# COMPUTING PROPERTIES OF INDEPENDENT SETS BY GENERIC PROGRAMMING TENSOR NETWORKS *

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**Abstract.** We introduce a method that uses generic programming tensor network to compute various properties of a class of hard graph problems that can be decribed by local constraints. Let the independent set problem be an example, we show how to compute, for example, the maximum several independent set sizes, the counting of independent sets of a give size, the enumeration of independent sets of a given size. By making use of generic programming, our algorithms are very simple to implement and one can in addition directly utilize recent advances in tensor network contraction techniques such as near-optimal contraction order finding and slicing to achieve high performance. The algorithmic complexity of this approach is $2^{\mathrm{tw}(G)}$, where $\mathrm{tw}(G)$ is the treewidth of the problem graph. Other hard graph problems solvable in our framework includes the cutting problem, the vertex coloring problem, the maximal clique problem, the dominating set problem, and satisfiability problem, among others. To demonstrate the versatility of this tool, we apply it to a few examples including the calculations of the entropy constant for some hardcore lattice gases on 2D square lattices and the study of the overlap gap property on three regular graphs. We show how our method helps people understand these hard problems better.

**Key words.** independent set, tensor network, maximum independent set, independence polynomial, generic programming

**AMS subject classifications.** 05C31, 14N07

[**ML: a comment**] and [~~**ML: a resolved comment**~~]

## 1. Introduction.

In graph theory and combinatorial optimization, there is an important class of problems that can be local constraints over a vertex and its neighborhood, including the independent set problem, the cutting problem, the vertex coloring problem, the satisfiability problem, the maximal clique problem, and the vertex cover problem et al [44]. Many decision and counting properties of these problems are in general intractable at large sizes (exponential runetime in problem size in the worst case), but it is nevertheless desirable to have high-performance algorithms because of their ubiquitous applications [13, 55].

The most studied version of the above problems is finding a maximum/minimum set satisfying the contraints and the corresponding set size, while many of them belong to the hardness category NP-hard [31], i.e. it is unlikely to solve them in a polynomial time. [**MC: Is MIS really the most studied NP-hard optimization problem? I would guess it is heavily studied, but not necessarily the most studied.**] [**JG: Here, we haven't mentioned the independent set, here "version" means, e.g. counting, enumeration, devision. I think finding one of the largest/smallest set and its cardinality in the above mentioned problems is the most studied?**] In this paper, we focus on the less studied *solution space property* computation which can be harder, e.g. counting independent sets of a general graph is in #P-complete [54], but is crutial towards understanding a hard problem. Here, the *solution space property* refers to a class of quantities that not only include the maximum/minimum set size, but also include the number of sets at a give size, enumeration of all sets at a give size or direct sampling of such sets when they are not enumeratable. For the weighted version of the above problems, it also includes finding largest/smallest $k$ sets and their sizes. Solution space property computation allows us to understand the solution space better. With the counting of sets at different sizes, one can related the computational hardness with the counting of sets at different sizes [56]. With the configuration

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enumeration/sampling at a given size, one can measure the overlap gap property better, while the configuration space connectivity also privides us an intuition about designing a better classical or quantum algortihms. [**MC: I would give examples of why we want to compute solution space properties. For instance, in statistical physics, computing thermal states and observables via the partition function. In complexity theory, proving limits on local algorithms (OGP).**][**JG: now?**]

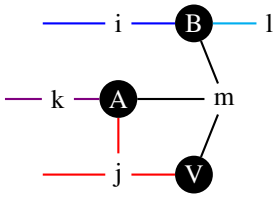
We propose to view the computation of all these properties from an abstract algebra perspective and use a unified framework, generic tensor-network, to solve these seeming unrelated properties all. Tensor network is also known as the sum product network in probabilistic modeling [10] or einsum in linear algebra libraries such as numpy. It is composed of a set of tensors and a set of labels for specifying the contraction of tensors, where the tensor element types are typically restricted to standard number types such as real numbers and complex numbers. We extend this concept to generic tensor network by generalizing the tensor element type to any type being a commutative semiring. Given a good contraction order, the space required to contract a tensor network is 2 power the treewidth of its line graph [43]. [**MC: I'd write out $2^{\mathrm{tw}(G)}$**][**JG: I feel it is hard to explain line graph without texts.**] Recent progress in simulating quantum circuits with random tensor networks [29, 46, 35] enables us to find such a good contraction order for a tensor network with thousands of tensors in a reasonable time. [**MC: Is the scaling of these algorithms known?**][**JG: They are not exact algorithms, the time can be any, typically a few minutes, will it be helpful to mention this?**] When using tensor network for solving one of the best sets with the maximum size, this time complexity is the same as the dynamic programming algorithm [16, 23]. These two algorithms are related but are not equivalent. Dynamic programming is more general purposed, while a tensor network has a richer algebraic structure, and this structure is crutial for solution space property computation. [**MC: Not clear how first part and second part of sentence are related**][**JG: now? or maybe just removing the comparison with dynamic programming?**]

To avoid the discussion being unnecessarily diversed, we mainly focus on the independent set problem, and discuss other combinatorial optimization problems, including the cutting problem, the matching problem, the vertex coloring problem, the satisfiability problem, the dominating set problem, the set packing problem and the maximal clique problem, in Appendix C. [~~**MC: More details on which combinatorial optimization problems this applies to?**~~] The paper is organized as follows. We first introduce the basic concepts of tensor networks and generic programming in Sec. 2 and Sec. 3. Then we show how to reduce an independent set problem to a tensor network contraction problem Sec. 4 and show how to engineer the element types in Sec. 6,Sec. 7 and Sec. 8 to count independent sets at a given size, enumerate/sample independent sets at a given size and find largest set sizes in weighted graphs. Lastly, we benchmark our algorithms in Sec. 9 and provide a few examples in Sec. 10 to demonstrate the versatility of our tool. We show how our method can help computing the entropy constant for some hardcore lattice gases on 2D square lattices and analyzing the presence of overlap gap property on three regular graphs.

**2. Tensor networks.** Tensor network [15, 45] is also known as einsum, factor graph or sum-product network [10] in different contexts; it can be viewed as a generalization of binary matrix multiplication to nary tensor contraction. Einstein's notation is often used to represent a tensor network, e.g. it represents the matrix multiplication between two matrices $A$ and $B$ as $C_{ik} = A_{ij}B_{jk}$, where we use a label in the subscript to represent a degree of freedom. One can enumerate these degrees of freedom and accumulate the product of tensor elements to the output tensor. In the standard Einstein's notation for tensor networks in physics, each index appears precisely twice, either both in input tensors (which will be summed over) or one in

a input tensor and another in the output tensor[~~MC: signifying which pairs of indices are summed over~~]. Hence a tensor network can be represented as a simple graph, where a tensor is mapped to a vertex and a label shared by two tensors is mapped to an edge. In this work, we do not impose such a restriction, so an index can appear an arbitrary number of times. The graphical representation of a generalized tensor network is a hypergraph, in which an edge (a label in subscript) can be shared by an arbitrary number of vertices (tensors). These two notations are equivalent in representation power, while the generalized tensor network might produce smaller contraction complexity, which will be illustrated in Appendix B. [~~MC: I feel that the $\delta$ tensors point is unnecessary to mention in the main text. Because not much detail is given, I internalized what it meant only on the third read-through.~~]

**Example 1.** $C_{ijk} = A_{jkm}B_{mil}V_{jm}$ is a tensor network that can be evaluated as $C_{ijk} = \sum_{ml} A_{jkm}B_{mil}V_{jm}$. Its hypergraph representation is shown below, where we use different colors to represent different hyperedges.




**3. Generic programming tensor contractions.** [**MC: On a second read of this section, I think that the clarity could be improved. My understanding is this is the flow: We would like to use generic programming, where we write code that works regardless of input type, and is optimized on all input types without sacrificing efficiency. In general, we can write code such that a function runs correctly regardless of the input data type. This is easy to do for dynamically typed languages like Python, which only verify and enforce the rules for the input data type at runtime (called type-checking). However, when the input data type is only checked at runtime (as opposed to when the code is compiled), type-specific optimization cannot be used. High efficiency is only achieved in statically typed languages, where modern compiling technology allows the function to be individually optimized for each input data type (then give C++/Julia examples).**][**JG: how about now?**] In previous works relating tensor networks and combinatoric problems [36, 9], the elements in the tensor networks are limited to standard number types such as floating point numbers and integers. The truth is, the elements in a tensor does not have to be a regular number type, or even a field (since division is not used in tensor contraction). One can use the same tensor contraction program for different purposes with different tensor element types, and this idea of using the same program for different purposes is also called the generic programming in computer science:

Definition 3.1 (Generic programming [52]). *Generic programming is an approach to programming that focuses on designing algorithms and data structures so that they work in the most general setting without loss of efficiency.*

[**MC: I think the following paragraph could be clarified. When you read the definition of generic programming, it's not clear what "in the most general setting" means. My understanding is it just means that the program will work regardless of the input data type - it would be good to say this explicitly.** ] [**JG: This definition is from the book I cited, I also do not like "in the most general setting", maybe we just use our version?**] [**MC: I also think the way it is written takes a while to understand what dynamically versus statically typed languages are. The definition, "When these**

languages "see" a new input type, the compiler can recompile the generic program for the new type." comes rather late in the paragraph.] [~~MC: Also, while I know what you mean, concepts like "inlining immutable elements" and "cache miss rate" would be lost on someone only with a physics background.~~] This definition of generic programming contains two major aspects: a single program works in the most general setting and efficiency. To understand the first aspect on generality, suppose we want to write a function that raises an element to a power, $f(x, n) := x^n$. One can easily write a function for standard number types that computes the power of $x$ in $O(\log(n))$ steps using the multiply and square trick. Generic programming does not require $x$ to be a standard number type, instead it treats $x$ as an element with an associative multiplication operation $\odot$ and a multiplicative identity $\mathbb{1}$. In such a way, when the program takes a matrix as an input, it computes the matrix power without extra efforts. The second aspect is about performance. For dynamically typed languages such as Python, one can easily write very general codes, but the efficiency is not guaranteed; for example, the speed of computing the matrix multiplication between two numpy arrays with python objects as elements is much slower than statically typed languages such as C++ and Julia [8]. C++ uses templates for generic programming while Julia takes advantage of just-in-time compilation and multiple dispatch. When these languages "see" a new input type, the compiler can recompile the generic program for the new type. A myriad of optimizations can be done during the compilation, such as optimize the memory layout of immutable elements with fixed sizes in an array to speed up the array indexing. In Julia, arrays with immutable elements with fixed sizes can even be compiled to GPU devices for faster computation [7].

This motivates us to think about what is the most general tensor element type allowed in a tensor network contraction program. We find that as long as the algebra of tensor elements forms a commutative semiring, the tensor network contraction result will be valid and be independent of the contraction order. A commutative semiring is a ring with its multiplication operation being commutative and without an additive inverse. To define a commutative semiring with the addition operation $\oplus$ and the multiplication operation $\odot$ on a set $R$, the following relations must hold for any arbitrary three elements $a, b, c \in R$.

$$
\begin{aligned}
(a \oplus b) \oplus c &= a \oplus (b \oplus c) \\
a \oplus \mathbb{0} &= \mathbb{0} \oplus a = a \\
a \oplus b &= b \oplus a
\end{aligned}
\qquad \triangleright \text{ commutative monoid } \oplus \text{ with identity } \mathbb{0}
$$

$$
\begin{aligned}
(a \odot b) \odot c &= a \odot (b \odot c) \\
a \odot \mathbb{1} &= \mathbb{1} \odot a = a \\
a \odot b &= b \odot a
\end{aligned}
\qquad \triangleright \text{ commutative monoid } \odot \text{ with identity } \mathbb{1}
$$

$$
\begin{aligned}
a \odot (b \oplus c) &= a \odot b \oplus a \odot c \\
(a \oplus b) \odot c &= a \odot c \oplus b \odot c
\end{aligned}
\qquad \triangleright \text{ left and right distributive}
$$

$$
a \odot \mathbb{0} = \mathbb{0} \odot a = \mathbb{0}
$$

We require the algebra being multiplicative commutative because the contraction order optimizer will change the multiplication order of elements, while we wish this contraction order does not change the contraction results. In the following sections, we show how to compute a number of properties of independent sets by designing tensor element types as specific commutative semirings without changing the tensor network contraction

| Element type | Solution space property |
|---|---|
| $\mathbb{R}$ | Counting of all independent sets |
| Polynomial (Eq. (5.2: PN)) | Independence polynomial |
| Tropical (Eq. (6.3: T)) | Maximum independent set size |
| Extended tropical of order $k$ (Eq. (8.1: T$k$)) | Largest $k$ independent set sizes |
| Polynomial truncated to $k$-th order (Eq. (6.2: P1) and Eq. (6.5: P2)) | $k$ largest independent sizes and their numbers [**MC: "and their counting" is gramatically confusing, can we say independence polynomial or degeneracy or something?**][**JG: Since you mentioned degeneracy is bad, what about "numbers"?**] |
| Set (Eq. (7.1: SN)) | Enumeration of independent sets |
| Sum Product Tree (Eq. (7.6: SPT)) | Sampling of independent sets |
| Polynomial truncated to highest order combined with Bit string (Eq. (7.5: S1)) | Maximum independent set size and one of such configurations |
| Polynomial truncated to $k$-th order combined with Set (Eq. (7.3: P1+SN)) | $k$ largest independent set sizes and their enumeration |

Table 1: Tensor element types and the independent set properties that can be computed using them.

program [52]. The Table 1 summarizes those properties that can be computed by various tensor element types.

**4. Tensor network representation of independent sets.** This section is about reducing the independent set problem to a tensor network contraction problem. For people with physics background, we suggest using an alternative approach described in Appendix A to understand this reduction from an energy model. Let $G = (V, E)$ be a weighted undirected graph with each vertex $v \in V$ being associated with a weight $w_v$. An independent set $I \subseteq V$ is a set of vertices that for any vertex pair $u, v \in I$, $(u, v) \notin E$, and we denote the maximum independent set (MIS) size $\alpha(G) \equiv \max_I \sum_{v\in I} w_v$. We map a vertex $v \in V$ to a label $s_v \in \{0, 1\}$ of dimension 2 in a tensor network, where we use 0 (1) to denote a vertex is absent (present) in the set. For each label $s_v$, we defined a parametrized rank-one vertex tensor $W(x_v, w_v)$ as

$$W(x_v, w_v) = \begin{pmatrix} 1_v \\ x_v^{w_v} \end{pmatrix}. \tag{4.1}$$

where we use subscripts to annotate different vertices, these annotation are only used in configuration enumeration and sampling. One can index tensor elements by subscripting tensors, e.g. $W(x_i, w_i)_0 = 1$ is the first element associated with $s_i = 0$ and $W(x_i, w_i)_1 = x_i^{w_i}$ is the second element associated with $s_i = 1$. Similarly, on each edge $(u, v)$, we define a matrix

$B$ indexed by $s_u$ and $s_v$ as

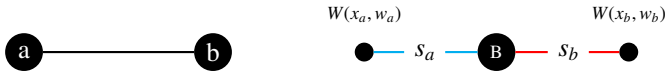
$$B = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}. \tag{4.2}$$

The corresponding tensor network contraction gives

$$P(G, \{x_1^{w_1}, x_2^{w_2}, \ldots, x_{|V|}^{w_{|V|}}\}) = \sum_{s_1, s_2, \ldots, s_{|V|}=0}^{1} \prod_{i=1}^{|V|} W(x_i, w_i)_{s_i} \prod_{(i,j)\in E(G)} B_{s_i s_j}, \tag{4.3}$$

where the summation runs over all vertex configurations $\{s_1, s_2, \ldots, s_{|V|}\}$ and accumulates the product of tensor elements to the output $P$ (see Example 3 for a concrete example). The edge tensor element $B_{s_i=1, s_j=1} = 0$ encodes the independent set constraint, meaning vertex $i$ and $j$ cannot be both in the independent set if they are connected by an edge $(i, j)$.

**Example 2.** In the following, we show a minimum example of mapping the independent problem of a 2 vertex complete graph K2 (left) to a tensor network (right).




In the graphical representation of tensor network on the right panel, we use a circle to represent a tensor, a hyperedge in cyan color to represent the degree of freedom $s_a$, and a hyperedge in red color to represent a degree of freedom $s_b$. Tensors sharing a same degree of freedom are connected by that hyperedge. The contraction of this tensor network can be evaluated manually:

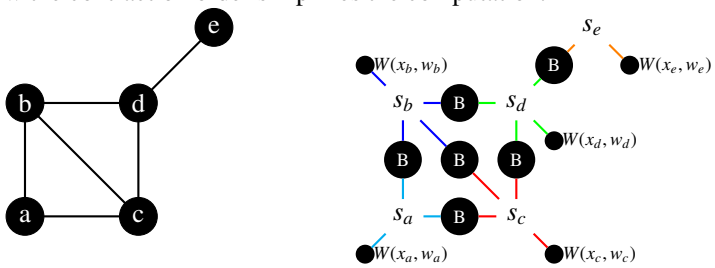
$$\begin{aligned} P(\mathrm{K2}, \{x_a^{w_a}, x_b^{w_b}\}) &= \begin{pmatrix} 1 & x_a^{w_a} \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ x_b^{w_b} \end{pmatrix} \\ &= 1 + x_a^{w_a} + x_b^{w_b} \end{aligned} \tag{4.4}$$

The resulting polynomial represents 3 different independent sets {}, $\{a\}$ and $\{b\}$, with weights being 0, $w_a$ and $w_b$ respectively.

It is in general not computational efficient to evaluate Eq. (4.3) by directly summing up the $2^{|V|}$ products, which scales exponentially as the number of vertices. [**MC: Perhaps explicitly say what this scales as?**][**JG: I am not sure explicitly saying "scales exponentially as the number of vertices" is helpful, because treewidth often scales linearly as number of vertices, so tensor network also scales exponentially as the number vertices in most cases.**] The standard approach to evaluate a tensor network is to contract two tensors at a time with a certain order utilizing the associativity and commutativity of tensor contraction. A fully optimized contraction order can reduce the time complexity significantly, while requiring a minimum space complexity $O(2^{\mathrm{tw}(G)})$ [43] to store intermediate contraction results. [**MC: Perhaps just say time and space complexity? Order of magnitude doesn't make sense to me in terms of scaling. Also, what is the time complexity of finding a good contraction order? Is there a known average-case complexity? This seems important.**][**JG: see added texts below.**] The pairwise tensor contraction also makes it possible to utilize basic linear algebra subprograms (BLAS) functions to speed up the computation for certain tensor element types. In practise, it is difficult to find an optimal contraction order for large tensor networks because finding the treewidth itself is NP-hard. However, it is easy to find a close to optimal contraction order in typically a few minutes with a heuristic contraction order finding algorithm [36, 35]. For large scale applications, it is also possible to slice over certain degrees of freedom to reduce

the space complexity, i.e. enumerating certain degrees of freedom in an external loop so that the space complexity of contracting a smaller tensor network inside the loop can be smaller.

**Example 3.** In the following, we mapping a 5 vertex graph (left) to a tensor network (right) and show how the contraction order simplifies the computation.




The contraction of this tensor network can be done in a pairwise order utilizing the associativity, additive commutativity, and multiplicative commutativity of tensor elements:

$$
\begin{aligned}
&\sum_{s_a,s_b,s_c,s_d,s_e} W(x_a,w_a)_{s_a} W(x_b,w_b)_{s_b} W(x_c,w_c)_{s_c} W(x_d,w_d)_{s_d} W(x_e,w_e)_{s_e} B_{s_a s_b} B_{s_b s_d} B_{s_c s_d} B_{s_a s_c} B_{s_b s_c} B_{s_d s_e} \\
=&\sum_{s_b,s_c}\left(\sum_{s_d}\left(\left(\left(\left(\sum_{s_e} B_{s_d s_e} W(x_e,w_e)_{s_e}\right) W(x_d,w_d)_{s_d}\right)\left(B_{s_b s_d} W(x_b,w_b)_{s_b}\right)\right)\left(B_{s_c s_d} W(x_c,w_c)_{s_c}\right)\right)\right. \\
&\left.\left(B_{s_b s_c}\left(\sum_{s_a} B_{s_a s_b}\left(B_{s_a s_c} W(x_a,w_a)_{s_a}\right)\right)\right)\right) \\
=&1 + x_a^{w_a} + x_b^{w_b} + x_c^{w_c} + x_d^{w_d} + x_e^{w_e} + x_a^{w_a} x_d^{w_d} + x_a^{w_a} x_e^{w_e} + x_c^{w_c} x_e^{w_e} + x_b^{w_b} x_e^{w_e}
\end{aligned}
$$

One can easily check the maximum tensor during computing is rank 2, and the total number of multiplication operations is reduced significantly.

[**MC: I have not checked this yet but will tomorrow. Is it really easy/simple enough to do without writing stuff down? Is this the simplest example possible? The equations look quite formidable at first glance, and it takes a lot of time to match the hyperedge labels in the equation to the physical graph.**][**JG: sometimes I am afraid the example is too trivial to be useful. The simplest example to show contraction order matters can be a 3-vertex one.**]

**5. Independence polynomial.** Let $x_i = x$ and $w_i = 1$, the evaluation of Eq. (4.3) corresponds to the independence polynomial [30, 21]. which is a useful graph characteristic related to, for example, the partition functions [37, 57] and Euler characteristics of the independence complex [11, 39]. The independence polynomial is an important graph polynomial that contains the counting information of independent sets. It is defined as

$$
I(G, x) = \sum_{k=0}^{\alpha(G)} a_k x^k, \tag{5.1}
$$

where $a_k$ is the number of independent sets of size $k$ in graph $G = (V, E)$. The total number of independent sets is thus equal to $I(G, 1)$. Its connection to Eq. (4.3) can be understood as follows: the product over vertex tensor elements produces a factor $x^k$, where $k = \sum_i s_i$ counts the set size, and the product over edge tensor elements gives a factor 1 for a configuration being in an independent set and 0 otherwise. The summation counts the number of independent sets of size $k$. By assigning a standard computer number to $x$, one can evaluate

this independence polynomial for this specific value by contracting this tensor network directly. [**MC: By feed in standard computer number types into the network, do you mean for x? Then, you look at multiple x, you can fit the independence polynomial to solve for the coefficients? It's not very explicit this procedure works at this point.**][**JG: how about now?**] However, instead of evaluating this polynomial for a certain value, we are more interested in finding the coefficients of this polynomial, because this quantity tells us the counting of independent sets at each size. [**MC: Does the previous technique (contracting the tensor network numerically) give the coefficients of the polynomial? The use of the word "however" here is confusing to me because it feels like you're saying that the previous technique doesn't give the coefficients, or it's very hard to obtain the coefficients.**][**JG: Yep, we haven't found the coefficients. I tried to modify words a bit, does it look better now?**] To achieve this, let us first elevate the tensor elements 0s and 1s in tensors $W(x, 1)$ and $B$ from integers and floating point numbers to the additive identity, $\mathbb{0}$, and multiplicative identity, $\mathbb{1}$, of a commutative semiring as discussed in Sec. 3. [**MC: I'd say that you're about to describe this semiring, otherwise it seems like you're going to use the general definition of the semiring rather than a specific type of semiring**][**JG: from $1$ to $\mathbb{1}$ and $0$ to $\mathbb{0}$ applies for a general semiring, I haven't change this part, let's discuss to make sure I understand your point.**] Let us create a polynomial type and represent a polynomial $a_0 + a_1 x + \ldots + a_k x^k$ as a coefficient vector $a = (a_0, a_1, \ldots, a_k) \in \mathbb{R}^k$, so, e.g., $x$ is represented as $(0, 1)$. We define the algebra between the polynomials $a$ of order $k_a$ and $b$ of order $k_b$ as

$$
\begin{aligned}
a \oplus b &= (a_0 + b_0, a_1 + b_1, \ldots, a_{\max(k_a,k_b)} + b_{\max(k_a,k_b)}),\\
a \odot b &= (a_0 + b_0, a_1 b_0 + a_0 b_1, a_2 b_0 + a_1 b_1 + a_0 b_2, \ldots, a_{k_a} b_{k_b}),\\
\mathbb{0} &= (),\\
\mathbb{1} &= (1).
\end{aligned}
\tag{5.2: PN}
$$

Here, the multiplication operation can be evaluated in time $O(k \log(k))$, where $k = \max k_a, k_b$, using the convolution theorem [51]. These operations are standard addition and multiplication operations of polynomials, and the polynomial type forms a commutative ring. The tensors $W$ and $B$ can thus be written as

$$
W^{\mathrm{PN}} = \begin{pmatrix} \mathbb{1} \\ (0, 1) \end{pmatrix}, \qquad B^{\mathrm{PN}} = \begin{pmatrix} \mathbb{1} & \mathbb{1} \\ \mathbb{1} & \mathbb{0} \end{pmatrix}. \tag{5.3}
$$

By contracting the tensor network with the polynomial type, we have the exact representation of the independence polynomial. In practise, using the polynomial type suffers a space overhead proportional to $\alpha(G)$ because each polynomial requires a vector of such size to store the coefficients. One may argue that one can first evaluate this polynomial at different $x$ being a standard number type, and then apply the gaussian elimination to fit the coefficients of this polynomial. This seemingly more time and space efficient approach suffers from severe issues in practise. The data ranges of standard integer types are too small to cover many practical using cases, while the floating point numbers may have round off error that much larger than the value itself, because the number of sets at different sizes may vary tens or even hundreds of orders and this makes the small coefficients can not be retrieved correctly by fitting. For the purpose of evaluating these coefficients, we refer readers to Appendix E, where we provide an accurate and memory efficient method to find the polynomial by fitting it in a finite field. Alternatively, one can use the method in Appendix F to fit this polynomial more time efficiently with complex numbers with controllable round off errors. For the purpose of discussion in the main text, let us stick to

this less efficient polynomial algebra. [**MC: It's not clear to me what we gain by using the polynomial semiring rather than floating points/integers here. Could you comment on how the compiler can optimize on this data type?**][**JG: I added some discussion here to address why we stick to polynomial number types, for short, it is a dynamic type that can be slow, so we do not use it a lot in practise. I mention it here because it is the base of the following discussion.**]

## 6. Maximum independent sets and its counting.

**6.1. Tropical algebra for finding the MIS size and counting MISs.** The MIS size $\alpha(G)$, or the independence number is an important graph characteristics. The method we use to compute this quantity is based on the following observations. Let $x = \infty$, the independence polynomial in the previous section becomes

$$I(G, \infty) = \lim_{x\to\infty} \sum_{k=0}^{\alpha(G)} a_k x^k = a_{\alpha(G)} \infty^{\alpha(G)}, \tag{6.1}$$

where the lower-order terms vanish. We can thus replace the polynomial type $a = (a_0, a_1, \ldots, a_k)$ with a new type with two fields: the largest exponent $k$ and its coefficient $a_k$. [**MC: I was initially confused because I thought $\mathbb{0} = (0, ?)$ where "?" could be anything positive since it's multiplied by zero. It confused me that ? could equal $-\infty$ since I thought you defined your ring for k positive, since a polynomial has positive exponents. If you have negative exponents I thought it is a Laurent polynomial or something. After re-reading I see why this doesn't matter, though.**][**JG: I let $\mathbb{0} = (1, -\infty)$ now, it is still correct, is it easier for understanding or I change it back?**] From this, we can define a new algebra as

$$\begin{aligned} a_x\infty^x \oplus a_y\infty^y &= \begin{cases} (a_x + a_y)\infty^{\max(x,y)}, & x = y \\ a_y\infty^{\max(x,y)}, & x < y \\ a_x\infty^{\max(x,y)}, & x > y \end{cases} \\ a_x\infty^x \odot a_y\infty^y &= a_x a_y \infty^{x+y} \\ \mathbb{0} &= 1\infty^{-\infty} \\ \mathbb{1} &= 1\infty^{0}. \end{aligned} \tag{6.2: P1}$$

To implement this algebra programmatically, we create a data type with two fields $(x, a_x)$ to store the MIS size and its counting, and define the above operations and constants correspondingly. If one is only interested in finding the MIS size, one can drop the counting field. The algebra of the exponents becomes the max-plus tropical algebra [41, 44]:

$$\begin{aligned} x \oplus y &= \max(x, y) \\ x \odot y &= x + y \\ \mathbb{0} &= -\infty \\ \mathbb{1} &= 0. \end{aligned} \tag{6.3: T}$$

Algebra Eq. (6.3: T) and Eq. (6.2: P1) are the same as those used in Liu et al. [40] to calculate and count spin glass ground states. For independent set calculations here, the vertex tensor and edge tensor becomes:

$$W^{\mathrm{T}} = \begin{pmatrix} \mathbb{1} \\ \infty \end{pmatrix}, \qquad B^{\mathrm{T}} = \begin{pmatrix} \mathbb{1} & \mathbb{1} \\ \mathbb{1} & \mathbb{0} \end{pmatrix}. \tag{6.4}$$

**6.2. Truncated polynomial algebra for counting independent sets of large size.** Instead of counting just the MISs, one may also be interested in counting the independent sets with largest several sizes. For example, if one is interested in counting only $a_{\alpha(G)}$ and $a_{\alpha(G)-1}$, we can define a truncated polynomial algebra by keeping only the largest two coefficients in the polynomial in Eq. (5.2: PN) as:

$$\begin{aligned} a \oplus b &= (a_{\max(k_a,k_b)-1} + b_{\max(k_a,k_b)-1}, a_{\max(k_a,k_b)} + b_{\max(k_a,k_b)}), \\ a \odot b &= (a_{k_a-1}b_{k_b} + a_{k_a}b_{k_b-1}, a_{k_a}b_{k_b}), \\ \mathbb{0} &= (), \\ \mathbb{1} &= (1). \end{aligned} \tag{6.5: P2}$$

In the program, we thus need a data structure that contains three fields, the largest order $k$, and the coefficients for the two largest orders $a_k$ and $a_{k-1}$. This approach can clearly be extended to calculate more independence polynomial coefficients and is more efficient than calculating the entire independence polynomial. Similarly, one can also truncate the polynomial and keep only its smallest several orders, which can be used for e.g. counting the maximal independent sets with smallest cardinality, where a maximal independent set is an independent set that can not be made larger by adding a new vertex into the it without violating the independence contraint. As will be shown below, this algebra can also be extended to enumerate those large-size independent sets.

## 7. Enumerating and sampling independent sets.

**7.1. Set algebra for configuration enumeration.** The configuration enumeration of independent sets includes, for example, the enumeration of all independent sets, the enumeration of all MISs and the enumeration of independent sets with maximum several sizes. The most studied enumeration of maximal independent sets [12, 19, 34] requires using a different tensor network structure, which is discussed in Appendix C.1. To enumerate all independent sets, we designed an algebra defined on sets of bit strings:

$$\begin{aligned} s \oplus t &= s \cup t \\ s \odot t &= \{\sigma \vee^{\circ} \tau \,|\, \sigma \in s, \tau \in t\} \\ \mathbb{0} &= \{\} \\ \mathbb{1} &= \{0^{\otimes |V|}\}. \end{aligned} \tag{7.1: SN}$$

where $s$ and $t$ are each a set of $|V|$-bit strings and $\vee^{\circ}$ is the bitwise OR operation over two bit strings.

**Example 4.** For elements being bit strings of length 5, we have the following set algebra

$$\{00001\} \oplus \{01110, 01000\} = \{01110, 01000\} \oplus \{00001\} = \{00001, 01110, 01000\}$$
$$\{00001\} \oplus \{\} = \{00001\}$$

$$\{00001\} \odot \{01110, 01000\} = \{01110, 01000\} \odot \{00001\} = \{01111, 01001\}$$
$$\{00001\} \odot \{\} = \{\}$$
$$\{00001\} \odot \{00000\} = \{00001\}.$$

To enumerate all independent sets, we initialize variable $x_i$ in the vertex tensor to $x_i = \{\boldsymbol{e}_i\}$, where $\boldsymbol{e}_i$ is a basis bit string of size $|V|$ that has only one non-zero value at location $i$. The

vertex and edge tensors are thus

$$W^{\mathrm{SN}}(\{\boldsymbol{e}_i\}) = \begin{pmatrix} \mathbb{1} \\ \{\boldsymbol{e}_i\} \end{pmatrix}, \qquad B^{\mathrm{SN}} = \begin{pmatrix} \mathbb{1} & \mathbb{1} \\ \mathbb{1} & \mathbb{0} \end{pmatrix}. \tag{7.2}$$

This set algebra can serve as the coefficients in Eq. (5.2: PN) to enumerate independent sets of all different sizes, Eq. (6.2: P1) to enumerate all MISs, or Eq. (6.5: P2) to enumerate all independent sets of size $\alpha(G)$ and $\alpha(G) - 1$. As long as the coefficients in a truncated polynomial forms a commutative semiring, the polynomial itself is still a commutative semiring. For example, to enumerate only the MISs, with the tropical algebra, we can define $s_k \infty^k$, where the coefficients follow the algebra in Eq. (7.1: SN) and the orders (exponents) follow the max-plus tropical algebra. The combined operations become:

$$\begin{aligned} s_x \infty^x \oplus s_y \infty^y &= \begin{cases} (s_x \cup s_y)\infty^{\max(x,y)}, & x = y \\ s_y \infty^{\max(x,y)}, & x < y \\ s_x \infty^{\max(x,y)}, & x > y \end{cases}, \\ s_x \infty^x \odot s_y \infty^y &= \{\sigma \vee^\circ \tau | \sigma \in s_x, \tau \in s_y\} \infty^{x+y}, \\ \mathbb{0} &= \{\} \infty^{-\infty}, \\ \mathbb{1} &= \{0^{\otimes |V|}\} \infty^0. \end{aligned} \tag{7.3: P1+SN}$$

Clearly, the vertex tensor and edge tensor become

$$W^{\mathrm{P1+SN}}(\{\boldsymbol{e}_i \infty^1\}) = \begin{pmatrix} \mathbb{1} \\ \{\boldsymbol{e}_i\} \infty^1 \end{pmatrix}, \qquad B^{\mathrm{P1+SN}} = \begin{pmatrix} \mathbb{1} & \mathbb{1} \\ \mathbb{1} & \mathbb{0} \end{pmatrix}. \tag{7.4}$$

The contraction of the corresponding tensor network yields an enumeration of all MIS configurations. Direct implementing this algebra for configuration MISs might incur significant space overheads for keeping too many intermediate states not contributing to the final maximum independent sets, one can avoid this issue by using the bounding technique in Appendix D.

If one is interested in obtaining only a single MIS configuration, one can just keep a single configuration in the intermediate computations to save the computational effort. Here is a new algebra defined on the bit strings, replacing the sets of bit strings in Eq. (7.1: SN),

$$\begin{aligned} \sigma \oplus \tau &= \mathrm{select}(\sigma, \tau), \\ \sigma \odot \tau &= (\sigma \vee^\circ \tau), \\ \mathbb{0} &= 1^{\otimes |V|}, \\ \mathbb{1} &= 0^{\otimes |V|}, \end{aligned} \tag{7.5: S1}$$

where the `select` function picks one of $\sigma$ and $\tau$ by some criteria to make the algebra commutative and associative, e.g. by picking the one with a smaller integer value.

**7.2. Sampling extremely large configuration space.** When the graph size goes large, the configurations might be impossible to fit into any type of storage. Then instead of using the set algebra, one can use a binary sum-product tree as a compact representation of the configurations. We use a quadruple $(type, data, left, right)$ to represent a node in the tree, where *type* is one of `LEAF`, `ZERO`, `SUM` and `PROD`, *data* is a bit string as the content in a `LEAF` node, $left$ and *right* are left and right operands of `SUM` and `PROD` nodes.

(7.6: SPT)
$$\begin{aligned} s \oplus t &= (\texttt{SUM}, /, s, t) \\ s \odot t &= (\texttt{PROD}, /, s, t) \\ \mathbb{0} &= (\texttt{ZERO}, /, /, /) \\ \mathbb{1} &= (\texttt{LEAF}, 0^{\otimes |V|}, /, /). \end{aligned}$$

[**MC: It might be nice to have a picture of an example tree if you have time. However, it is pretty clear from the definition, it would just help to visualize. Do you ever use the zero element?**][**JG: now we have an example, but it does not include a zero element, do you think I should use a more concrete one instead of an abstract one?**] The vertex tensor and edge tensor become

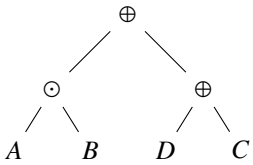
(7.7)
$$W^{\text{SPT}}((\texttt{LEAF}, \boldsymbol{e}_i, /, /)) = \begin{pmatrix} \mathbb{1} \\ (\texttt{LEAF}, \boldsymbol{e}_i, /, /) \end{pmatrix}, \qquad B^{\text{SPT}} = \begin{pmatrix} \mathbb{1} & \mathbb{1} \\ \mathbb{1} & \mathbb{0} \end{pmatrix}.$$

This algebra is a commutative semiring because we define the equivalence of two sum-product trees by comparing their expanded (using Eq. (7.1: SN)) forms, rather than their storages. Although one is probably unable to enumerate the configurations represented by this tree due to the extremely large configuration space size, but he can directly sample configurations from this tree. This is because once we have this sum-product representation of the configuration space, either generate by using this algebra directly or serve as the coefficients of (truncated) polynomials, one can compute the number of configurations in each branch rigorously and efficiently. [**MC: To clarify - is the sum-product tree now the coefficients on the polynomial? I am a little confused on how we would, for instance, use this to compute the MISs**][**JG: added one more descriptive sentence, does it resolve your concern?**] To generate samples, one just descends this sum product tree to left or right sibling with probability decided by the size of each branch while doing the computation specified by the first field. [~~**MC: How do we compute the size of each branch?**~~]

**Example 5.** Let us consider the following sum product tree

$$(\texttt{SUM}, /, (\texttt{PROD}, /, A, B), (\texttt{SUM}, /, C, D)),$$

where siblings $A, B, C$ and $D$ can be any four types of nodes. It can be represented diagramatically as the following.




The left and right sibling of root node has size $|A| \times |B|$ and $|C| + |D|$ respectively, and since the root node has type SUM, its size can be computed as $|A| \times |B| + |C| + |D|$. One can compute the sizes of $A, B, C$ and $D$ recursively until the program meets either a the LEAF node or a ZERO node, which has a known size of 1 or 0 respectively.

**8. Weighted graphs.** In the previous discussion, we have limited ourselves to unweighted graphs. For integer weighted graphs, all results still holds, while for general weighted graphs, the independence polynomial is not computable anymore. For general weighted graphs, we are more interested to know the $k$ most weighted sets and their sizes. Hence we define the extended tropical numbers as the following

(8.1: T$k$)
$$\begin{aligned} s \oplus t &= \texttt{largest}(s \cup t, k) \\ s \odot t &= \texttt{largest}(\{a+b | a \in s, b \in t\}, k) \\ \mathbb{0} &= -\infty^{\otimes k} \\ \mathbb{1} &= -\infty^{\otimes k-1} \otimes 0 \end{aligned}$$

where $\texttt{largest}(s,k)$ means truncating the set by only keeping $k$ largest values in the set $s$. The computation of $s \odot t$ is a maximum sum combination problem which can be done in time $\sim k\log(k)$, one can find an implementation in Appendix H. The vertex tensor and edge tensor become

(8.2)
$$W^{\mathrm{T}k}(-\infty^{\otimes k-1} \otimes 1, w_v) = \begin{pmatrix} \mathbb{1} \\ -\infty^{\otimes k-1} \otimes w_v \end{pmatrix}, \qquad B^{\mathrm{T}k} = \begin{pmatrix} \mathbb{1} & \mathbb{1} \\ \mathbb{1} & \mathbb{0} \end{pmatrix},$$

where we have used the relation $(-\infty^{\otimes k-1} \otimes 1)^{w_v} = -\infty^{\otimes k-1} \otimes w_v$. Similar to the tropical numbers, we can combine it with a bit string sampler (Eq. (7.5: S1)) for finding the configuration of each size. Since the $\odot$ operation of configuration sampler is not used, the resulting configurations are deterministic and complete.

**9. Performance benchmarks.** We run a single thread benchmark on CPU Intel(R) Xeon(R) CPU E5-2686 v4 @ 2.30GHz, and its CUDA version on a GPU Tesla V100-SXM2 16G. The results are summarized in Figure 1. The graphs that we use in benchmarks are random three regular graphs, a typical type of sparse graphs that has a small treewidth that asymptotically smaller than $|V|/6$ [22]. In this benchmark, we do not include traditional algorithms for finding the MIS size like the branching algorithms [53, 50] and dynamic programming based algorithms [16, 23], because to the best of our knowledge, most of the properties mentioned in this paper are not computable within these frameworks. The main goal of this section is to show the relative timing for computing different properties.

Figure 1(a) shows the time and space complexity of tensor network contraction for different graph sizes, where the space complexity is the same as the treewidth of the problem graph. Here, we assume our contraction order finding program has been converged to the optimal treewidth. The contraction order is obtained using the local search algorithm in Ref. [35]. In practice, slicing technique [35] is used for graphs with treewidth greater than 27 to fit the computation into a 16GB memory. One can see that all the computing times in figure 1(b), (c) and (d) have a strong correlation with the treewidth, while in panel (d), the timing of certain computing tasks also strongly correlates with other factors like the configuration space size. [**MC: with the number of vertices, and therefore the treewidth**][**JG: not sure it is safe to say this, because they do not always have a nice linear relation**]. [~~**MC: Does this say anything about how optimized the contraction order is? If so, it might be worth explicitly saying. Some of the quantities in panel d look like they might be superexponential in the number of vertices (tree-width).**~~] Among these benchmarks, computational tasks with data types tropical number of on CPU and real and complex numbers on both CPU and GPU can utilize fast BLAS functions to evaluate tensor contractions, hence are much faster comparing to non-BLAS element types in the same category. [~~**MC: It might be worth explicitly saying the data types the first time they're mentioned (for example, I don't know what T is. Also, it might be worth adding a couple descriptor words on bounding.**~~] GPU computes much faster than CPU in all cases when the problem scale is large enough such that the actual computing time is comparable or larger than the launching overhead of CUDA kernels. Most algebras can be computed on a GPU, except those requiring dynamic sized structures, i.e. types with algebra

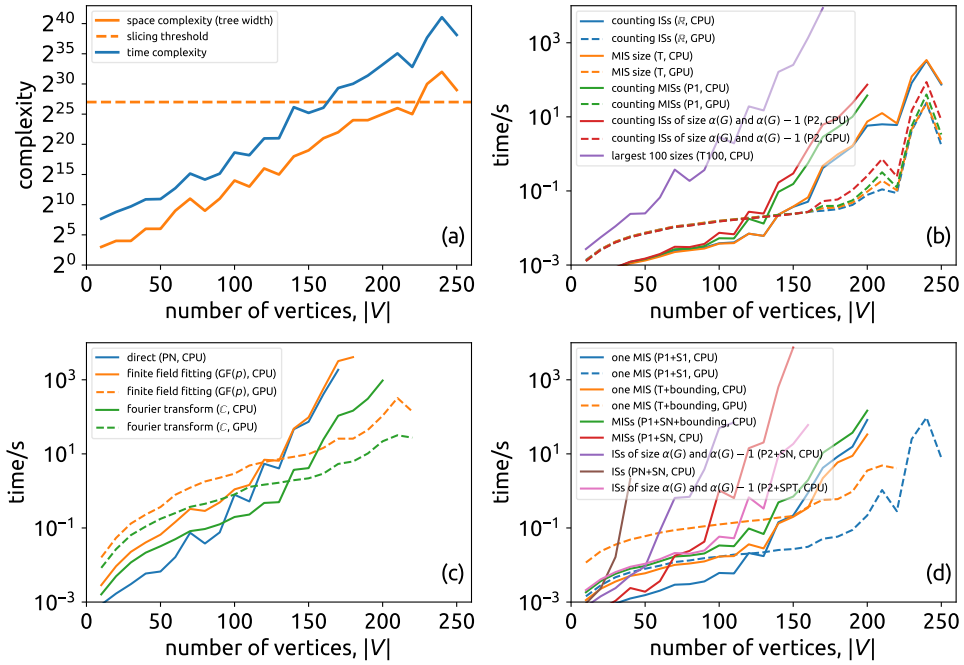



Figure 1: Benchmark results for computing different properties of independent sets of a random three regular graph with different tensor element types. The time in these plots only includes tensor network contraction, without taking into account the contraction order finding and just-in-time compilation time. Legends are properties, algebra and devices that we used in the computation; one can find the corresponding computed solution space property in Table 1. (a) time and space complexity versus the number of vertices for the benchmarked graphs. (b) The computing time for calculating the MIS size and for counting of the number of all independent sets (ISs), the number of MISs, the number of independent sets having size $\alpha(G)$ and $\alpha(G) - 1$, and finding 100 largest sets sizes. (c) The computing time for calculating the independence polynomials with different approaches. (d) The computing time for configuration enumeration, including the enumeration of all independent set configurations, a single MIS configuration, all MIS configurations, all independent set configurations having size $\alpha(G)$ and $\alpha(G) - 1$, and all independent set configurations having size $\alpha(G)$ and $\alpha(G) - 1$ in the sum product tree format, with or without bounding the enumeration space.

defined in Eq. (5.2: PN), Eq. (7.1: SN), Eq. (8.1: T$k$) and Eq. (7.6: SPT). In figure 1(c), one can see the Fourier transformation based method is the fastest in computing the independence polynomial, but it may suffer from round-off errors (Appendix F)[**MC: Can the round-off error thing be seen from Figure c?**][**JG: it is hard, so I added a ref to the appendix, is it more informative?**]. The finite field (GF($p$)) approach is the only method that does not have round-off errors and can be run on a GPU. In figure 1(d), one can see the technique to bound the enumeration space improves the performance for more than one order of magnitude in enumerating the MISs. Bounding can also reduce the memory usage significantly, without which the largest computable graph size is only $\sim 150$ on a device with 32GB main memory.

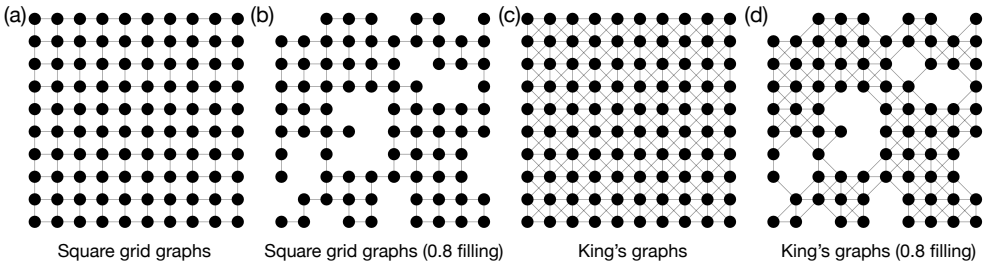



Figure 2: The types of graphs used in the case study in section 10.1. The lattice dimensions are $L \times L$. (a) Square grid graphs. (b) Square grid graphs with a filling factor $p = 0.8$. (c) King's graphs. (d) King's graphs with a filling factor $p = 0.8$.

**10. Example case studies.** In this section, we give a few examples where the different properties of independence sets are used.

**10.1. Number of independent sets and entropy constant for some hardcore lattice gases.** We compute the counting of all independent sets for graphs shown in Figure 2, where vertices are all placed on square lattices with lattice dimensions $L \times L$. The types of graphs include: the square grid graphs (Figure 2(a)); the square grid graphs with a filling factor $p = 0.8$, which means $\lfloor pL^2 \rceil$ square grids are occupied with vertices (Figure 2(b)); the King's graphs (Figure 2(c)); the King's graphs with a filling factor $p = 0.8$ (Figure 2(d)). The number of independent sets for square grid graphs of size $L \times L$ form a well-known integer sequence (OEIS A006506), which is thought as a two-dimensional generalization of the Fibonacci numbers. We computed the integer sequence for $L = 38$ and $L = 39$, which, to the best of our knowledge, is not known before. In the computation, we used the finite-field algebra for contracting arbitrarily high precision integer tensor networks.

A theoretically interesting number that can be computed using the number of independent sets is the entropy constant for the hardcore lattice gases on these graphs, which can tell us thermal dynamic properties of these lattices at the high temperature limit. [**MC: Why is it useful and what does it tell us about the physical system?**][**JG: It is probably useless, so: useful -> theoretically interesting**] For the square grid graphs, it is called the *hard square entropy constant* (OEIS A085850), which is defined as $\lim_{L\to\infty} F(L,L)^{1/L^2}$, where $F(L,L)$ is the number of independent sets of a given lattice dimensions $L \times L$. This quantity arises in statistical mechanics of hard-square lattice gases [6, 47] and is used to understand phase transitions for these systems. This entropy constant is not known to have an exact representation, but it is accurately known in many digits. Similarly, we can define entropy constants for other lattice gases. In Fig. 3, we look at how $F(L,L)^{1/\lfloor pL^2 \rceil}$ scales as a function of the grid size $L$ for all types of graphs shown in Figure 2. Our results match the known results for the non-disordered square grid and King's graphs. For disordered square grid and King's graphs with a filling factor $p = 0.8$, we randomly sample 1000 graph instances. To our knowledge, the entropy constants for these disordered graphs have not been studied before. Interestingly, the variations due to different random instances are negligible for this entropy quantity.

**10.2. The overlap gap property.** With the tool to enumerate configurations, one can try to understand the structure of the independent set configuration space, such as the optimization landscape for finding the MISs and the geometry of the solution space. One of the known barriers for finding the MIS is the so-called overlap gap property [26, 25].

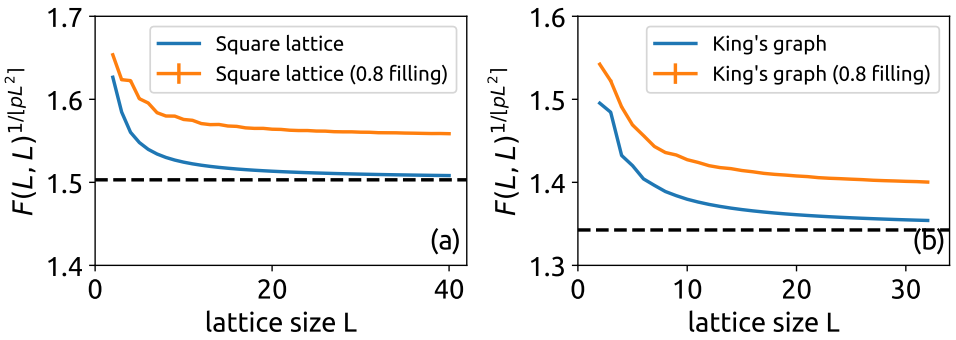
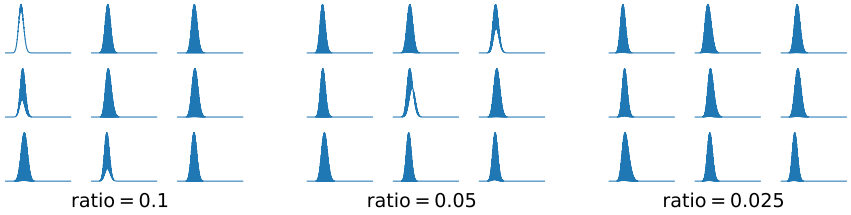


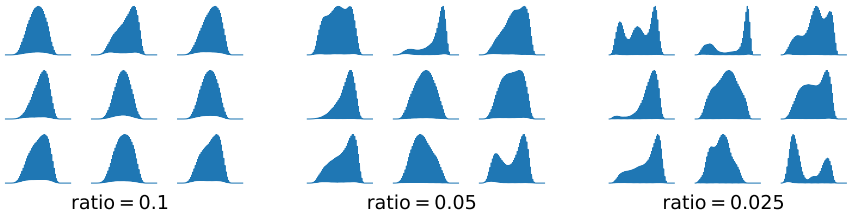

Figure 3: Mean entropy for lattice gases on graphs defined in Fig. 2. We sampled 1000 instances for $p = 0.8$ lattices and the error bar is too small to be visible. The horizontal black dashed lines are for $\lim_{L\to\infty} F(L,L)^{1/L^2}$ for the corresponding non-disordered square grid and King's graphs.

Intuitively, if the overlap gap property is present, it means every two large independent sets either have a significant intersection or very small intersection; it implies that large independent sets are clustered together. This clustering property has been used to prove the limitations of local algorithms in finding the MISs [26, 25]. It was shown that for finding MISs of $d$ regular graphs with $d$ and graph sizes both being large, there exists overlap gap property [49, 24]. However, it is not yet clear whether for small $d$, e.g. three regular graphs, this statement is still true. Here, we direct sample from the computed configurations of large independent sets to investigate the presence or absence of the overlap gap property for some given graphs. We do no explore the full configurations space because the number of configurations is too large to fit into a storage, so we have to use the sum product tree representation to store it in a compact format and draw samples from it. We compare two categories of graphs, one is the King's graph at 0.8 filling, a type of unit disk graph having no overlap gap property, [**JG: @Maddie, do you have a good reference to justify this statement about unit disk graph OGP?**] another is the vertex 3-regular graph that we want to investigate. Each category contains 9 randomly generated instances, due to the limitation of computing resources, the size of King's graph is $20 \times 20$ (320 vertices) and the size of 3-regular graphs are 110. In particular, in Fig. 4, we sample two sets of $10^4$ configurations from the ISs at sizes $\geq$ ratio $\times \lfloor \alpha(G) \rfloor$ for each instance and show the pairwise Hamming distance distribution for the enumerated configurations. In Fig. 4(a), we observed a clear single peak structure at a fixed distance normalized by the MIS size for the King's graphs. While in Fig. 4(b), we observed the multiple peak structure as the ratio becomes small for the 3-regular graphs. This indicates the presence of the overlap gap property and disconnected clusters exist in the configuration space for large independent sets. We expect our numerical tool can be used to understand this phenomenon better and to further investigate the graph properties and the geometry of the configuration spaces for a variety of graph instances.

**10.3. Visualizing experimental quantum algorithm outputs for solving Maximum Independent Set.** The ability to enumerate configurations can also be used to understand the distribution of outputs from algorithms for solving the Maximum Independent Set problem. This can give detailed insights to performance of the algorithm, such as if the




(a) 9 King's graphs of size $20 \times 20$, 0.8 filling.




(b) 9 Random three regular graphs of size 110.

Figure 4: The distribution of pairwise Hamming distances for configurations sampled from independent sets with sizes $\geq \lfloor \text{ratio} \times \alpha(G) \rfloor$. In each plot, the $x$-axis is the hamming distance normalized by the total number of vertices and the $y$-axis is the probability.

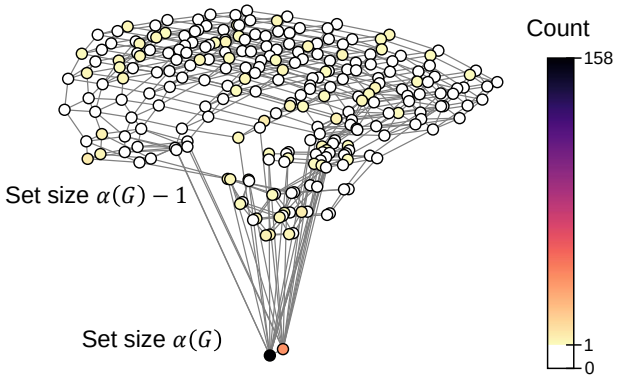



Figure 5: A visualization of experimental outputs of a quantum algorithm for solving the Maximum Independent Set problem. Each vertex represents an independent set, with edges between independent sets with pairwise Hamming distance $\leq 2$.

algorithm is likely to return independent sets from certain clusters of local or global minima in the solution space. As an example, we show in Figure 5 how our algorithm can be used to visualize experimental outputs of a quantum algorithm for solving the Maximum Independent Set problem using a programmable Rydberg atom array quantum computer [18]. The structure of the solution space for a King's graph with 39 vertices and filling factor $\rho = 0.8$ can be visualized on a graph where each vertex represents a large independent set, with edges between independent sets with a small pairwise Hamming

distance $\leq 2$. The algorithm either finds the largest independent set with size $\alpha(G)$ with high probability, or returns a suboptimal independent set, usually with size $\alpha(G) - 1$. The algorithm does not appear to return local minima with large Hamming distance from the MISs as suggested by [**?**], but samples from local minima with a wide range of Hamming distances from the MISs. Consistent with Sec. 10.2, there are no disconnected clusters in the solution space for this particular King's graph.

**11. Discussion and conclusion.** In this paper, we introduce a method to use generic programming tensor networks to compute a number of different properties of a hard problem, including the largest several independent sets sizes, the counting of independent sets of a given size and the enumeration of independent sets of a given size. For each solution space property, we design an algebra being a commutative semiring and let it be the tensor element type. With different algebras, the contraction of the same tensor network gives us the different properties. The data types introduced in the main text is summarized in the diagram in Fig. 6. Other than the case with real numbers, we have polynomials and truncated polynomials. We combine them with the bit string algebra, the set algebra, and sum product tree algebra for finding, enumeration, and sampling of independent sets at a given size. These algebras are of generic use: they can be utilized to compute properties of maximal independent sets and a variety of other combinatorial problems such as the matching problem, the k-coloring problem, the max-cut problem, and the set packing problem, as detailed in Appendix C. Moreover, since the independence polynomial is closely related to the matching polynomial [38], the clique polynomial [32], and the vertex cover polynomial [4], our algorithm to compute the independence polynomial can also be used to compute these graph polynomials. By adapting to the style of generic programming, we can implement all the algorithms without much effort. We show some of the Julia language implementations in Appendix I. A complete implementation can be found in our Github repository [1]. We expect our tool can be used to understand and study many interesting applications of independent sets and beyond. We also hope this approach of generic tensor networks can inspire future works on tensor network computations.

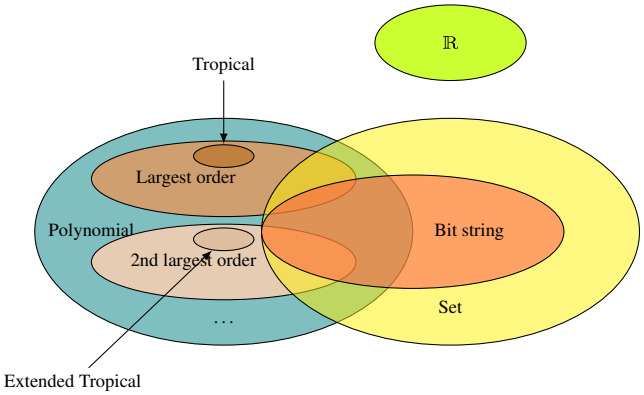



Figure 6: The the tensor network element types used in this work, while the purpose of these element types can be found in Table 1. The overlap between two algebra indicates that a new algebra can be created by combining those two types of algebra.

**[MC: It's not clear what some words mean on this diagram, such as "highest order" and "extended tropical"] [JG: the extended tropical is defined in Sec. 8, should I emphasis it more? also, "highest"->"largest"]**

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**Appendix A. An alternative way to construct the tensor network.**

Let us characterize the independent set problem on graph $G = (V, E)$ as an energy model

$$\mathcal{E}(G, s) = -\sum_{i\in V(G)} w_i s_i + \infty \sum_{\langle i,j\rangle\in E(G)} s_i s_j \tag{A.1}$$

where $s_i$ is a spin on vertex $i \in V$ and $w_i$ is an onsite energy term associated with it. The first term is the energy that corresponds to the inverse of the independent set size and the second term describes the independence contraint. In physical systems, this contraint term usually corresponds to the Rydberg blockade [48, 18] in cold atom arrays or the repulsive force in hard core lattice model [17, 20]. Its partition function is defined as

$$\begin{aligned} Z(G,\beta) &= \sum_{s} e^{-\beta\mathcal{E}(G,s)} = \sum_{s\in\mathcal{I}(G)} e^{\beta\sum w_i s_i} \\ &= \sum_{k=0}^{\alpha(G)} a(k) e^{\beta k} \qquad (k = \sum w_i s_i) \end{aligned} \tag{A.2}$$

where $\mathcal{I}(G)$ is the set of independent sets of graph $G$. $\alpha(G)$ is the absolute value of the minimum energy (maximum independent set size). $a(k)$ is the number of spin configurations with energy $-k$ (independent sets of size $k$). The partition function can be evaluated as a tensor network contraction, where the tensor network is constructed by placing a vertex tensor on each spin $i$

$$W(\beta, w_i) = \begin{pmatrix} 1 \\ e^{\beta w_i} \end{pmatrix}, \tag{A.3}$$

and an edge tensor on each bond

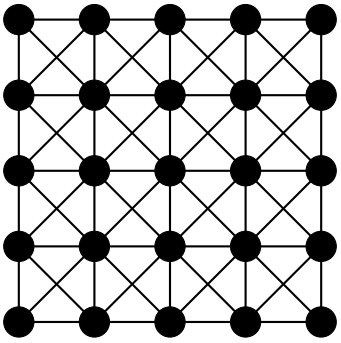
$$B = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}, \tag{A.4}$$

where the 0 in the bond tensor coming from $e^{-\beta\infty}$ in the second term of Eq. (A.1). By letting $x = e^{\beta}$, we get the tensor network for computing the independence polynomial as described by Eq. (4.1) and Eq. (4.2), and by letting $w_i = 1$, the second line of Eq. (A.2) is the independence polynomial.

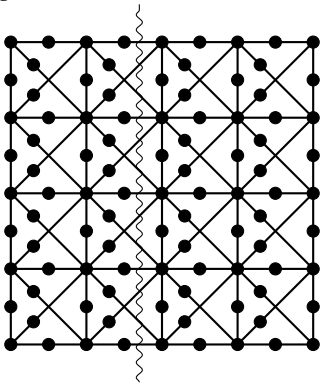
**Appendix B. An example of contraction complexity increase due to introducing $\delta$ tensors.** As we have mentioned in the main text, a standard tensor network notation is equivalent to the generalized tensor network by introducing $\delta$ tensors, where a $\delta$ tensor of rank $d$ is defined as

$$\delta_{i_1,i_2,\ldots,i_d} = \begin{cases} 1, & i_1 = i_2 = \ldots = i_d, \\ 0, & \text{otherwise.} \end{cases} \tag{B.1}$$

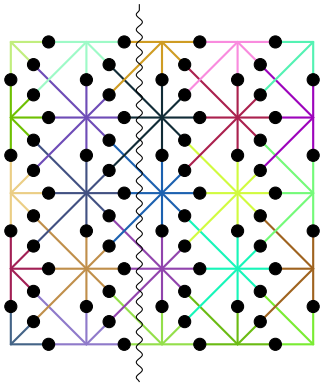
In the following, we are going to show introducing $\delta$ tensors might increase the contraction complexity of a tensor network. Let us consider the following King's graph.



By mapping the independent set problem to a standard tensor network with $\delta$ tensors, we have the following graphical representation.



In this diagram, the circle on each vertex in the original graph is a $\delta$ tensor of rank 8 or less. If we contract this tensor network in a naive column-wise order, the maximum intermediate tensor has rank $\sim 3L$, requiring a storage of size $\approx 2^{3L}$. If we relax the restriction that each label must appears exactly twice, we have the following hypergraph representation of a generalized tensor network.



Here, we use different colors to distinguish different hyperedges. A vertex tensor always has rank 1 and is not shown here since it does not change the contraction complexity. If we contract this tensor network in the column-wise order, the maximum intermediate tensor rank is $\sim L$, which can be seen by counting the number of colors at the cut.

## Appendix C. Hard problems and tensor networks.

**C.1. Maximal independent sets and maximal cliques.** Since finding maximal cliques of a graph is equivalent to finding the maximal independent sets of its complement graph, in

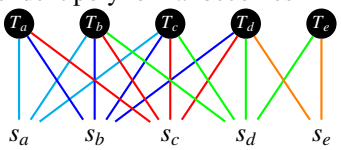
the following, we limit our discussion to finding maximal independent sets. Let us denote the neighborhood of a vertex $v$ as $N(v)$ and the closed neighborhood of $v$ as $N[v] = N(v) \cup \{v\}$. A maximal independent set $I_m$ is an independent set where there does exist a vertex $v \in V$ such that $I_m \cap N[v] = \emptyset$, i.e. an independent set that can not become a larger one by adding a new vertex. To characterize the maximal independence restriction, one can quantify over a local set $N[v]$ with a local tensor:

$$T(x_v, w_v)_{s_1,s_2,\ldots,s_{|N(v)|},s_v} = \begin{cases} s_v x_v^{w_v} & s_1 = s_2 = \ldots = s_{|N(v)|} = 0, \\ 1 - s_v & \text{otherwise.} \end{cases} \tag{C.1}$$

Intuitively, it means if all the neighbourhood vertices are not in $I_m$, i.e., $s_1 = s_2 = \ldots = s_{|N(v)|} = 0$, then $v$ should be in $I_m$ and contribute a factor $x_v$, otherwise, if any of the neighbourhood vertices is in $I_m$, then $v$ cannot be in $I_m$. As an example, for a vertex of degree 2, the resulting rank-3 tensor is

$$T(x_v, w_v) = \begin{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix} \\ \begin{pmatrix} x_v^{w_v} & 0 \\ 0 & 0 \end{pmatrix} \end{pmatrix}. \tag{C.2}$$

Let us consider the example in Sec. 3: its corresponding tensor network structure for computing the maximal independent polynomial becomes




One can see that the average rank of a tensor is increased. The computational complexity of this new tensor network contraction is often greater than the one for computing the independence polynomial.

By contracting this tensor network with generic element types, we can compute the maximal independent set properties such as the maximal independence polynomial and the enumeration of maximal independent sets. Similar to the independence polynomial, the maximal independence polynomial counts the number of maximal independent sets of various sizes [33]. Let $G = (V, E)$ be a graph, its maximal independence polynomial is defined as

$$D_m(G, x) = \sum_{k=0}^{\alpha(G)} b_k x^k, \tag{C.3}$$

where $b_k$ is the number of maximal independent sets of size $k$. Comparing with the independence polynomial in Eq. (5.1), we have $b_k \leq a_k$ and $b_{\alpha(G)} = a_{\alpha(G)}$. $D_m(G, 1)$ counts the total number of maximal independent sets [27, 42], which to our knowledge, the best algorithm gives a time complexity $O(1.3642^{|V|})$ [27]. If we want to find an MIS, $b_k$ can, in some cases, provide hints on the difficulty of finding the MIS using local algorithms [18].

We show the benchmark of computing the maximal independent set properties in Fig. 7, including a comparison to the Bron-Kerbosch algorithm from Julia package Graphs [2]. The treewidth of this tensor network is significantly larger, so benchmark with only a smaller graph size is feasible. The time for the tensor network approach and the Bron-Kerbosch approach to enumerate all maximal independent sets are comparable, while the tensor network does counting much more efficiently. Due to the memory limit, this Bron-Kerbosch algorithm is only feasible up to a graph size around 70.

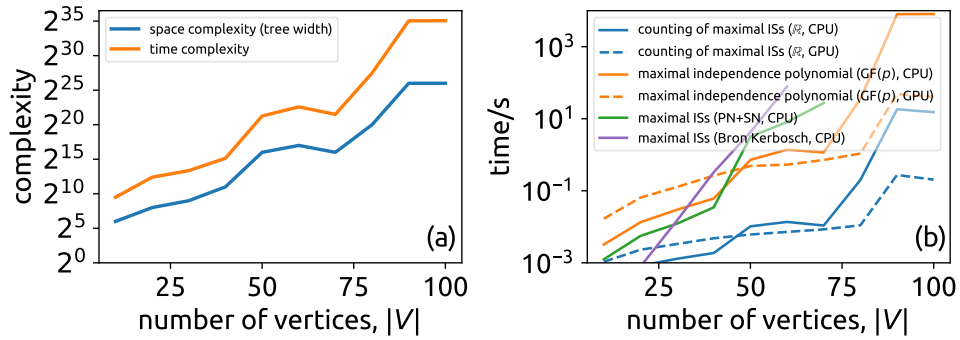



Figure 7: Benchmark results for computing different properties of maximal independent sets on a random three regular graph with different tensor element types. (a) treewidth versus the number of vertices for the benchmarked graphs. (b) The computing time for calculating the number of independent sets and enumerate all MISs.

**C.2. Matching problem.** A $k$-matching in a graph $G = (V, E)$ is a set of $k$ edges, no two of which have a vertex in common. We map an edge $(u, v) \in E$ to a degree of freedom $\langle u, v\rangle \in \{0, 1\}$ in a tensor network, where 1 means this edge is in the set and 0 otherwise. To characterize the matching, one can define a tensor of rank $d(v) = |N(v)|$ on vertex $v$

$$W_{\langle v,n_1\rangle,\langle v,n_2\rangle,\ldots,\langle v,n_{d(v)}\rangle} = \begin{cases} 1, & \sum_{i=1}^{d(v)} \langle v, n_i\rangle \leq 1, \\ 0, & \text{otherwise}, \end{cases} \tag{C.4}$$

and a tensor of rank 1 on the bond

$$B(w_{\langle u,v\rangle})_{\langle u,v\rangle} = \begin{cases} 1, & \langle u, v\rangle = 0 \\ x_{\langle u,v\rangle}^{w_{\langle u,v\rangle}}, & \langle u, v\rangle = 1, \end{cases} \tag{C.5}$$

where label $\langle v, u\rangle$ is equivalent to $\langle u, v\rangle$. The vertex tensor specifies the constraint that a vertex cannot be shared by two edges in the matched set, while an edge tensor carries the weights as the target to optimize. Let $x_{\langle u,v\rangle}^{w_{\langle u,v\rangle}} = x$, the tensor network contraction gives us the matching polynomial

$$M(G, x) = \sum_{k=1}^{|V|/2} c_k x^k, \tag{C.6}$$

where $k$ is the size of a matched edges set, and a coefficients $c_k$ is the number of $k$-matchings.

**C.3. Vertex coloring.** Let $G = (V, E)$ be a graph, a vertex coloring is an assignment of colors to each vertex $v \in V$ such that no edge connects two identically colored vertices. In a $k$-coloring problem, the number of different colors can be used is limited to less or equal to $k$. Let us use the 3-coloring problem as an example to show how to characterize with local tensors. For each vertex $v \in V$, we associate a degree of freedom $c_v \in \{0, 1, 2\}$ to it. Then we define a vertex tensor labelled by it as

$$W(v) = \begin{pmatrix} r_v \\ g_v \\ b_v \end{pmatrix}, \tag{C.7}$$

where $r_v$, $g_v$ and $b_v$ are colors for labeling the configurations. For each edge $(u, v)$, we specify the constraint carrying a weight $w_{uv}$ on it by defining an edge tensor labelled by $(c_u, c_v)$ as

$$B(x, w_{uv}) = \begin{pmatrix} 0 & x^{w_{uv}} & x^{w_{uv}} \\ x^{w_{uv}} & 0 & x^{w_{uv}} \\ x^{w_{uv}} & x^{w_{uv}} & 0 \end{pmatrix}. \tag{C.8}$$

The number of possible colorings can be obtained by contracting this tensor network by setting $r_v, g_v$ and $b_v$ to 1. Let $x^{w_{uv}} = x$, we have a graph polynomial, in which the $k$-th coefficient is the number of coloring with $k$ bonds satisfied. If a graph is colorable, the maximum order of this polynomial should be equal to the number of edges in this graph. Similarly, one can define the $k$-coloring problem on edges by defining the tensor network on the line graph of $G$.

**C.4. Cutting problem.** In graph theory, a cut is a partition of the vertices of a graph into two disjoint subsets, which is also known as the boolean spin glass problem in statistic physics. Let $G = (V, E)$ be a graph, to reduce the cutting problem on $G$ to the contraction of a tensor network, we first define a boolean degree of freedom $s_v \in \{0, 1\}$ for each vertex $v \in V$. Then for each edge $(u, v) \in E$, we define an edge matrix labelled by $s_u s_v$ as

$$B(x, w_{uv}) = \begin{pmatrix} 1 & x_v^{w_{uv}} \\ x_u^{w_{uv}} & 1 \end{pmatrix}, \tag{C.9}$$

where variables $x_u$ and $x_v$ represents a cut on this edge or a domain wall in an spin glass. Let $x_u^{w_{uv}} = x_v^{w_{uv}} = x$, we have a graph polynomial similar to previous ones, where its $k$th coefficient is two times the number of cuts with size $k$ (i.e. cutting $k$ edges).

**C.5. Dominating Set.** In graph theory, a dominating set for a graph $G = (V, E)$ is a subset $D \subseteq V$ such that every vertex not in $D$ is adjacent to at least one member of $D$. To reduce this problem to the contraction of a tensor network, we first map a vertex $v \in V$ to a boolean degree of freedom $s_v \in \{0, 1\}$. Then for each vertex $v \in V$ we define a tensor on its closed neighborhood $\{v\} \cup N(v)$ as

$$T(x, w_v)_{s_1, s_2, \ldots, s_{|N(v)|}, s_v} = \begin{cases} 0_v & s_1 = s_2 = \ldots = s_{|N(v)|} = s_v = 0, \\ 1_v & s_v = 0, \\ x^{w_v} & \text{otherwise}, \end{cases} \tag{C.10}$$

where $w_v$ is the weight of vertex $v$. This tensor means if both $v$ and its neighbouring vertices are not in $D$, i.e., $s_1 = s_2 = \ldots = s_{|N(v)|} = s_v = 0$, this configuration is forbidden because $v$ is not adjacent to any member in the set. Otherwise, if $v$ is in $D$, this tensor contributes a multiplicative factor $x_v^{w_v}$ to the output. The graph polynomial for the dominating set problem is known as the domination polynomial [5], which is defined as

$$D(G, x) = \sum_{k=0}^{\gamma(G)} d_k x^k, \tag{C.11}$$

where $d_k$ is the number of dominating sets of size $k$.

**C.6. Boolean satisfiability Problem.** The boolean satisfiability problem is the problem of determining if there exists an interpretation that satisfies a given boolean formula. One can specify a satisfiable problem in the conjuctive normal form (CNF): a conjuction of disjunctions of boolean literals, where a disjunction of boolean literals is also

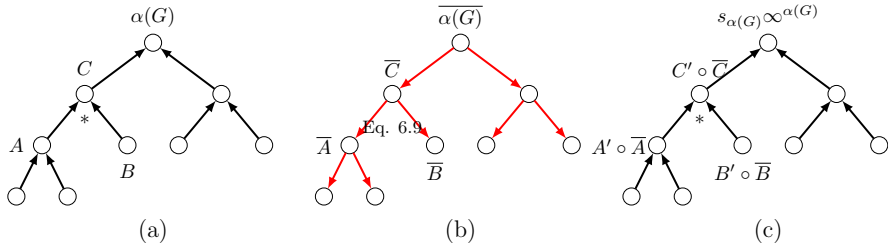



Figure 8: Bounded enumeration of maximum independent sets. In these graphs, a circle is a tensor, an arrow specifies execution direction of a function and $\circ$ is the Hadamard (element-wise) multiplication. $\overline{A}$ means the boolean mask of $A$. (a) is the forward pass with algebra Eq. (6.3: T) for computing $\alpha(G)$. (b) is the backward pass for computing boolean gradients as masks. (c) is the masked forward pass with algebra Eq. (7.3: P1+SN) for enumerating configurations.

named a clause. To reduce the problem of solving CNF to a tensor network contraction, we first map a boolean literal $a$ and its negation $\neg a$ to a same degree of freedom (label) $s_a \in \{0, 1\}$, where 0 stands for variable $a$ having value `false` while 1 stands for having value `true`. Then we map a clause to a tensor. For example, the $k$-th clause $\neg a \vee b \vee \neg c$ can be mapped to a tensor labeled by $(s_a, s_b, s_c)$.

$$C_k = \begin{pmatrix} \begin{pmatrix} x^{w_k} & x_b^{w_k} \\ x_a^{w_k} & x_{ab}^{w_k} \end{pmatrix} \\ \begin{pmatrix} x_c^{w_k} & x_{bc}^{w_k} \\ 1_{ac} & x_{abc}^{w_k} \end{pmatrix} \end{pmatrix}, \tag{C.12}$$

where a weight $w_k$ is associated with a clause. There is only one entry $(s_a, s_b, s_c) = (1, 0, 1)$ that makes this clause unsatisfied. If we contract this tensor network, we will get a multiplicative factor $x$ whenever there is a clause satisfied. Let $x_{\dots}^{w_k} = x$, one can get a polynomial, in which the $k$-th coefficient gives the number of assignments with $k$ clauses satisfied.

**C.7. Set packing.** Set packing is the hypergraph generalization of the maximum independent set problem, where a set corresponds to a vertex and an element corresponds to a hyperedge. To solve the set packing problem, we can just remove the rank-2 restriction of the edge tensor in Eq. (4.2)

$$B_{s_u, s_v, \dots, s_w} = \begin{cases} 1, & s_u + s_v + \dots + s_w \leq 1, \\ 0, & \text{otherwise.} \end{cases} \tag{C.13}$$

**Appendix D. Bounding the MIS enumeration space.**

When we use the algebra in Eq. (7.3: P1+SN) to enumerate all MIS configurations, we find that the program stores significantly more intermediate configurations than necessary and thus incur significant overheads in space. To speed up the computation and reduce space overhead, we bound the searching space using the information from the computation of the MIS size $\alpha(G)$. As shown in Fig. 8, (a) we first compute the value of $\alpha(G)$ with tropical algebra and cache all intermediate tensors. (b) Then, we compute a boolean mask for each cached tensor, where we use a boolean true to represent a tensor element having a contribution to the MIS (i.e. with a non-zero gradient) and boolean false otherwise. (c)

Finally, we perform masked tensor network contraction (i.e. discarding the unnecessary intermediate configurations) using the element type with the algebra in Eq. (7.3: P1+SN) to obtain all MIS configurations. Note that these masks in fact correspond to tensor elements with non-zero gradients with respect to the MIS size; we compute these masks by back propagating the gradients. To derive the back-propagation rule for tropical tensor contraction, we first reduce the problem to finding the back-propagation rule of a tropical matrix multiplication $C = AB$. Since $C_{ik} = \bigoplus_j A_{ij} \odot B_{jk} = \max_j A_{ij} \odot B_{jk}$ with tropical algebra, we have the following inequality

$$A_{ij} \odot B_{jk} \leq C_{ik}. \tag{D.1}$$

Here $\leq$ on tropical numbers are the same as the real-number algebra. The equality holds for some $j'$, which means $A_{ij'}$ and $B_{j'k}$ have contributions to $C_{ik}$. Intuitively, one can use this relation to identify elements with nonzero gradients in $A$ and $B$, but if doing this directly, one loses the advantage of using BLAS libraries [3] for high performance. Since $A_{ij} \odot B_{jk} = A_{ij} + B_{jk}$, one can move $B_{jk}$ to the right hand side of the inequality:

$$A_{ij} \leq C_{ik} \odot B_{jk}^{\circ -1} \tag{D.2}$$

where $^{\circ -1}$ is the element-wise multiplicative inverse on tropical algebra (which is the additive inverse on real numbers). The inequality still holds if we take the minimum over $k$:

$$A_{ij} \leq \min_k (C_{ik} \odot B_{jk}^{\circ -1}) = \left(\max_k \left(C_{ik}^{\circ -1} \odot B_{jk}\right)\right)^{\circ -1} = \left(\bigoplus_k \left(C_{ik}^{\circ -1} \odot B_{jk}\right)\right)^{\circ -1} = \left(C^{\circ -1} B^{\mathsf{T}}\right)_{ij}^{\circ -1}. \tag{D.3}$$

On the right hand side, we transform the operation into a tropical matrix multiplication so that we can utilize the fast tropical BLAS routines [3]. Again, the equality holds if and only if the element $A_{ij}$ has a contribution to $C$ (i.e. having a non-zero gradient). Let the gradient mask for $C$ be $\overline{C}$; the back-propagation rule for gradient masks reads

$$\overline{A}_{ij} = \delta\left(A_{ij}, \left(\left(C^{\circ -1} \circ \overline{C}\right) B^{\mathsf{T}}\right)_{ij}^{\circ -1}\right), \tag{D.4}$$

where $\delta$ is the Dirac delta function that returns one if two arguments have the same value and zero otherwise, $\circ$ is the element-wise product, boolean false is treated as the tropical number $\mathbb{0}$, and boolean true is treated as the tropical number $\mathbb{1}$. This rule defined on matrix multiplication can be easily generalized to tensor contraction by replacing the matrix multiplication between $C^{\circ -1} \circ \overline{C}$ and $B^{\mathsf{T}}$ by a tensor contraction. With the above method, one can significantly reduce the space needed to store the intermediate configurations by setting the tensor elements masked false to zero during contraction.

**Appendix E. The fitting approach to computing the independence polynomial.** In this section, we propose to find the independence polynomial by fitting $\alpha(G)+1$ random pairs of $x_i$ and $y_i = I(G, x_i)$. One can then compute the independence polynomial coefficients $a_i$ by solving the linear equation:

$$\begin{pmatrix} 1 & x_0 & x_0^2 & \dots & x_0^{\alpha(G)} \\ 1 & x_1 & x_1^2 & \dots & x_1^{\alpha(G)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{\alpha(G)} & x_{\alpha(G)}^2 & \dots & x_{\alpha(G)}^{\alpha(G)} \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_{\alpha(G)} \end{pmatrix} = \begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_{\alpha(G)} \end{pmatrix}. \tag{E.1}$$

With this approach, we do not incur the linear overhead in space. However, because the independence polynomial coefficients can have a huge order-of-magnitude range, if we use

floating point numbers in the computation, the round-off errors can be significant for the counting of large-size independent sets. In addition, the number could easily overflow if we use fixed-width integer types. The big integer type is also not a good option because big integers with varying width can be very slow and is incompatible with GPU devices. These problems can be solved by introducing a finite-field algebra GF($p$):

$$\begin{aligned} x \oplus y &= x + y \pmod{p}, \\ x \odot y &= xy \pmod{p}, \\ \mathbb{0} &= 0, \\ \mathbb{1} &= 1. \end{aligned} \tag{E.2: GF($p$)}$$

With a finite-field algebra, we have the following observations:

1. One can use Gaussian elimination [28] to solve the linear equation Eq. (E.1) since it is a generic algorithm that works for any elements with field algebra. The multiplicative inverse of a finite-field algebra can be computed with the extended Euclidean algorithm.
2. Given the remainders of a larger unknown integer $x$ over a set of co-prime integers $\{p_1, p_2, \ldots, p_n\}$, $x \pmod{p_1 \times p_2 \times \ldots \times p_n}$ can be computed using the Chinese remainder theorem. With this, one can infer big integers from small integers.

With these observations, we develop Algorithm E.1 to compute the independence polynomial exactly without introducing space overheads. The algorithm iterates over a sequence of large prime numbers until convergence. In each iteration, we choose a large prime number $p$, and contract the tensor networks to evaluate the polynomial for each variable $\chi = (x_0, x_1, \ldots, x_{\alpha(G)})$ on GF($p$) and denote the outputs as $(y_0, y_1, \ldots, y_{\alpha(G)}) \pmod{p}$. Then we solve Eq. (E.1) using Gaussian elimination on GF($p$) to find the coefficient modulo $p$, $A_p \equiv (a_0, a_1, \ldots, a_{\alpha(G)}) \pmod{p}$. As the last step of each iteration, we apply the Chinese remainder theorem to update $A \pmod{P}$ to $A \pmod{P \times p}$, where $P$ is a product of all prime numbers chosen in previous iterations. If this number does not change compared with the previous iteration, it indicates the convergence of the result and the program terminates. All computations are done with integers of fixed width $W$ except the last step of applying the Chinese remainder theorem, where we use arbitrary precision integers to represent the counting.

**Algorithm E.1** Computing the independence polynomial exactly without integer overflow

Let $P = 1$, $W$ be the integer width, vector $\chi = (0, 1, 2, \ldots, \alpha(G))$, matrix $X_{ij} = (\chi_i)^j$, where $i, j = 0, 1, \ldots, \alpha(G)$
**while** *true* **do**
  compute the largest prime $p$ that $\gcd(p, P) = 1$ and $p < 2^W$
  **for** $i = 0 \ldots \alpha(G)$ **do**
    $y_i \pmod{p}$ = contract_tensor_network($\chi_i \pmod{p}$) ; // on GF($p$)
  **end**
  $A_p = (a_0, a_1, \ldots, a_{\alpha(G)}) \pmod{p}$ = gaussian_elimination($X, (y_0, y_1, \ldots, y_{\alpha(G)}) \pmod{p}$)
  $A_{P\times p}$ = chinese_remainder($A_P, A_p$)
  **if** $A_P = A_{P\times p}$ **then**
    **return** $A_P$ ; // converged
  **end**
  $P = P \times p$
**end**

## Appendix F. The discrete Fourier transform approach to computing the independence polynomial.

In section 5, we show that the independence polynomial can be obtained by solving the linear equation Eq. (E.1). Since the coefficients of the independence polynomial can range many orders of magnitude, the round-off errors in fitting can be significant if we use random floating point numbers for $x_i$. In the main text, we propose to use a finite field GF($p$) to circumvent integer overflow and round-off errors. One drawback of using finite field algebra is its matrix multiplication is less computational efficient compared with floating point matrix multiplication. Here, we give an alternative method based on discrete Fourier transform with controllable round off errors. Instead of choosing $x_i$ as random numbers, we can choose them such that they form a geometric sequence in the complex domain $x_j = r\omega^j$, where $r \in \mathbb{R}$ and $\omega = e^{-2\pi i/(\alpha(G)+1)}$. The linear equation thus becomes

$$\begin{pmatrix} 1 & r & r^2 & \dots & r^{\alpha(G)} \\ 1 & r\omega & r^2\omega^2 & \dots & r^{\alpha(G)}\omega^{\alpha(G)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & r\omega^{\alpha(G)} & r^2\omega^{2\alpha(G)} & \dots & r^{\alpha(G)}\omega^{\alpha(G)^2} \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_{\alpha(G)} \end{pmatrix} = \begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_{\alpha(G)} \end{pmatrix}. \tag{F.1}$$

Let us rearrange the coefficients $r^j$ to $a_j$, the matrix on the left side becomes the discrete Fourier transform matrix. Thus, we can obtain the coefficients by inverse Fourier transform $\vec{a}_r = \text{FFT}^{-1}(\omega)\cdot\vec{y}$, where $(\vec{a}_r)_j = a_j r^j$. By choosing different $r$, one can obtain better precision in low independent set size region by choosing $r < 1$ or high independent set size region by choosing $r > 1$.

**Appendix G. Integer sequence formed by the number of independent sets.** We computed the number of independent sets on square lattices and King's graphs with our generic tensor network contraction algorithm on GPUs. The tensor element type is finite-field algebra so that we can reach arbitrary precision. We also computed the independence polynomial exactly for these lattices which can be found in our Github repo.

Table 2: The number of independent sets for square grid graphs of size $L \times L$. This forms the integer sequence OEIS A006506. Here we only include two updated entries for $L = 38, 39$, which, to our knowledge, has not been computed before [14].

| $L$ | square grid graphs |
|---|---|
| 38 | 616 412 251 028 728 207 385 738 562 656 236 093 713 609 747 387 533 907 560 081 990 229 746 115 948 572 583 817 557 035 128 726 922 565 913 748 716 778 414 190 432 479 964 245 067 083 441 583 742 870 993 696 157 129 887 194 203 643 048 435 362 875 885 498 554 979 326 352 127 528 330 481 118 313 702 375 541 902 300 956 879 563 063 343 972 979 |
| 39 | 29 855 612 447 544 274 159 031 389 813 027 239 335 497 014 990 491 494 036 487 199 167 155 042 005 286 230 480 609 472 592 158 583 920 411 213 748 368 073 011 775 053 878 033 685 239 323 444 700 725 664 632 236 525 923 258 394 737 964 155 747 730 125 966 370 906 864 022 395 459 136 352 378 231 301 643 917 282 836 792 261 715 266 731 741 625 623 207 330 411 607 |

**Appendix H. Computing maximum sum combination.** Given two sets $A$ and $B$ of the same size $n$. It is known that the maximum $n$ sum combination of $A$ and $B$ can be computed in time $n\log(n)$. The standard approach to solve the sum combination problem requires storing the variables in a heap - a highly dynamic binary tree structure which can can be much slower to manipulate than arrays. In the following, we show an algorithm that has roughly the same complexity (given the data range is not exponentially large) but does not need a heap. This

algorithm first sorts both $A$ and $B$, then use the bisection to find the $n$-th largest value in the sum combination. The key point is we can count the number of entries greater than a specific value in the sum combination of $A$ and $B$ in linear time. We summarize the algorithm as in Algorithm H.1.

**Algorithm H.1** Fast sum combination without using heap

Let $A$ and $B$ be two sets of size $n$
`// sort A and B in ascending order`
$A \leftarrow$ sort($A$)
$B \leftarrow$ sort($B$)
`// use bisection to find the n-th largest value in sum combination`
high $\leftarrow A_n + B_n$
low $\leftarrow A_1 + B_n$
**while** *true* **do**
    mid $\leftarrow$ (high + low)/2
    $c \leftarrow$ `count_geq`($n, A, B,$ mid)
    **if** $c > n$ **then**
        low $\leftarrow$ mid
    **else if** $c = n$ **then**
        **return** `collect_geq`($n, A, B,$ mid)
    **else**
        high $\leftarrow$ mid
    **end**
**end**
**function** `count_geq`*(n, A, B, v)*
    $k \leftarrow 1$ ; `// number of entries in A s.t.` $a + b \geq v$
    $a \leftarrow A_n$ ; `// the smallest entry in A s.t.` $a + b \geq v$
    $c \leftarrow 0$ ; `// the counting of sum combinations s.t.` $a + b \geq v$
    **for** $q = n, n-1 \ldots 1$ **do**
        $b \leftarrow B_{n-q+1}$
        **while** $k < n$ ***and*** $a + b \geq v$ **do**
            $k \leftarrow k + 1$
            $a \leftarrow A_{n-k+1}$
        **end**
        **if** $a + b \geq v$ **then**
            $c \leftarrow c + k$
        **else**
            $c \leftarrow c + k - 1$
        **end**
    **end**
    **return** c
**end**

Function `collect_geq` is similar the `count_geq` except the counting is replace by the item collection. Note in function `count_geq`, variable $k$ monotoneously increase while $q$ monotoneously decrease in each iteration, the total number of iterations must be smaller or equal to $2n$. Here for simplicity, we do not handle the $-\infty$s in $A$ and $B$ and the degeneracy in the sums. They need to be taken seriously in practical implementations.

**Appendix I. Technical guide.** This project depends on multiple open source packages in the Julia ecosystem. We list the Julia packages that play important roles in our code base as follows:

**OMEinsum and OMEinsumContractionOrders** are packages providing the support for Einstein's (or tensor network) notation and contraction order optimizations.

`OMEinsumContractionOrders` implements state-of-the-art algorithms for finding the optimal contraction order for a tensor network, including the KaHypar+Greedy [29, 46] and local transformation based approaches [35],

**TropicalNumbers and TropicalGEMM** are packages providing tropical number and efficient tropical matrix multiplication,

**Graphs** is a package providing graph utilities, like random regular graph generator,

**Polynomials** is a package providing polynomial algebra and polynomial fitting,

**Mods and Primes** are packages providing finite field algebra and prime number generations.

One can install these packages by opening a Julia REPL, type `]` to enter the `pkg>` mode and type, e.g.

```
pkg> add OMEinsum Graphs Mods Primes Polynomials TropicalNumbers OMEinsumContractionOrders
```

The reader may find it surprising that the Julia implementation of the algorithms introduced in this work is so short that except the bounding algorithm, all are contained in this appendix. This is due to the power of generic programming. After installing the required packages, one can open a Julia REPL and copy the following codes into it.

```julia
using OMEinsum, OMEinsumContractionOrders
using Graphs
using Random

# generate a random regular graph of size 100, degree 3
graph = (Random.seed!(2); Graphs.random_regular_graph(50, 3))

# generate einsum code, i.e. the labels of tensors
code = EinCode(([minmax(e.src,e.dst) for e in Graphs.edges(graph)]..., # labels for edge tensors
                [(i,) for i in Graphs.vertices(graph)]...), ())        # labels for vertex
     tensors

# an einsum contraction without a contraction order specified is called `EinCode`,
# an einsum contraction having a contraction order (specified as a tree structure) is called `
     NestedEinsum`.
# assign each label a dimension-2, it will be used in the contraction order optimization
# `uniquelabels` function extracts the tensor labels into a vector.
size_dict = Dict([s=>2 for s in uniquelabels(code)])
# optimize the contraction order using the `TreeSA` method; the target space complexity is 2^17
optimized_code = optimize_code(code, size_dict, TreeSA())
println("time/space complexity is $(OMEinsum.timespace_complexity(optimized_code, size_dict))")

# a function for computing the independence polynomial
function independence_polynomial(x::T, code) where {T}
   xs = map(getixsv(code)) do ix
        # if the tensor rank is 1, create a vertex tensor.
        # otherwise the tensor rank must be 2, create a bond tensor.
        length(ix)==1 ? [one(T), x] : [one(T) one(T); one(T) zero(T)]
    end
    # both `EinCode` and `NestedEinsum` are callable, inputs are tensors.
   code(xs...)
end

########## COMPUTING THE MAXIMUM INDEPENDENT SET SIZE AND ITS COUNTING/DEGENERACY ###########

# using Tropical numbers to compute the MIS size and the MIS degeneracy.
using TropicalNumbers
mis_size(code) = independence_polynomial(TropicalF64(1.0), code)[]
println("the maximum independent set size is $(mis_size(optimized_code).n)")

# A `CountingTropical` object has two fields, tropical field `n` and counting field `c`.
mis_count(code) = independence_polynomial(CountingTropical{Float64,Float64}(1.0, 1.0), code)[]
println("the degeneracy of maximum independent sets is $(mis_count(optimized_code).c)")

########## COMPUTING THE INDEPENDENCE POLYNOMIAL ###########
```

```
# using Polynomial numbers to compute the polynomial directly
using Polynomials
println("the independence polynomial is $(independence_polynomial(Polynomial([0.0, 1.0]),
      optimized_code)[])")

########## FINDING MIS CONFIGURATIONS ###########

# define the set algebra
struct ConfigEnumerator{N}
    # NOTE: BitVector is dynamic and it can be very slow; check our repo for the static version
    data::Vector{BitVector}
end
function Base.:+(x::ConfigEnumerator{N}, y::ConfigEnumerator{N}) where {N}
    res = ConfigEnumerator{N}(vcat(x.data, y.data))
    return res
end
function Base.:*(x::ConfigEnumerator{L}, y::ConfigEnumerator{L}) where {L}
    M, N = length(x.data), length(y.data)
    z = Vector{BitVector}(undef, M*N)
    for j=1:N, i=1:M
        z[(j-1)*M+i] = x.data[i] .| y.data[j]
    end
    return ConfigEnumerator{L}(z)
end
Base.zero(::Type{ConfigEnumerator{N}}) where {N} = ConfigEnumerator{N}(BitVector[])
Base.one(::Type{ConfigEnumerator{N}}) where {N} = ConfigEnumerator{N}([falses(N)])

# the algebra sampling one of the configurations
struct ConfigSampler{N}
    data::BitVector
end

function Base.:+(x::ConfigSampler{N}, y::ConfigSampler{N}) where {N}  # biased sampling: return
      `x`
    return x  # randomly pick one
end
function Base.:*(x::ConfigSampler{L}, y::ConfigSampler{L}) where {L}
    ConfigSampler{L}(x.data .| y.data)
end

Base.zero(::Type{ConfigSampler{N}}) where {N} = ConfigSampler{N}(trues(N))
Base.one(::Type{ConfigSampler{N}}) where {N} = ConfigSampler{N}(falses(N))

# enumerate all configurations if `all` is true; compute one otherwise.
# a configuration is stored in the data type of `StaticBitVector`; it uses integers to represent
       bit strings.
# `ConfigTropical` is defined in `TropicalNumbers`. It has two fields: tropical number `n` and
      optimal configuration `config`.
# `CountingTropical{T,<:ConfigEnumerator}` stores configurations instead of simple counting.
function mis_config(code; all=false)
    # map a vertex label to an integer
    vertex_index = Dict([s=>i for (i, s) in enumerate(uniquelabels(code))])
    N = length(vertex_index)  # number of vertices
    xs = map(getixsv(code)) do ix
        T = all ? CountingTropical{Float64, ConfigEnumerator{N}} : CountingTropical{Float64,
     ConfigSampler{N}}
        if length(ix) == 2
            return [one(T) one(T); one(T) zero(T)]
        else
            s = falses(N)
            s[vertex_index[ix[1]]] = true  # one hot vector
            if all
                [one(T), T(1.0, ConfigEnumerator{N}([s]))]
            else
                [one(T), T(1.0, ConfigSampler{N}(s))]
            end
        end
    end
   return code(xs...)
end

println("one of the optimal configurations is $(mis_config(optimized_code; all=false)[].c.data)"
      )
```

```
# direct enumeration of configurations can be very slow; please check the bounding version in
    our Github repo.
println("all optimal configurations are $(mis_config(optimized_code; all=true)[].c)")
```

For better performance, we recommend checking our GitHub repository for the full featured version: https://github.com/Happy-Diode/GraphTensorNetworks.jl. It can be installed in a similar style to other packages.