q$. Since $r_q = \operatorname{rank}\bigl(\flat_{i_q j_q}(T)\bigr)$,

$$\dim \operatorname{span}\{P_{ik} : i = 1, \dots, r_p,\ k = 1, \dots, r\} = r_q,$$

and so we may find $P_1, \dots, P_{r_q}$ such that each P_{ik} is a linear combination of $P_1, \dots, P_{r_q}$. Thus for each $i = 1, \dots, r_p$, R_i can be written as

$$R_i = \sum\nolimits_{k=1}^{r_q} P_k \otimes Q'_{ki}, \quad P_k \in \bigotimes\nolimits_{h \in V(i_p, i_q)} \mathbb{V}_h, \quad Q'_{ki} \in \bigotimes\nolimits_{h \in V(i_p, j_q)} \mathbb{V}_h, \quad k = 1, \dots, r_q,$$

[6] These components are also connected trees and so the subsequent argument may be repeated on each of them.

where each Q'_{ki} is a linear combination of the Q_{ki}'s in (34). Then we may write T as

$$\begin{aligned} T &= \kappa_G\Bigl(\Bigl[\sum_{i=1}^{r_p}\Bigl(\sum_{k=1}^{r_q} P_k\otimes f_k\Bigr)\otimes\Bigl(\sum_{l=1}^{r_q} f_l^*\otimes Q'_{li}\Bigr)\otimes e_i\Bigr]\otimes\Bigl[\sum_{j=1}^{r_p} e_j^*\otimes S_j\Bigr]\Bigr)\\ &= \kappa_G\Bigl(\Bigl[\sum_{k=1}^{r_q} P_k\otimes f_k\Bigr]\otimes\Bigl[\sum_{i,l=1}^{r_p,r_q} f_l^*\otimes Q'_{li}\otimes e_i\Bigr]\otimes\Bigl[\sum_{j=1}^{r_p} e_j^*\otimes S_j\Bigr]\Bigr), \end{aligned}$$

where $f_1,\dots,f_{r_q}$ is a basis of $\mathbb{E}_q$ and $f_1^*,\dots,f_{r_q}^*$ is the corresponding dual basis of $\mathbb{E}_q^*$.

Repeating the process in the previous paragraph until we exhaust all edges, we obtain $T = \kappa_G(T_1\otimes\cdots\otimes T_d)$ for some

$$T_i \in \Bigl(\bigotimes_{j\in\textsc{in}(i)}\mathbb{E}_j\Bigr)\otimes\mathbb{V}_i\otimes\Bigl(\bigotimes_{k\in\textsc{out}(i)}\mathbb{E}_k^*\Bigr),\quad \dim\mathbb{E}_j = r_j,\quad i=1,\dots,d,\ j=1,\dots,c.$$

and thus $T\in\textsc{tns}(G;r_1,\dots,r_c;\mathbb{V}_1,\dots,\mathbb{V}_d)$, establishing (i).

Suppose $(s_1,\dots,s_c)\le(r_1,\dots,r_c)$ is such that $T\in\textsc{tns}(G;s_1,\dots,s_c;\mathbb{V}_1,\dots,\mathbb{V}_d)$, i.e., $T = \kappa_G(T_1\otimes\cdots\otimes T_d)$ for some

$$T_i \in \Bigl(\bigotimes_{j\in\textsc{in}(i)}\mathbb{F}_j\Bigr)\otimes\mathbb{V}_i\otimes\Bigl(\bigotimes_{k\in\textsc{out}(i)}\mathbb{F}_k^*\Bigr),\quad \dim\mathbb{F}_j = s_j,\quad i=1,\dots,d,\ j=1,\dots,c.$$

However, for each $p=1,\dots,c$, we can also write

$$T = \kappa_G\Bigl(\Bigl[\bigotimes_{h\in V(i_p)} T_h\Bigr]\otimes\Bigl[\bigotimes_{h\in V(j_p)} T_h\Bigr]\Bigr)$$

where

$$\begin{aligned} \Bigl[\bigotimes_{h\in V(i_p)} T_h\Bigr] &\in \Bigl(\bigotimes_{h\in V(i_p)}\Bigl(\bigotimes_{j\in\textsc{in}(h)}\mathbb{F}_j\otimes\mathbb{V}_h\otimes\bigotimes_{j\in\textsc{out}(h),j\ne p}\mathbb{F}_j^*\Bigr)\Bigr)\otimes\mathbb{F}_p^*,\\ \Bigl[\bigotimes_{h\in V(j_p)} T_h\Bigr] &\in \mathbb{F}_p\otimes\Bigl(\bigotimes_{k\in V(j_p)}\Bigl(\bigotimes_{j\in\textsc{in}(k),j\ne p}\mathbb{F}_j\otimes\mathbb{V}_k\otimes\bigotimes_{j\in\textsc{out}(k)}\mathbb{F}_j^*\Bigr)\Bigr). \end{aligned}$$

This together with Lemma 8.7 imply that $r_p = \operatorname{rank}\bigl(\flat_{i_pj_p}(T)\bigr)\le s_p$ and therefore $r_p = s_p$, establishing (ii). □

A weaker form of Theorem 8.8 that establishes the upper bound $\operatorname{rank}_G(T)\le(r_1,\dots,r_c)$ in (33) under the assumption that $\mathbb{V}_1,\dots,\mathbb{V}_d$ are Hilbert spaces appeared in [2, Theorem 3.3]. An immediate consequence of Theorem 8.8 is the following.

Corollary 8.9 (TTNS as an algebraic variety)**.** *Let $G=(V,E)$ be a tree with d vertices and c edges. For any $(n_1,\dots,n_d)\in\mathbb{N}^d$ and $(r_1,\dots,r_c)\in\mathbb{N}^c$, $\textsc{tns}(G;r_1,\dots,r_c;n1,\dots,n_d)$ is an irreducible algebraic variety in $\mathbb{C}^{n_1\times\cdots\times n_d}$ with vanishing ideal generated by all $(r_p+1)\times(r_p+1)$ minors of the flattening map* (32) *for $\{i_p,j_p\}\in E$, taken over all $p=1,\dots,c$.*

We will see in the next section that when G contains a cycle, G-rank cannot be computed as matrix ranks of flattening maps and $\textsc{tns}(G;r_1,\dots,r_c;n_1,\dots,n_d)$ is not Zariski closed in general.

9. Matrix product states

We will restrict our attention in this section to the case where $G=C_d$, the cyclic graph on d vertices in Figure 4. This gives us the matrix product states — one of the most widely used class of tensor network states. We start by stating the dimensions of MPS in the supercritical and subcritical cases. Theorem 9.1 and Corollary 9.2 appear as [39, Theorem 4.10 and Corollary 4.11].

Theorem 9.1 (Dimension of MPS)**.** *Let C_d be the cycle graph with $d\ge 3$ vertices and d edges. Let $(r_1,\dots,r_d)\in\mathbb{N}^d$ be such that $\textsc{tns}(C_d;r_1,\dots,r_d;n_1,\dots,n_d)$ is supercritical or critical. Then*

$$\dim\textsc{tns}(C_d;r_1,\dots,r_d;n_1,\dots,n_d) = \sum_{i=1}^d r_ir_{i+1}n_i - \sum_{i=1}^d r_i^2 + 1,$$

where $r_{d+1}\coloneqq r_1$.

It follows from the above dimension count that every element in $\mathbb{C}^{m\times n\times mn}$ is an MPS state.

Corollary 9.2. *Let C_3 be the three-vertex cycle graph and*

$$\dim \mathbb{V}_1 = n_1, \quad \dim \mathbb{V}_2 = n_2, \quad \dim \mathbb{V}_3 = n_1 n_2.$$

Then

$$\overline{\text{TNS}}(C_3; n_1, n_2, 1; \mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3) = \mathbb{V}_1 \otimes \mathbb{V}_2 \otimes \mathbb{V}_3.$$

Theorem 9.3 (Generic C_3-ranks of MPS)**.** *Let C_3 be the cycle graph on three vertices. If $\dim \mathbb{V}_i = n_i$, $i = 1, 2, 3$ and $n_2 n_3 \geq n_1, n_1 n_3 \geq n_2$, then $\mathbb{V}_1 \otimes \mathbb{V}_2 \otimes \mathbb{V}_3$ has generic C_3-rank $(n_1, n_2, 1)$.*

Proof. First we have

$$\text{TNS}(C_3; n_1, n_2, 1; \mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3) = \text{TNS}(P_3; n_1, n_2; \mathbb{V}_1, \mathbb{V}_3, \mathbb{V}_2) = \mathbb{V}_1 \otimes \mathbb{V}_2 \otimes \mathbb{V}_3,$$

where the first equality follows from Proposition 3.5 and the second follows from Proposition 3.2. Next, we claim that there does not exist $(r_1, r_2, 1) \in \mathbb{N}^3$ such that

$$\overline{\text{TNS}}(C_3; r_1, r_2, 1; \mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3) = \mathbb{V}_1 \otimes \mathbb{V}_2 \otimes \mathbb{V}_3$$

and that $r_1 \leq n_1$, $r_2 \leq n_2$ with at least one strict inequality. Take $r_1 < n_1$ for example (the other case may be similarly argued). Again by Proposition 3.5,

$$\dim \text{TNS}(C_3; r_1, r_2, 1; \mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3) = \dim \text{TNS}(P_3; r_1, r_2; \mathbb{V}_1, \mathbb{V}_3, \mathbb{V}_2).$$

By Proposition 3.3,

$$\begin{aligned} \dim \text{TNS}(P_3; r_1, r_2; \mathbb{V}_1, \mathbb{V}_3, \mathbb{V}_2) &= \dim \operatorname{Gr}(r_1, n_1) + \dim \text{TNS}(P_2; r_2; r_1 n_3, n_2) \\ &\leq r_1(n_1 - r_1) + r_1 n_2 n_3 < n_1 n_2 n_3 \end{aligned}$$

as $n_2 n_3 \geq n_1 > r_1$. Thus

$$\text{TNS}(C_3; r_1, r_2, 1; \mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3) \subsetneq \mathbb{V}_1 \otimes \mathbb{V}_2 \otimes \mathbb{V}_3.$$

Hence $(n_1, n_2, 1)$ is a generic C_3-rank of $\mathbb{V}_1 \otimes \mathbb{V}_2 \otimes \mathbb{V}_3$. $\square$

Corollary 9.4. *If $\dim \mathbb{V}_1 = \dim \mathbb{V}_2 = \dim \mathbb{V}_3 = n$, then $(n, n, 1)$, $(1, n, n)$, and $(n, 1, n)$ are all the generic C_3-ranks of $\mathbb{V}_1 \otimes \mathbb{V}_2 \otimes \mathbb{V}_3$.*

Proof. Apply Theorem 9.3 to the case $n_1 = n_2 = n_3 = n$ to see that $(n, n, 1)$ is a generic rank of $\mathbb{V}_1 \otimes \mathbb{V}_2 \otimes \mathbb{V}_3$. Now we may permute $\mathbb{V}_1, \mathbb{V}_2$ and $\mathbb{V}_3$ to obtain the other two generic C_3-ranks. $\square$

In case the reader is led to the false belief that the sums of entries of generic C_3-ranks are always equal, we give an example to show that this is not the case.

Example 9.5. Let $\mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3$ be of dimensions n_1, n_2, n_3 where

$$n_2 \neq n_3 \quad \text{and} \quad n_i n_j \geq n_k \text{ whenever } \{i, j, k\} = \{1, 2, 3\}.$$

By Theorem 9.3, we see that $(1, n_2, n_1)$ and $(n_1, 1, n_3)$ are both generic C_3-ranks of $\mathbb{V}_1 \otimes \mathbb{V}_2 \otimes \mathbb{V}_3$ but $1 + n_2 + n_1 \neq n_1 + 1 + n_3$.

The following provides a necessary condition for generic C_d-rank of supercritical MPS.

Theorem 9.6 (Test for generic C_d-rank)**.** *Let $(n_1, \dots, n_d) \in \mathbb{N}^d$ and $(r_1, \dots, r_d) \in \mathbb{N}^d$ be such that $\text{TNS}(C_d; r_1, \dots, r_d; n_1, \dots, n_d)$ is supercritical, i.e., $n_i \geq r_i r_{i+1}, i = 1, \dots, d$, where $r_{d+1} \coloneqq r_1$. If $(r_1, \dots, r_d)$ is a generic C_d-rank of $\mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$, then there exists $j \in \{1, \dots, d\}$ such that*

$$\prod\nolimits_{i \neq j} n_i < d n_j. \tag{35}$$

Proof. Fix $(r_1, \dots, r_d) \in \mathbb{N}^d$ and consider the function

$$f(n_1, \dots, n_d) \coloneqq \prod\nolimits_{i=1}^d n_i - \sum\nolimits_{i=1}^d r_i r_{i+1} n_i + \sum\nolimits_{i=1}^d r_i^2 - 1.$$

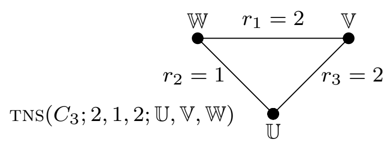
We have

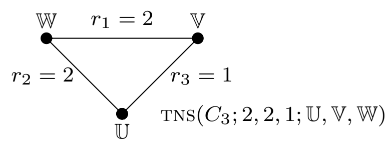
$$f(n_1, \dots, n_d) \geq \prod\nolimits_{i=1}^d n_i - \sum\nolimits_{i=1}^d n_i^2 + \sum\nolimits_{i=1}^d r_i^2 - 1 = \sum\nolimits_{i=1}^d \frac{1}{d} \prod\nolimits_{i=1}^d (n_i - n_i^2) + \sum\nolimits_{i=1}^d r_i^2 - 1.$$

If $(r_1, \dots, r_d)$ is a generic C_3-rank, then $f(n_1, \dots, n_d) = 0$ by Theorem 9.1. This implies that for some $j = 1, \dots, d$, we must have (35). $\square$

The next example shows that intersection of MPS are more intricate than that of TTNS. In particular, Lemma 8.1 does not hold for MPS.

Example 9.7 (Intersection of MPS)**.** Let $\mathbb{U}$, $\mathbb{V}$, $\mathbb{W}$ be two-dimensional vector spaces associated respectively to vertices 1, 2, 3 of C_3. Let $r_i \in \mathbb{N}$ be the weight of the edge *not* adjacent to the vertex $i \in V = \{1, 2, 3\}$.





By Corollary 9.4, we see that

$$\text{TNS}(C_3; 2, 1, 2; \mathbb{U}, \mathbb{V}, \mathbb{W}) = \text{TNS}(C_3; 2, 2, 1; \mathbb{U}, \mathbb{V}, \mathbb{W}) = \mathbb{U} \otimes \mathbb{V} \otimes \mathbb{W}.$$

Observe that an element in $\text{TNS}(C_3; 2, 1, 2; \mathbb{U}, \mathbb{V}, \mathbb{W})$ takes the form

$$u_1 \otimes v_1 \otimes w_1 + u_1 \otimes v_2 \otimes w_2 + u_2 \otimes v_3 \otimes w_1 + u_2 \otimes v_4 \otimes w_2$$

where $u_1, u_2 \in \mathbb{U}$, $v_1, v_2, v_3, v_4 \in \mathbb{V}$, $w_1, w_2 \in \mathbb{W}$. By symmetry, an element in $\text{TNS}(C_3; 2, 2, 1; \mathbb{U}, \mathbb{V}, \mathbb{W})$ takes the form

$$u_1 \otimes v_1 \otimes w_1 + u_1 \otimes v_2 \otimes w_2 + u_2 \otimes v_1 \otimes w_3 + u_2 \otimes v_2 \otimes w_4$$

where $u_1, u_2 \in \mathbb{U}$, $v_1, v_2 \in \mathbb{V}$, $w_1, w_2, w_3, w_4 \in \mathbb{W}$. However, $\text{TNS}(C_3; 1, 1, 2; \mathbb{U}, \mathbb{V}, \mathbb{W})$ is a proper subset of $\mathbb{U} \otimes \mathbb{V} \otimes \mathbb{W}$ since an element in $\text{TNS}(C_3; 1, 1, 2; \mathbb{U}, \mathbb{V}, \mathbb{W})$ takes the form

$$u_1 \otimes v_1 \otimes w + u_2 \otimes v_2 \otimes w$$

where $u_1, u_2 \in \mathbb{U}$, $v_1, v_2 \in \mathbb{V}$, $w \in \mathbb{W}$. Hence

$$\text{TNS}(C_3; 2, 1, 2; \mathbb{U}, \mathbb{V}, \mathbb{W}) \cap \text{TNS}(C_3; 2, 2, 1; \mathbb{U}, \mathbb{V}, \mathbb{W}) \supsetneq \text{TNS}(C_3; 2, 1, 1; \mathbb{U}, \mathbb{V}, \mathbb{W})$$

and thus Lemma 8.1 does not hold for C_3.

The main difference between tensor network states associated to trees and those associated to cycle graphs is that one may apply Proposition 3.2 to trees but not to graphs containing cycles. In particular, the induction argument used to prove Lemma 8.1 fails for non-acyclic graphs.

Example 9.7 generalizes to the following proposition, i.e., Theorem 8.2 is always false for MPS.

Proposition 9.8 (Intersection of MPS)**.** *Let $d \ge 3$ and C_d be the cycle graph with d vertices. Then there exists $\mathbb{V}_1, \dots, \mathbb{V}_d$ and $\underline{r} = (r_1, \dots, r_d)$, $\underline{s} = (s_1, \dots, s_d) \in \mathbb{N}^d$ such that*

$$\text{TNS}(C_d; \underline{t}; \mathbb{V}_1, \dots, \mathbb{V}_d) \subsetneq \text{TNS}(C_d; \underline{r}; \mathbb{V}_1, \dots, \mathbb{V}_d) \cap \text{TNS}(C_d; \underline{s}; \mathbb{V}_1, \dots, \mathbb{V}_d), \tag{36}$$

where $\underline{t} = (t_1, \dots, t_d) \in \mathbb{N}^d$ is given by $t_i = \min(r_i, s_i)$, $i = 1, \dots, d$.

Proof. Let all $\mathbb{V}_i$'s be two-dimensional. If d is odd, set

$$\underline{r} = (2, 1, 2, 1, \dots, 2, 1, 2), \quad \underline{s} = (2, 2, 1, 2, \dots, 1, 2, 1), \quad \underline{t} = (2, 1, 1, 1, \dots, 1, 1, 1),$$

and it is easy to check that (36) holds with strict inclusion. If $d \equiv 0 \pmod 4$, write $d = 4m$, set

$$\underline{r} = (\overbrace{1, 2, \dots, 1, 2}^{2m}, \overbrace{2, 1, \dots, 2, 1}^{2m}), \quad \underline{s} = (\overbrace{2, 1, \dots, 2, 1}^{2m}, \overbrace{1, 2, \dots, 1, 2}^{2m});$$

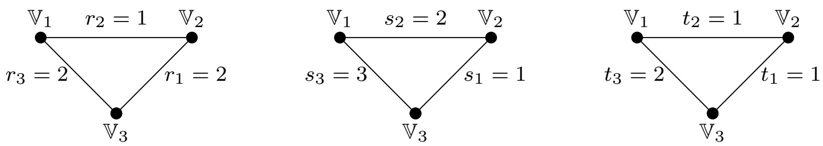
if $d \equiv 2 \pmod 4$, write $d = 4m + 2$, set

$$\underline{r} = (\overbrace{1, 2, \dots, 1, 2}^{2m}, 1, 1, \overbrace{2, 1, \dots, 2, 1}^{2m}), \quad \underline{s} = (\overbrace{2, 1, \dots, 2, 1}^{2m}, 2, 2, \overbrace{1, 2, \dots, 1, 2}^{2m}).$$

In both cases, we have $\underline{t} = (1, \dots, 1)$ and it is easy to verify (36). $\square$

We saw that generic C_d-rank is not unique. The next example shows, nonconstructively, that there are tensors with nonunique C_d-ranks. We give explicitly constructed examples in Section 10.

Example 9.9 (MPS-rank not unique up to permutation)**.** Let $\dim \mathbb{V}_1 = \dim \mathbb{V}_2 = 2$ and $\dim \mathbb{V}_3 = 3$. Consider the MPS's of C_3-ranks $\underline{r} = (2,1,2)$, $\underline{s} = (1,2,3)$, and $\underline{t} = (1,1,2)$ respectively:



It is straightforward to see that

$$\operatorname{TNS}(C_3;1,1,2;\mathbb{V}_1,\mathbb{V}_2,\mathbb{V}_3) \subsetneq \operatorname{TNS}(C_3;2,1,2;\mathbb{V}_1,\mathbb{V}_2,\mathbb{V}_3) \cap \operatorname{TNS}(C_3;1,2,3;\mathbb{V}_1,\mathbb{V}_2,\mathbb{V}_3),$$
$$\overline{\operatorname{TNS}}(C_3;2,1,2;\mathbb{V}_1,\mathbb{V}_2,\mathbb{V}_3) = \overline{\operatorname{TNS}}(C_3;1,2,3;\mathbb{V}_1,\mathbb{V}_2,\mathbb{V}_3) = \mathbb{V}_1 \otimes \mathbb{V}_2 \otimes \mathbb{V}_3.$$

Thus a generic $T \in \mathbb{V}_1 \otimes \mathbb{V}_2 \otimes \mathbb{V}_3$ such that $T \notin \operatorname{TNS}(C_3;1,1,2;\mathbb{V}_1,\mathbb{V}_2,\mathbb{V}_3)$ has at least two C_3-ranks $(2,1,2)$ and $(1,2,3)$.

As we saw in Theorem 8.5 and Corollary 8.6, for an acyclic G, G-rank is closed, i.e., border G-rank and G-rank are equivalent. We will see here that this is always false when G is not acyclic. In the following, we show that MPS-rank is never closed by constructing a d-tensor whose border C_d-rank is strictly less than C_d-rank for each $d \geq 3$, extending [17, Theorem 2].

Let $\mathbb{V} = \mathbb{C}^{n\times n}$ and let $\{E_{ij} \in \mathbb{C}^{n\times n} : i,j = 1,\dots,n\}$ be the standard basis as in the proof of Theorem 5.1. For each $d \geq 3$, define

$$T \coloneqq \sum\nolimits_{i,j,k=1}^{n} (E_{ij} \otimes E_{jj} + E_{ii} \otimes E_{ij}) \otimes E_{jk} \otimes R_{ki} \in \mathbb{V}^{\otimes d}, \tag{37}$$

where for each $k, i = 1,\dots,n$,

$$R_{ki} \coloneqq \sum\nolimits_{j_1,\dots,j_{d-4}=1}^{n} E_{kj_1} \otimes E_{j_1 j_2} \otimes \cdots \otimes E_{j_{d-5} j_{d-4}} \otimes E_{j_{d-4} i} \in \mathbb{V}^{\otimes(d-3)}.$$

We adopt the convention that $E_{jk} \otimes R_{ki} = E_{ji}$ in (37) when $d = 3$ and $R_{ki} = E_{ki}$ if $d = 4$. The following is a straightforward generalization of [17, Theorem 2], with a similar proof.

Theorem 9.10. *Let $d \geq 3$ and T be defined as above. Then (i) $T \in \overline{\operatorname{TNS}}(C_d;n,\dots,n;\mathbb{V},\dots,\mathbb{V})$; (ii) $T \notin \operatorname{TNS}(C_d;n,\dots,n;\mathbb{V},\dots,\mathbb{V})$; (iii) $T \notin \operatorname{Sub}_{m_1,\dots,m_d}(\mathbb{V},\dots,\mathbb{V})$ whenever $m_i \leq n^2$, $i = 1,\dots,d$, with at least one strict inequality.*

Corollary 9.11. $\overline{\operatorname{rank}}_{C_d}(T) = (n,\dots,n)$ *but* $\operatorname{rank}_{C_d}(T) \neq (n,\dots,n)$.

Proof. By Theorem 9.10, we have $\operatorname{rank}_{C_d}(T) \neq (n,\dots,n)$ and $\overline{\operatorname{rank}}_{C_d}(T) \leq (n,\dots,n)$. It remains to establish equality in the latter. Suppose not, then $\overline{\operatorname{rank}}_{C_d}(T) = (r_1,\dots,r_d)$ where $r_i \leq n$, $i = 1,\dots,d$, with at least one strict inequality. Assume without loss of generality that $r_1 < n$. Then $r_1 r_2 < n^2$ and thus

$$T \in \operatorname{Sub}_{n^2, r_1 r_2, n^2,\dots,n^2}(\mathbb{V},\dots,\mathbb{V}),$$

contradicting Theorem 9.10(iii). $\square$

Theorem 9.12 (Nonacyclic G-rank is not closed)**.** *Let $G = (V,E)$ be a connected graph with d vertices and c edges that contains a cycle subgraph C_b for some $b \leq d$, i.e., there exist b vertices $i_1,\dots,i_b \in V$ such that the b edges $(i_1,i_2),\dots,(i_{b-1},i_b),(i_b,i_1) \in E$. Then there exists $S \in \mathbb{V}^{\otimes d}$ such that*

$$\overline{\operatorname{rank}}_G(S) = (s_1,\dots,s_c) \leq (r_1,\dots,r_c) = \operatorname{rank}_G(S),$$

with $s_i < r_i$ for at least one $i \in \{1,\dots,c\}$.

Proof. Relabeling the vertices if necessary, we may assume that $i_1 = 1, \dots, i_b = b$, i.e., the first b vertices of G form the cycle subgraph C_b. Relabeling the edges if necessary, we may also assume that $r_1, \dots, r_b$ are the weights associated to $(1,2), \dots, (b,1)$, i.e., the edges of C_b. Let $r_1 = \cdots = r_b = n$ and $r_{b+1} = \cdots = r_c = 1$. Let $T \in \mathbb{V}^{\otimes b}$ be as defined in (37) (with b in place of d) and let $S = T \otimes v^{\otimes(d-b)} \in \mathbb{V}^d$ where $v \in \mathbb{V}$ is a nonzero vector. Then

$$S \in \overline{\text{TNS}}(G; \underbrace{n, \dots, n}_{b}, \underbrace{1, \dots, 1}_{c-b}; n^2, \dots, n^2).$$

So $\overline{\operatorname{rank}}_G(S) \le (n, \dots, n, 1, \dots, 1) \in \mathbb{N}^b \times \mathbb{N}^{c-b} = \mathbb{N}^c$. On the other hand, if $(r_1, \dots, r_b, 1, \dots, 1) \in \mathbb{N}^c$ is a border G-rank of S such that $r_i \le n$, $i = 1, \dots, b$, with at least one strict inequality, then $S \in \operatorname{Sub}_{m_1,\dots,m_d}(\mathbb{V}, \dots, \mathbb{V})$ where $m_i \le n^2$, $i = 1, \dots, b$, with at least one strict inequality. But this contradicts Theorem 9.10(iii). Hence $\overline{\operatorname{rank}}_G(S) = (n, \dots, n, 1, \dots, 1) \in \mathbb{N}^b \times \mathbb{N}^{c-b} = \mathbb{N}^c$. Lastly, by the way S is constructed, if $(r_1, \dots, r_b) \in \mathbb{N}^b$ is a C_b-rank of T, then $(r_1, \dots, r_b, 1, \dots, 1) \in \mathbb{N}^c$ is a G-rank of S. Since by Corollary 9.11, $\operatorname{rank}_{C_b}(T) = (r_1, \dots, r_b) \in \mathbb{N}^b$ where $n \le r_i$, $i = 1, \dots, b$, with at least one strict inequality, this completes the proof. ☐

10. Tensor network ranks of common tensors

We will compute some G-ranks of some well-known tensors from different fields:

- **Algebra:** G-rank of decomposable tensors and monomials, S_n-ranks of decomposable symmetric and skew-symmetric tensors (Section 10.1);
- **Physics:** P_d-rank and C_d-rank of the d-qubit W and GHZ states (Section 10.2);
- **Computing:** P_3-rank and C_3-rank of the structure tensor for matrix-matrix product (Section 10.3).

10.1. **Tensors in algebra.**

The following shows that the term 'rank-one' is unambiguous — all rank-one tensors have G-rank one regardless of G, generalizing Example 7.3.

Proposition 10.1. *Let G be a connected graph with d vertices and c edges. Let $0 \ne v_1 \otimes \cdots \otimes v_d \in \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_d$ be a rank-one tensor. Then the G-rank of $v_1 \otimes \cdots \otimes v_d$ is unique and equals $(1, \dots, 1) \in \mathbb{N}^c$.*

Proof. As usual, let $\dim \mathbb{V}_i = n_i$, $i = 1, \dots, n_d$. It follows easily from Definition 2.1 that

$$\text{TNS}(G; 1, \dots, 1; n_1, \dots, n_d) = \operatorname{Seg}(\mathbb{V}_1, \dots, \mathbb{V}_d), \tag{38}$$

and so $(1, \dots, 1)$ is a G-rank of $v_1 \otimes \cdots \otimes v_d$. Conversely, if $(r_1, \dots, r_c)$ is a G-rank of $v_1 \otimes \cdots \otimes v_d$, then $(r_1, \dots, r_c)$ is minimal in $\mathbb{N}^c$ such that $v_1 \otimes \cdots \otimes v_d \in \text{TNS}(G; r_1, \dots, r_c; n_1, \dots, n_d)$. However, by (38), $v_1 \otimes \cdots \otimes v_d \in \text{TNS}(G; 1, \dots, 1; n_1, \dots, n_d)$, and obviously $1 \le r_i$, $i = 1, \dots, c$, implying that $r_i = 1$, $i = 1, \dots, c$. ☐

We next discuss *decomposable symmetric tensors* and *decomposable skew-symmetric tensors*. For those unfamiliar with these notions, they are defined respectively as

$$v_1 \circ \cdots \circ v_d \coloneqq \frac{1}{d!} \sum\nolimits_{\sigma \in \mathfrak{S}_d} v_{\sigma(1)} \otimes \cdots \otimes v_{\sigma(d)} \in \mathsf{S}^d(\mathbb{V}) \subseteq \mathbb{V}^d,$$
$$v_1 \wedge \cdots \wedge v_d \coloneqq \frac{1}{d!} \sum\nolimits_{\sigma \in \mathfrak{S}_d} \varepsilon(\sigma) v_{\sigma(1)} \otimes \cdots \otimes v_{\sigma(d)} \in \mathsf{\Lambda}^d(\mathbb{V}) \subseteq \mathbb{V}^d,$$

where $v_1, \dots, v_d \in \mathbb{V}$, an n-dimensional vector space, and where $\varepsilon(\sigma)$ denotes the sign of the permutation $\sigma \in \mathfrak{S}_d$.

Theorem 10.2 (STNS-rank of decomposable (skew-)symmetric tensors)**.** *Let S_n be the star graph with vertices $1, \dots, n$ and with 1 as the root vertex. If $d = n$ and $v_1, \dots, v_n \in \mathbb{V}$ are linearly independent, then $v_1 \circ \cdots \circ v_n$ and $v_1 \wedge \cdots \wedge v_n$ both have S_n-rank $(n, \dots, n) \in \mathbb{N}^n$.*

Proof. Since $\text{TNS}(S_n; n, \dots, n; n, \dots, n) = \mathbb{V}^{\otimes n}$,

$$v_1 \circ \cdots \circ v_n,\ v_1 \wedge \cdots \wedge v_n \in \text{TNS}(S_n; n, \dots, n; n, \dots, n). \tag{39}$$

It remains to show that there does not exist $(r_1, \dots, r_n)$ such that $r_i \le n$, $i = 1, \dots, n$, with at least one strict inequality, such that $v_1 \circ \cdots \circ v_n$ and $v_1 \wedge \cdots \wedge v_n \in \text{TNS}(S_n; r_1, \dots, r_n; n, \dots, n)$. But this is clear as $v_1 \circ \cdots \circ v_n$ and $v_1 \wedge \cdots \wedge v_n$ are nondegenerate tensors in $\mathbb{V}^{\otimes n}$. ☐

It is easy to construct explicit S_n-decompositions of $v_1 \circ \cdots \circ v_n$ and $v_1 \wedge \cdots \wedge v_n$ in Theorem 10.2. Let $\mathbb{E}$ be n-dimensional with basis $e_1, \dots, e_n$ and dual basis $e_1^*, \dots, e_n^*$. Consider

$$\Sigma = \frac{1}{n!} \sum\nolimits_{\sigma \in \mathfrak{S}_n} v_{\sigma(1)} \otimes e_{\sigma(2)} \otimes \cdots \otimes e_{\sigma(n)} \in \mathbb{V} \otimes \mathbb{E}^{\otimes (n-1)},$$
$$\Lambda = \frac{1}{n!} \sum\nolimits_{\sigma \in \mathfrak{S}_n} \varepsilon(\sigma) v_{\sigma(1)} \otimes e_{\sigma(2)} \otimes \cdots \otimes e_{\sigma(n)} \in \mathbb{V} \otimes \mathbb{E}^{\otimes (n-1)},$$

and $M = \sum_{i=1}^n e_j^* \otimes v_j \in \mathbb{E}^* \otimes \mathbb{V}$. Then

$$\kappa_{S_n}(\Sigma \otimes M^{\otimes (n-1)}) = v_1 \circ \cdots \circ v_n \qquad \text{and} \qquad \kappa_{S_n}(\Lambda \otimes M^{\otimes (n-1)}) = v_1 \wedge \cdots \wedge v_n.$$

A *monomial* of degree d in n variables $x_1, \dots, x_n$ may be regarded [15] as a decomposable symmetric d-tensor over an n-dimensional vector space $\mathbb{V}$:

$$x_1^{p_1} \cdots x_n^{p_n} = v_1^{\otimes p_1} \circ \cdots \circ v_n^{\otimes p_n} \in \mathsf{S}^d(\mathbb{V}),$$

where $p_1, \dots, p_n$ are nonnegative integers such that $p_1 + \cdots + p_n = d$. If $d = n$ and $p_1 = \cdots = p_d = 1$, then $v_1 \circ \cdots \circ v_d = x_1 \cdots x_d$, i.e., a decomposable symmetric tensor is a special case.

Proposition 10.3 (G-rank of monomials)**.** *Let G be a connected graph with d vertices and c edges. Let $n \le d$ and $p_1 + \cdots + p_n = d$. Let $\mathbb{U}$ be a d-dimensional vector space with basis $u_1, \dots, u_d$ and $\mathbb{V}$ an n-dimensional vector space with basis $v_1, \dots, v_n$. If $u_1 \circ \cdots \circ u_d \in \text{TNS}(G; r_1, \dots, r_c; d, \dots, d)$, then $v_1^{\otimes p_1} \circ \cdots \circ v_n^{\otimes p_n} \in \text{TNS}(G; r_1, \dots, r_c; n, \dots, n)$, i.e.,*

$$\operatorname{rank}_G(v_1^{\otimes p_1} \circ \cdots \circ v_n^{\otimes p_n}) \le \operatorname{rank}_G(u_1 \circ \cdots \circ u_d). \tag{40}$$

Proof. Let $\varphi : \mathbb{U} \to \mathbb{V}$ be the linear map that sends $u_{p_i+1}, \dots, u_{p_{i+1}}$ to v_{i+1}, $i = 0, \dots, n-1$, where $p_0 \coloneqq 0$. Let $\varphi^{\otimes d} : \mathbb{U}^{\otimes d} \to \mathbb{V}^{\otimes d}$ be the linear map induced by φ. Observe that $\varphi^{\otimes d}(u_1 \circ \cdots \circ u_d) = v_1^{\otimes p_1} \circ \cdots \circ v_n^{\otimes p_n}$. Also, $\varphi^{\otimes d}\bigl(\text{TNS}(G; r_1, \dots, r_c; d, \dots, d)\bigr) \subseteq \text{TNS}(G; r_1, \dots, r_c; d, \dots, d)$. Hence $v_1^{\otimes p_1} \circ \cdots \circ v_n^{\otimes p_n} \in \text{TNS}(G; r_1, \dots, r_c; d, \dots, d) \cap (\mathbb{V}^{\otimes p_1} \otimes \cdots \otimes \mathbb{V}^{\otimes p_n}) = \text{TNS}(G; r_1, \dots, r_c; n, \dots, n)$. ☐

The case where number of variables is larger than degree, i.e., $n > d$, reduces to Proposition 10.3. In this case, a monomial $x_1^{p_1} \cdots x_n^{p_n}$ of degree d will not involve all variables $x_1, \dots, x_n$ and, as a tensor, $v_1^{\otimes p_1} \circ \cdots \circ v_n^{\otimes p_n} \in \mathsf{S}^d(\mathbb{W})$ where $\mathbb{W} \subseteq \mathbb{V}$ is an appropriate subspace of dimension $\le d$.

For comparison, the *Waring rank*[7] or *symmetric tensor rank* of a monomial $v_1^{\otimes p_1} \circ \cdots \circ v_n^{\otimes p_n}$ where $p_1 \ge p_2 \ge \cdots \ge p_n > 0$, is $\prod_{i=1}^{n-1}(p_i + 1)$, whereas its *Waring border rank* is $\prod_{i=2}^{n}(p_i + 1)$ [18, 27]; its multilinear rank is easily seen[8] to be $(n, \dots, n)$. The monomials include $v_1 \circ \cdots \circ v_n$ as a special case. As for $v_1 \wedge \cdots \wedge v_n$, tensor rank and border rank are still open but its multilinear rank is also easily seen to be $(n, \dots, n)$.

[7]The Waring rank of a polynomial f of degree d is the smallest r such that $f = \sum_{i=1}^r l_i^d$ for linear forms $l_1, \dots, l_r$. Its Waring border rank is the smallest r such that f is a limit of a sequence of polynomials of Waring rank r.

[8]The first flattening $\flat_1(v_1^{\otimes p_1} \circ \cdots \circ v_n^{\otimes p_n})$, as a linear map, sends v_i to $v_1^{p_1} \circ \cdots \circ v_i^{p_i - 1} \circ \cdots v_n^{p_n}$, $i = 1, \dots, n$. It has full rank n since $v_1^{p_1} \circ \cdots \circ v_i^{p_i - 1} \circ \cdots v_n^{p_n}$, $i = 1, \dots, n$, are linearly independent. Ditto for other flattenings.

10.2. **Tensors in physics.** Let $\mathbb{V}$ be two-dimensional and v_1, v_2 be a basis. For any $d \geq 3$, the d-tensors in $\mathbb{V}^d$ defined by

$$\mathrm{W}_d := \sum\nolimits_{i=1}^{d} v_1^{\otimes(i-1)} \otimes v_2 \otimes v_1^{\otimes(d-i)} \qquad \text{and} \qquad \mathrm{GHZ}_d := v_1^{\otimes d} + v_2^{\otimes d},$$

are called the d-qubit *W state* and *GHZ state* (for Werner and Greenberger–Horne–Zeilinger) respectively.

Observe that $\mathrm{W}_d = v_1^{d-1} \circ v_2$ is a decomposable symmetric tensor corresponding to the monomial $x_1^{d-1}x_2$. By (39) and Proposition 10.3, we obtain $\mathrm{W}_d \in \mathrm{TNS}(S_d; d, \dots, d; 2, \dots, 2)$ but this also trivially follows from $\mathrm{TNS}(S_d; d, \dots, d; 2, \dots, 2) = \mathrm{TNS}(S_d; 2, \dots, 2; 2, \dots, 2) = \mathbb{V}^d$, which shows that the inequality can be strict in (40).

We start with the P_d-rank of W_d. Let the vertices of P_d be $1, \dots, d$ and edges be oriented $(1,2), (2,3), \dots, (d-1, d)$. Let $\mathbb{E}_i \simeq \mathbb{E}$ be a two-dimensional vector space associated to $(i, i+1)$, $i = 1, \dots, d-1$, with basis e_1, e_2 and dual basis e_1^*, e_2^*. Note that $\mathrm{W}_d = \kappa_{P_d}(A \otimes B^{\otimes(d-2)} \otimes C) \in \mathrm{TNS}(P_d; 2, \dots, 2; 2, \dots, 2)$ with $A = v_1 \otimes e_1^* + v_2 \otimes e_2^* \in \mathbb{V} \otimes \mathbb{E}^*$, $B = e_1 \otimes (v_1 \otimes e_1^* + v_2 \otimes e_2^*) + e_2 \otimes v_1 \otimes e_2^* \in \mathbb{V} \otimes \mathbb{E}^* \otimes \mathbb{E}$, $C = v_1 \otimes e_2 + v_2 \otimes e_1 \in \mathbb{V} \otimes \mathbb{E}$. So if $\mathrm{rank}_{P_d}(\mathrm{W}_d) = (r_1, \dots, r_{d-1})$, then we must have $r_i = 1$ or 2 for $i = 1, \dots, d-1$. Let $r_0 = r_d = 1$. Suppose $r_{i-1}r_i = 1$ for some $i \in \{1, \dots, d\}$. Then $\mathrm{W}_d \in \mathbb{V}^{\otimes(i-1)} \otimes \mathbb{W} \otimes \mathbb{V}^{\otimes(d-i)}$ where $\mathbb{W} \subseteq \mathbb{V}$ is a one-dimensional subspace, which is impossible by the definition of W_d. Thus we obtain the following.

Lemma 10.4. *If* $\mathrm{rank}_{P_d}(\mathrm{W}_d) = (r_1, \dots, r_{d-1})$*, then* $r_i \in \{1, 2\}$ *and* $r_{i-1}r_i \geq 2$*,* $i = 1, \dots, d$*, where* $r_0 = r_d = 1$*.*

Theorem 10.5 (TT-rank of W state)**.** *Let* $d \geq 3$*. Then* $\mathrm{rank}_{P_d}(\mathrm{W}_d) = (2, \dots, 2) \in \mathbb{N}^{d-1}$*.*

Proof. Suppose not. By Lemma 10.4, there exists $i \in \{2, \dots, d-2\}$ such that $r_i = 1$, $r_j = 2$ for all $j \neq i$, and

$$\mathrm{W}_d \in \mathrm{TNS}(P_d; \overbrace{2, \dots, 2}^{i-1}, 1, \overbrace{2, \dots, 2}^{d-i-1}; 2, \dots, 2).$$

This implies that $\mathrm{W}_d = X \otimes Y$ for some $X \in \mathbb{V}^{\otimes i}$ and $Y \in \mathbb{V}^{\otimes(d-i)}$, i.e., W_d is a rank-one 2-tensor in $\mathbb{V}^{\otimes i} \otimes \mathbb{V}^{\otimes(d-i)}$, which is impossible by the definition of W_d. □

We next deduce the C_d-ranks of W_d. Let the vertices of C_d be $1, \dots, d$ and edges be oriented $(1,2), (2,3), \dots, (d, d+1)$, with $d+1 := 1$. Let $\mathbb{E}_i \simeq \mathbb{E}$ be a two-dimensional vector space associated to $(i, i+1)$, $i = 1, \dots, d$, with basis e_1, e_2 and dual basis e_1^*, e_2^*. Note that $\mathrm{W}_d = \kappa_{C_d}(A \otimes B^{\otimes(d-2)} \otimes C) \in \mathrm{TNS}(C_d; 2, \dots, 2; 2, \dots, 2)$ with $A = e_1 \otimes v_1 \otimes e_1^* + e_2 \otimes v_2 \otimes e_2^*$, $B = e_1 \otimes (v_1 \otimes e_1^* + v_2 \otimes e_2^*) + e_2 \otimes v_1 \otimes e_2^*$, $C = e_2 \otimes v_1 \otimes (e_1^* + e_2^*) + e_1 \otimes v_2 \otimes e_1^*$, all in $\mathbb{E} \otimes \mathbb{V} \otimes \mathbb{E}^*$.

Theorem 10.6 (MPS-rank of W state)**.** *Let* $d \geq 3$*. Then* $\mathrm{rank}_{C_d}(\mathrm{W}_d) = (r_1, \dots, r_d) \in \mathbb{N}^d$ *if and only if* $r_i = 1$ *for some* $i \in \{1, \dots, d\}$ *and all other* $r_j = 2$*,* $j \neq i$*.*

Proof. The "if" part follows from Theorem 10.5. Since $\mathrm{W}_d \in \mathrm{TNS}(C_d; 2, \dots, 2; 2, \dots, 2)$, if $(r_1, \dots, r_d)$ is a C_d-rank of W_d with $r_i \geq 2$ for all $i = 1, \dots, d$, then $r_i = 2$ for all $i = 1, \dots, d$. However, we also have $\mathrm{TNS}(C_d; r_1, \dots, r_d; 2, \dots, 2) \subseteq \mathrm{TNS}(C_d; 2, \dots, 2; 2, \dots, 2)$ for $1 \leq r_1, \dots, r_d \leq 2$. This implies that $(2, \dots, 2)$ cannot be a C_d-rank of W_d, showing the "only if" part. □

We now proceed to the GHZ state. $\mathrm{GHZ}_2 = v_1^{\otimes 2} + v_2^{\otimes 2} \in \mathbb{V} \otimes \mathbb{V}$ is known as the *Bell state*, a rank-two 2×2 matrix. For the only connected graph with two vertices, P_2, and it is clear that $\mathrm{rank}_{P_2}(\mathrm{GHZ}_2) = 2$. For $d \geq 3$, the arguments for deducing the P_d-rank and C_d-rank of GHZ_d are very similar to those used for W_d and we will be brief. First observe that $\mathrm{GHZ}_d = \kappa_{P_d}(A \otimes B^{\otimes(d-2)} \otimes C) \in \mathrm{TNS}(P_d; 2, \dots, 2; 2, \dots, 2)$ with $A = v_1 \otimes e_1^* + v_2 \otimes e_2^*$, $B = e_1 \otimes v_1 \otimes e_1^* + e_2 \otimes v_2 \otimes e_2^*$, $C = e_1 \otimes v_1 + e_2 \otimes v_2$, and we may obtain the following analogue of Theorem 10.5.

Theorem 10.7 (TT-rank of GHZ state)**.** *Let* $d \geq 3$*. Then* $\mathrm{rank}_{P_d}(\mathrm{GHZ}_d) = (2, \dots, 2) \in \mathbb{N}^{d-1}$*.*

Likewise, $\mathrm{GHZ}_d = \kappa_{C_d}(D^{\otimes d}) \in \mathrm{TNS}(C_d; 2, \dots, 2; 2, \dots, 2)$ with $D = e_1 \otimes v_1 \otimes e_1^* + e_2 \otimes v_2 \otimes e_2^*$, and we obtain the following analogue of Theorem 10.6

Theorem 10.8 (MPS-rank of GHZ state)**.** *Let $d \geq 3$. Then* $\operatorname{rank}_{C_d}(\mathrm{GHZ}_d) = (r_1, \dots, r_d) \in \mathbb{N}^d$ *if and only if $r_i = 1$ for some $i \in \{1, \dots, d\}$ and all other $r_j = 2$, $j \neq i$.*

For comparison, note that W_d and GHZ_d are respectively the monomial $x^{d-1}y$ and the binary form $x^d + y^d$ regarded as symmetric tensors. By our discussion at the end of Section 10.1, the Waring rank of W_d is d while that of GHZ_d is at most $2(d+1)$; the border rank and multilinear rank of both states are 2 and $(2, \dots, 2)$ respectively.

10.3. **Tensors in computing.** Let $\mathbb{U} = \mathbb{C}^{m\times n}$, $\mathbb{V} = \mathbb{C}^{n\times p}$, and $\mathbb{W} = \mathbb{C}^{m\times p}$. Let $\mu_{m,n,p} \in \mathbb{U}^* \otimes \mathbb{V}^* \otimes \mathbb{W} \cong \mathbb{C}^{mn\times np\times mp}$ be the structure tensor for the product of $m \times n$ and $n \times p$ rectangular matrices [40], i.e.,

$$\mu_{m,n,p} = \sum\nolimits_{i,j,k=1}^{n} u_{ik}^* \otimes v_{kj}^* \otimes w_{ij} \tag{41}$$

where $\{u_{ij} \in \mathbb{U} : i = 1, \dots, m,\ j = 1, \dots, n\}$, $\{v_{jk} \in \mathbb{V} : j = 1, \dots, n,\ k = 1, \dots, p\}$, $\{w_{ki} \in \mathbb{W} : k = 1, \dots, p,\ i = 1, \dots, p\}$ are the standard bases of the respective spaces (e.g., u_{ij} is the $m \times n$ matrix with one in the (i, j) entry and zeroes everywhere else). The reader might remember that we have encountered a special case of this tensor in (18) — that is the structure tensor for product of square matrices, i.e., $m = n = p$ and we wrote $\mu_n = \mu_{n,n,n}$.

The structure tensor for matrix-matrix product is widely regarded as the most important tensor in algebraic computational complexity theory; its tensor rank quantifies the optimum complexity for matrix-matrix product and has a current best-known bound of $O(n^{2.3728639})$ [19]. We will establish the P_3-rank and C_3-rank of $\mu_{m,n,p}$ in the following. For comparison, note that its multilinear rank is (mn, np, mp).

Theorem 10.9 (TT-rank of Strassen tensor)**.** *Let $m, n, p \geq 2$. Then* $\operatorname{rank}_{P_3}(\mu_{m,n,p}) = (mn, mp)$.

Proof. Clearly $\mu_{m,n,p} \in \operatorname{TNS}(P_3; mn, mp; mn, np, mp) = \mathbb{U}^* \otimes \mathbb{V}^* \otimes \mathbb{W}$. As $\mu_{m,n,p}$ is nondegenerate, $\mu_{m,n,p} \notin \operatorname{TNS}(P_3; r_1, r_2; mn, np, mp)$ if $r_1 < mn, r_2 = mp$ or if $r_1 = mn, r_2 < mp$. ☐

Theorem 10.10 (MPS-rank of Strassen tensor)**.** *Let $m, n, p \geq 2$. Then (m, n, p), $(mn, mp, 1)$, $(mn, 1, np)$, $(1, mp, np)$ are all C_3-ranks of $\mu_{m,n,p}$.*

Proof. By Proposition 3.5 and Theorem 10.9, we see that $(mn, mp, 1)$, $(mn, 1, np)$, $(1, mp, np)$ are C_3-ranks of $\mu_{m,n,p}$. It remains to show that (m, n, p) is also a C_3-rank of $\mu_{m,n,p}$. Let $\{e_1, \dots, e_m\}$, $\{f_1, \dots, f_n\}$, $\{g_1, \dots, g_p\}$ be any bases of vector spaces $\mathbb{E}$, $\mathbb{F}$, $\mathbb{G}$ respectively. Then $\mu_{m,n,p} = \kappa_{C_3}(A \otimes B \otimes C) \in \operatorname{TNS}(C_3; m, n, p; mn, np, mp)$ with

$$A = \sum\nolimits_{i,j=1}^{m,n} e_i \otimes u_{ij} \otimes f_j^* \in \mathbb{E} \otimes \mathbb{U} \otimes \mathbb{F}^*, \quad B = \sum\nolimits_{j,k=1}^{n,p} f_j \otimes v_{jk} \otimes g_k^* \in \mathbb{F} \otimes \mathbb{V} \otimes \mathbb{G}^*,$$

$$C = \sum\nolimits_{k,i=1}^{p,m} g_k \otimes w_{ki} \otimes e_i^* \in \mathbb{G} \otimes \mathbb{W} \otimes \mathbb{E}^*.$$

Now let $(r_1, r_2, r_3) \leq (m, n, p)$ such that $\mu_{m,n,p} \in \operatorname{TNS}(C_3; r_1, r_2, r_3; mn, np, mp)$. If, for example, $r_1 < m$, then $r_1 r_2 < mn$ and thus $\mu_{m,n,p} \in \operatorname{TNS}(C_3; r_1, r_2, r_3; r_1 r_2, np, mp) \subseteq \mathbb{C}^{r_1 r_2} \otimes \mathbb{C}^{np} \otimes \mathbb{C}^{mp}$, which is impossible by the definition of $\mu_{m,n,p}$. Similarly, we may exclude other cases, concluding that $(r_1, r_2, r_3) = (m, n, p)$. ☐

In general, we do not know if there might be other C_3-ranks of $\mu_{m,n,p}$ aside from the four in Theorem 10.10 although for the case $m = n = p = 2$, we do have

$$\operatorname{rank}_{C_3}(\mu_{2,2,2}) = \{(2, 2, 2), (1, 4, 4), (4, 1, 4), (4, 4, 1)\}.$$

To see this, note that if (r_1, r_2, r_3) is a C_3-rank of $\mu_{2,2,2}$ with $r_i \geq 2$, $i = 1, 2, 3$, then $r_1 = r_2 = r_3 = 2$ by minimality of C_3-ranks; whereas if $r_i = 1$ for some i, say $r_1 = 1$, then $\mu_{2,2,2} \in \operatorname{TNS}(C_3; 1, r_2, r_3; 2, 2, 2) = \operatorname{TNS}(P_3; r_2, r_3; 2, 2, 2)$, and as $\operatorname{rank}_{P_3}(\mu_{2,2,2}) = (4, 4)$, we get $r_2 = r_3 = 4$.

One may wonder if proofs of Theorems 10.9 and 10.10 could perhaps give a new algorithm for matrix-matrix product along the lines of Strassen's famous algorithm. The answer is no: the proofs in fact only rely on the decomposition of $\mu_{m,n,p}$ given by the standard algorithm for matrix-matrix product.

11. Tensor network ranks versus tensor rank and multilinear rank

In Section 4, we saw that G-ranks may be regarded as 'interpolants' between tensor rank and multilinear rank. We will conclude this article by showing that they are nevertheless distinct notions, i.e., tensor and multilinear ranks cannot be obtained as G-ranks. This is already evident in 3-tensors and we may limit our discussions to this case. Since $d = 3$ and there are only two connected graphs with three vertices, we have only two choices for G — either C_3 or P_3.

Proposition 11.1. *Let $\mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3$ be of dimensions ≥ 4 and let the following sets be in $\mathbb{V}_1 \otimes \mathbb{V}_2 \otimes \mathbb{V}_3$. There exists $r \in \mathbb{N}$ such that*

$$\overline{\{T : \operatorname{rank}(T) \leq r\}} \tag{42}$$

is not equal to

$$\overline{\{T : \operatorname{rank}_{P_3} \leq (r_1, r_2)\}} \quad \text{or} \quad \overline{\{T : \operatorname{rank}_{C_3}(T) \leq (r_1, r_2, r_3)\}} \tag{43}$$

for any $r_1, r_2, r_3 \in \mathbb{N}$.

Proof. Note that the set on the left of (43) is $\overline{\mathrm{TNS}}(P_3; r_1, r_2; \mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3) =: X_{r_1,r_2}$, the one on the right is $\overline{\mathrm{TNS}}(C_3; r_1, r_2, r_3; \mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3) =: Y_{r_1,r_2,r_3}$, and the set in (42) is $\sigma\bigl(\operatorname{Seg}(\mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3)\bigr) =: \Sigma_r$.

It suffices to take $r = 2$. Suppose $\Sigma_2 = X_{r_1,r_2}$ for some positive integers r_1, r_2. Then a generic element in X_{r_1,r_2} must have rank 2, which implies that $r_1, r_2 \leq 2$. By Example 7.2, we see that

$$X_{r_1,r_2} = \operatorname{Sub}_{2,4,2}(\mathbb{V}_1, \mathbb{V}_2, \mathbb{V}_3),$$

which implies that a generic $T \in X_{r_1,r_2}$ has $\mu\mathrm{rank}(T) = (2, 4, 2)$; but this gives a contradiction as any $T \in \Sigma_2$ must have $\mu\mathrm{rank}(T) \leq (2, 2, 2)$.

Next we show that $\Sigma_2 \neq Y_{r_1,r_2,r_3}$. We may assume that $r_1, r_2, r_3 \geq 2$ or otherwise Y_{r_1,r_2,r_3} becomes X_{r_1,r_2}, X_{r_1,r_3}, or X_{r_2,r_3} by (13). So we have

$$Y_{2,2,2} \subseteq Y_{r_1,r_2,r_3},$$

which implies that the structure tensor μ_2 for 2×2 matrix-matrix product (cf. (18) and (41)) is contained in Y_{r_1,r_2,r_3}. It is well-known [16] that $\overline{\operatorname{rank}}(T) = 7$ and thus $T \notin \Sigma_2$ (since that would mean $\overline{\operatorname{rank}}(T) \leq 2$). Hence $\Sigma_2 \neq Y_{r_1,r_2,r_3}$. $\square$

Proposition 11.2. *Let $\mathbb{V}$ be of dimension $n \geq 4$ and let the following sets be in $\mathbb{V} \otimes \mathbb{V} \otimes \mathbb{V}$. There exist $s_1, s_2, s_3 \in \mathbb{N}$ such that*

$$\{T : \mu\mathrm{rank}(T) \leq (s_1, s_2, s_3)\} \tag{44}$$

is not equal to

$$\overline{\{T : \operatorname{rank}_{P_3} \leq (r_1, r_2)\}} \quad \text{or} \quad \overline{\{T : \operatorname{rank}_{C_3}(T) \leq (r_1, r_2, r_3)\}}$$

for any $r_1, r_2, r_3 \in \mathbb{N}$.

Proof. We adopt the shorthands in the proof of Proposition 11.1. In addition, note that the set in (44) is $\operatorname{Sub}_{s_1,s_2,s_3}(\mathbb{V}, \mathbb{V}, \mathbb{V}) =: Z_{s_1,s_2,s_3}$. It suffices to take $(s_1, s_2, s_3) = (2, 2, 2)$. It is obvious that for any $r_1, r_2 \in \mathbb{N}$,

$$Z_{2,2,2} \neq Z_{r_1,r_1 r_2,r_2} = X_{r_1,r_2}$$

where the second equality follows from Example 7.2. Next, suppose

$$Z_{2,2,2} = Y_{r_1,r_2,r_3},$$

then a generic T in Y_{r_1,r_2,r_3} has $\mu\mathrm{rank}(T) = (2, 2, 2)$. However since $T \in Y_{r_1,r_2,r_3}$ has the form

$$T = \sum\nolimits_{i,j,k=1}^{r_1,r_2,r_3} u_{ij} \otimes v_{jk} \otimes w_{ki},$$

we have $\mu\mathrm{rank}(T) = (\min\{r_1 r_2, n\}, \min\{r_2 r_3, n\}, \min\{r_1 r_3, n\})$ and therefore

$$r_1 r_2 = r_2 r_3 = r_3 r_1 = 2,$$

which cannot hold for any positive integers r_1, r_2, r_3. Hence $Z_{2,2,2} \neq Y_{r_1,r_2,r_3}$. $\square$

12. Conclusion

We hope this article provides a convincing explanation as to why G-rank can be a better alternative to rank under many circumstances, and how it underlies the efficacy of tensor networks in computational physics and other applications. We also hope that the formalism introduced in this article would help establish a mathematical foundation for tensor networks, the study of which has thus far relied more on physical intuition, computational heuristics, and numerical experiments; but suffers from a lack of mathematically precise results built upon unambiguous definitions and rigorous proofs.

A word about MERA. A notable omission from this article is the *multiscale entanglement renormalization ansatz* or MERA, often also regarded as a tensor network state in physics literature. From a mathematical perspective, MERA differs in important ways from other known tensor networks like TT, MPS, PEPS, and every other example discussed in our article — these can all be defined purely using tensor contractions but MERA will require additional operations known as 'isometries' and 'disentanglers' in physics [35, 36, 42, 43]. From a physics perspective, the discussion in [43, Section III] also highlights a critical difference: while other tensor network states are derived from the *physical geometry*, MERA is derived from the *holographic geometry* of the quantum system.

Although our definition of a tensor network state can be readily adapted to allow for more operations and thereby also include MERA, in this article we restricted ourselves to tensor network states that can be constructed out of the three standard operations on tensors — sums, outer products, contractions — in multilinear algebra and leave MERA to furture work.

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