

COMPUTING PROPERTIES OF INDEPENDENT SETS BY GENERIC PROGRAMMING TENSOR NETWORKS *

XXX[†] AND YYY[‡]

Abstract. We introduce a new approach to compute various properties of independent sets by encoding the problems into tensor networks with different tensor element algebra. The type of graph problems that can be computed using this method includes: independence number, the number of independent sets, independence polynomial, maximal independence polynomial, and enumeration of the maximum independence set configurations. Although the computational complexity inevitably scales exponentially with the graph size, the performance of our method using tensor network contraction with generic programming is on par or outperforms state-of-the-art, sophisticated methods; on the other hand, our algorithms are very simple to implement and one can directly utilize recent advances in tensor network contraction techniques. To demonstrate the versatility of this tool, we apply it to a few examples including the calculations of the hard-square entropy constant, Euler characteristics of the independence complex, partition functions, and finite-temperature phase transitions on square-lattice graphs.

Key words. independent set, tensor network, maximum independent set, independence polynomial

AMS subject classifications. 05C31, 14N07

1. Introduction. [JG: overlap gap property [19, 18], independence polynomial at -1 [7, 29], branching algorithm [41, 38]] In graph theory and combinatorics, there are many interesting but hard computational problems concerning properties of independent sets. An independent set is a set of vertices in a graph where no two vertices are adjacent to each other. More formally, given an undirected graph $G = (V, E)$, an independent set $I \subseteq V$ is a set that for any $u, v \in I$, there is no edge connecting u and v in G . The problem of finding an independent set of the largest possible size, the maximum independent set (MIS), is a paradigmatic NP-complete problem [24]. The size of the MIS of a graph G is called the independence number, denoted as $\alpha(G) \equiv \max_I |I|$.

Finding $\alpha(G)$ is a hard computational problem; moreover, it is NP-hard to even approximate $\alpha(G)$ within a factor $|V|^{1-\epsilon}$ for an arbitrarily small positive ϵ . Naive exhaustive search for the MIS requires time $O(2^{|V|})$. More efficient exact algorithms include the branching algorithms and dynamic programming. Sophisticated branching algorithms can reduce the base of the exponential time scaling to, e.g., $1.1996^n n^{O(1)}$ [43]. Dynamic programming approaches [11, 17] works better for graphs with a small treewidth $\text{tw}(G)$; these methods can produce algorithms of complexity $O(2^{\text{tw}(G)} \text{tw}(G) |V|)$.

The independent set problem is closely related to the clique problem and the vertex cover problem [34]; more concretely, an MIS of a graph G corresponds to a maximum clique in the complement graph of G , and the complement vertex set of an MIS corresponds to a minimum vertex cover of the graph G . Together, these problems find a wide range of applications in scheduling, logistics, social network analysis, bioinformatics, wireless networks and telecommunication, map labelling, computer vision, etc. [9, 42]. Besides the standard MIS problem, there are many other interesting problems pertaining to independent sets, such as the number of independent sets, independence polynomial, maximal independence polynomial, and enumeration of optimal and sub-optimal configurations. Some of these problems are of great interest in physics applications such as the hard-core lattice gas model [12, 14] in statistical mechanics and the Rydberg hamiltonian with neutral atoms [37] [ST: cite experiment when it's ready]; they can, for example, be used to

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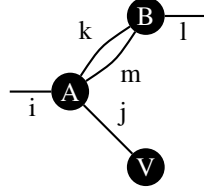
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understand phase transitions and to identify harder graphs in an ensemble of graphs [ST: cite experiment].

In this work, we introduce a tensor-network based framework to compute the various properties pertaining to independent sets. We map different problems into generic tensor network contraction with various tensor element algebra. Our approach does not necessarily provide a better time complexity compared to dynamic programming, but the tensor network approach is highly versatile so different problems can be generically solved with minimal implementation efforts. We benchmark our algorithms, the implementation of which benefits from recent advances in tensor-network contraction for the purposes of quantum circuit simulations [22, 36]. Lastly, we provide a few examples and show that the toolbox can be used to calculate the hard-square entropy constant, Euler characteristics of the independence complex, partition functions, and finite-temperature phase transitions on square-lattice graphs.

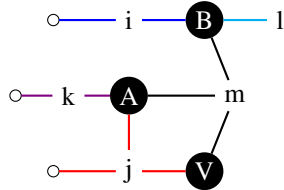
2. Tensor networks. A tensor network [10, 35] can be viewed as a generalization of matrix multiplication to multi-dimensional tensor contraction. Let A, B be two matrices; the matrix multiplication is defined as $C_{ik} = \sum_j A_{ij} B_{jk}$. Using the Einstein notation, we can write $C_{ik} = A_{ij} B_{jk}$, where j is implicitly summed over. In the standard notation, each index can appear at most twice. A tensor network consists of multiple tensors performing the sum-product operation, i.e., contraction, and the tensor network can be represented as a multigraph with open edges by viewing a tensor as a vertex, a label pairing two tensors as an edge, and the remaining unpaired labels as open edges.

Example 1. A tensor network $C_{il} = A_{ijkm} B_{kml} V_j$ has the following multigraph representation.



One can generalize the tensor network notation by removing the restriction that each index can appear at most twice. The notation can be considered as a generalized Einstein notation, which is sometimes called einsum, sum-product network or factor graph [6] in different contexts. The graphical representation of a tensor network we use in this paper is a hypergraph, where an edge (label) can be shared by an arbitrary number of vertices (tensors).

Example 2. $C_{ijk} = A_{jkm} B_{mil} V_{jm}$ is a tensor network representing $C_{ijk} = \sum_{ml} A_{jkm} B_{mil} V_{jm}$ [ST: I've changed this. please check. The original was $C_{ijk} = A_{jkm} B_{mil} V_{jm}$ and $C_{ijk} = \sum_{ml} A_{jkm} B_{mil} V_{jm}$]. [JG: changed back because l is not an open edge. Is it still confusing if I introduce open circles for open edges?] Its hypergraph representation is shown below, where we use different colors to annotate different hyperedges and open circles to denote open edges.



In the main text, we use the generalized tensor network notation. The generalized tensor network can be easily translated to the standard notation by adding identity tensors denoted

as δ tensors. The example above can be written as $C_{ijkl} = A_{jkm}B_{mil}V_{jm} = A_{ukm}B_{pil}V_{vq}\delta_{mpq}\delta_{juv}$ in the standard notion. However, by adding the δ tensors, one may unnecessarily increase the contraction complexity of a graph, which we illustrate in Appendix B.

3. Generic programming. [ST: I suggest we have a section on generic programming, putting both the semiring stuff and the summary table to this section, since generic programming is one of the highlights of this paper as well. I think it doesn't need to be long. Jinguo, could you write one or two paragraphs introducing generic programming?][JG: I wrote a draft here, does it look ok in general?] In previous works combining tensor network and combinatoric problems [27, 5], the elements in tensor networks are limited to regular number types such as floating point numbers and integers. As the development of modern compiling technology, we do not need to limit our imaginations to regular number types anymore. The key technology playing the role is called the generic programming:

DEFINITION 3.1 (Generic programming). *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.* [40]

This definition of generic programming contains two major pieces, one is a single program for the general setting, and another is about efficiency. To understand the first point, suppose we want to write a function to take the power of an element $f(x, n) := x^n$. One can easily write a function for regular numbers that computes the power of x in $\log(n)$ steps using the multiply and square trick. A generic programmer does not assume x being a regular number type, instead it treats x as an element with an associative multiplication operation \odot and multiplicative identity $\mathbb{1}$. In such a way, when the program takes a matrix as input, it computes the matrix power without extra efforts. The second point about performance. For dynamic typed languages like Python, one can easily write very general codes, however, the efficiency is not guaranteed. Imagine the speed of computing the matrix multiplication between two numpy arrays with python objects as elements. The generic programming that we want to discuss is those in static types languages like C++, and Julia [4]. C++ uses templates for generic programming while Julia has just in time compiling and multiple dispatch. When they “sees” a new input type, the compiler recompiles the generic program for the new type. A lot optimization can be done during the compiling, like inlining immutable elements with fixed sizes in an array to decrease the cache miss rate when accessing data. In Julia, these inlined arrays can even be compiled to GPU devices for faster computation [3].

This leads us to think about what is the most general element type that allowed in a tensor network contraction program. Our finding is: as long as the tensor elements form a commutative semiring, the tensor network contraction result can be contraction order independent. So what is a commutative semiring? A semiring is a ring without additive inverse, while a commutative semiring is a semiring where the multiplication operation is commutative. 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 arbitrary three

elements $a, b, c \in R$.

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

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

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

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

The requirement of being commutative is for the tensor contraction result to be independent of the contraction order, which could be relaxed in certain cases. In the following sections, we show how to compute the independence polynomial, the maximal independence polynomial, independence number, the number of independent sets, and enumeration of the MIS configurations of a general graph G by designing tensor element types as commutative semirings while keeping the tensor network generic [40]. Table 1 summarizes the problems that can be solved by various tensor element types.

4. Independence polynomial and maximal independence polynomial.

4.1. Independence polynomial. The independence polynomial is an important graph polynomial that contains the counting information of independent sets. It is defined as

$$(4.1) \quad I(G, x) = \sum_{k=0}^{\alpha(G)} a_k x^k,$$

where a_k is the number of independent sets of size k in G , and $\alpha(G)$ is the independence number. The total number of independent sets is thus equal to $I(G, 1)$. The problem of computing the independence polynomial belongs to the complexity class #P-hard. One approach to exactly compute the independence polynomial requires a computational time of $O(1.442^{|V|})$ [15] [JG: I am not sure about this complexity, this is based on the naive analysis of theorem 2.2 in [15]]. There are some interesting works on efficiently approximating the independence polynomial [23], but in this work, we focus on exact methods to compute the independence polynomial.

The independence polynomial is closely related to the matching polynomial, the clique polynomial, and the vertex cover polynomial. In fact, the independence polynomial can be viewed as a generalization of the matching polynomial, since the matching polynomial of a graph G is the same as the independence polynomial of the line graph of G [28]. Thus, our algorithm to compute the independence polynomial can also be used to compute the above graph polynomials. Some properties of the independence polynomial, such as the uni-modality, log-concavity, and roots of the polynomial, are well studied in the literature for special classes of graphs [28]. We hope our algorithms to calculate the independence polynomial can also help further research in these directions.

element type	purpose
real number	counting all independent sets
tropical number (Eq. (5.2))	finding the independence number
tropical number with counting (Eq. (5.2))	finding the independence number and the number of MISs
tropical number with configurations (Eq. (6.5))	finding the independence number and one MIS
tropical number with sets (Eq. (6.3))	finding the independence number and enumeration of all MISs
polynomial (Eq. (4.4))	computing the independence polynomial exactly
truncated polynomial (Eq. (5.4))	counting MISs and independent sets of size $\alpha(G) - 1$
complex number	fitting the independence polynomial with fast Fourier transform
finite-field algebra (Eq. (4.7))	fitting the independence polynomial exactly using number theory

Table 1: Tensor element types and their purposes in calculating various independent set properties.

To compute the independence polynomial of a graph G , we encode it to a tensor network. On the vertex i of the graph G , we place a rank-one vertex tensor, $W(x_i)$, of size 2 parametrized by x_i and a rank-two edge tensor, B , of size 2×2 on an edge (i, j) [ST: I removed the indices s_i etc, on the right of the equations, since that looks confusing to me. If I understand correctly, s_i, s_j just denotes the index of the vector/matrix.] [JG: To be consistent, we should also remove the index on the LHS. It is better not removing the label information.]

$$(4.2) \quad W(x_i)_{s_i} = \begin{pmatrix} 1 \\ x_i \end{pmatrix}, \quad B_{s_i s_j} = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix},$$

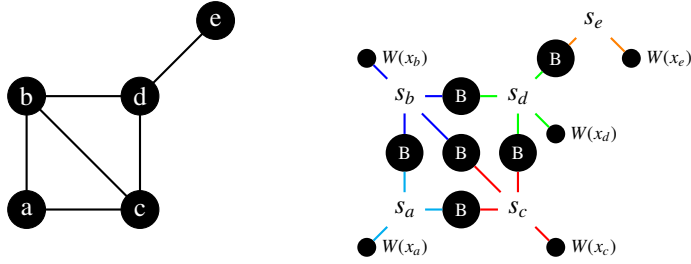
where the tensor index s_i is a boolean variable; $s_i = 1$ corresponds that the vertex i is in the independent set, and $s_i = 0$ means otherwise. Let us assume the tensor elements are real numbers for now. The edge tensor element $B_{s_i=1, s_j=1} = 0$ encodes the independent set constraint, meaning vertex i and j cannot be both in the independent set if they are connected by an edge (i, j) . The contraction of the tensor network representing G gives

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

where the summation runs over all vertex configurations $\{s_1, s_2, \dots, s_{|V|}\}$ and accumulates the product of tensor elements to the scalar output P (see Example 3 for a concrete example). In the special case of $x_i = x$, the contraction result directly corresponds to the independence polynomial. The connection 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. In the implementation of the algorithm, we benefit from recent advances in tensor network contraction, where researchers working on quantum circuit simulation evaluate the tensor network by pairwise contracting tensors in a good heuristic order [22, 36]. A good contraction order can reduce the time complexity significantly, at the cost of having a space overhead of $O(2^{\text{tw}(G)})$ [33]. 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.

Example 3. Mapping a graph (left) to a tensor network (right) that encodes the independence polynomial. In the generalized tensor network's graphical representation, a vertex is mapped to a hyperedge, and an edge is mapped to an edge tensor. **[ST: a vertex is mapped to a hyperedge?][JG: ✓]**



The contraction of this tensor network can be done in a pairwise order:

$$\begin{aligned}
& \sum_{s_a, s_b, s_c, s_d, s_e} W(x_a)_{s_a} W(x_b)_{s_b} W(x_c)_{s_c} W(x_d)_{s_d} W(x_e)_{s_e} B_{s_a s_b} B_{s_b s_d} B_{s_c s_d} B_{s_a s_c} B_{s_b s_c} B_{s_d s_e} \\
&= \sum_{s_b, s_c} \left(\sum_{s_d} \left(\left(\left(\sum_{s_e} B_{s_d s_e} W(x_e)_{s_e} \right) W(x_d)_{s_d} \right) (B_{s_b s_d} W(x_b)_{s_b}) \right) (B_{s_c s_d} W(x_c)_{s_c}) \right) \\
& \quad \left(B_{s_b s_c} \left(\sum_{s_a} B_{s_a s_b} (B_{s_a s_c} W(x_a)_{s_a}) \right) \right) \\
&= 1 + x_a + x_b + x_c + x_d + x_e + x_a x_d + x_a x_e + x_c x_e + x_b x_e \\
&= 1 + 5x + 4x^2 \quad (x_i = x)
\end{aligned}$$

Before contracting the tensor network and evaluating the independence polynomial numerically, let us first elevate the tensor elements 0s and 1s in tensors $W(x)$ 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. The most natural approach is to treat the tensor elements as polynomials and evaluate the polynomial directly. Let us create a polynomial type, and represent a polynomial $a_0 + a_1 x + \dots + a_k x^k$ as a coefficient vector $(a_0, a_1, \dots, a_k) \in \mathbb{R}^k$, 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

$$\begin{aligned}
(4.4) \quad & a \oplus b = (a_0 + b_0, a_1 + b_1, \dots, a_{\max(k_a, k_b)} + b_{\max(k_a, k_b)}), \\
& a \odot b = (a_0 + b_0, a_1 b_0 + a_0 b_1, a_2 b_0 + a_1 b_1 + a_0 b_2, \dots, a_{k_a} b_{k_b}), \\
& \mathbb{0} = (), \text{ [ST: should this be } (\mathbb{0})? \text{][JG : both are ok]} \\
& \mathbb{1} = (1).
\end{aligned}$$

We can see 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

$$(4.5) \quad W_{s_i}^{\text{poly}} = \begin{pmatrix} 1 \\ (0, 1) \end{pmatrix}, \quad B_{s_i s_j}^{\text{poly}} = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}.$$

By contracting the tensor network with the polynomial type, the final result is the exact representation of the independence polynomial. One way to efficiently evaluate the multiplication operation is to use the convolution theorem [39], but this approach suffers from a space overhead proportional to $\alpha(G)$ because each polynomial requires a vector of such size to store the coefficients.

Here, we propose to find the independence polynomial by fitting $\alpha(G) + 1$ random values 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:

$$(4.6) \quad \begin{pmatrix} 1 & x_0 & x_0^2 & \dots & x_0^{\alpha(G)} \\ 1 & x_1 & x_1^2 & \dots & x_1^{\alpha(G)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{\alpha(G)} & x_{\alpha(G)}^2 & \dots & x_{\alpha(G)}^{\alpha(G)} \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_{\alpha(G)} \end{pmatrix} = \begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_{\alpha(G)} \end{pmatrix}.$$

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 independent set sizes. 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 graphics processing unit (GPU) devices. These problems can be solved by introducing a finite-field algebra $\text{GF}(p)$:

$$(4.7) \quad \begin{aligned} x \oplus y &= x + y \pmod{p}, \\ x \odot y &= xy \pmod{p}, \\ 0 &= 0, \\ 1 &= 1. \end{aligned}$$

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

1. One can use Gaussian elimination [21] to solve the linear equation Eq. (4.6) 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 $\{p_1, p_2, \dots, p_n\}$, $x \pmod{p_1 \times p_2 \times \dots \times p_n}$ can be computed using the Chinese remainder theorem. With this, one can infer big integers from small integers.

With these observations, we develop Algorithm 4.1 to compute the independence polynomial exactly without introducing space overheads. This is an iterative algorithm that tries different prime numbers p until convergence. In each iteration, we contract tensor networks to evaluate the polynomial for each $x \in X$ on the finite field algebra $\text{GF}(p)$. Let us denote the results as Y , then we solve a linear equation $Y = \hat{X}A_p$ using the gaussian elimination on $\text{GF}(p)$ to find the coefficient modulus $A_p \equiv A \pmod{p}$. Finally we apply the Chinese remainder theorem to get $A \pmod{P}$, where P is a product of all prime numbers chosen in current and previous iterations. If this number does not change comparing with the previous iteration, it indicates

a convergent result. All computations are done with integers of fixed width W except the last step of applying Chinese remainder theorem. In Appendix D, we provide another method to solve the linear equation using discrete Fourier transform.

Algorithm 4.1 Compute the independence polynomial exactly without integer overflow

Let $P = 1$, W be the integer width, vector $X = (0, 1, 2, \dots, \alpha(G))$, matrix $\hat{X}_{ij} = X_i^j$, where $i, j = 0, 1, \dots, \alpha(G)$

while true do

 compute the largest prime p that $\gcd(p, P) = 1$ and $p \leq 2^W$

 compute the tensor contraction for each $x = X_i \pmod p$ on $\text{GF}(p)$ and obtain $Y = (y_0, y_1, \dots, y_{\alpha(G)}) \pmod p$

$A_p = (a_0, a_1, \dots, a_{\alpha(G)}) \pmod p = \text{gaussian_elimination}(\hat{X}, Y \pmod p)$

$A_{P \times p} = \text{chinese_remainder}(A_p, A_p)$

if $A_p = A_{P \times p}$ **then**

return A_p ; // converged

end

$P = P \times p$

end

[ST: discuss this algorithm table, X_{ij} , etc.][JG: done]

4.2. Maximal independence polynomial. [ST: It might be helpful to add a figure of the tensor network for computing the maximal independence polynomial.] [JG: done]

Sometimes people are interested in knowing maximal solutions to understand why their programs are trapped in a local minimal. In this paper, the word “maximal” is different with the “maximum” discussed the previous discussion in such a way that it is not necessarily refer to the gloal optimum. Instead of counting all independent sets, the maximal independence polynomial counts the number of maximal independent sets of various sizes [25]. Concretely, it is defined as

$$(4.8) \quad I_{\max}(G, x) = \sum_{k=0}^{\alpha(G)} b_k x^k,$$

where b_k is the number of maximal independent sets of size k in G . Obviously, $b_k \leq a_k$ and $b_{\alpha(G)} = a_{\alpha(G)}$. $I_{\max}(G, 1)$ counts the total number of maximal independent sets [20, 32], where the fastest algorithm currently has a runtime of $O(1.3642^{|V|})$ [20]. For the problem of finding the MIS, b_k counts the number of local optimum at size $k < \alpha(G)$, and can, in some cases, provide hints on the difficulty of finding the MIS using local algorithms [ST: cite experiment]. The uni-modality, log-concavity, and real-rootness properties of the maximal independence polynomial for special classes of graphs have also been studied [25].

Let us denote the neighborhood of a vertex v as $N(v)$ and denote $N[v] = N(v) \cup \{v\}$. A maximal independent set I_m is an independent set where there exists no vertex v such that $I_m \cap N[v] = \emptyset$. We can modify the tensor network for computing the independence polynomial to include this restriction. Instead of defining the restriction on vertices and edges, it is more natural to define it on $N[v]$:

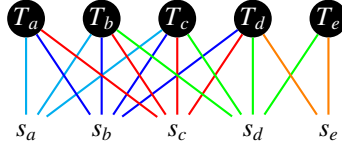
$$(4.9) \quad T(x_v)_{s_1, s_2, \dots, s_{|N(v)|}, s_v} = \begin{cases} s_v x_v & s_1 = s_2 = \dots = s_{|N(v)|} = 0, \\ 1 - s_v & \text{otherwise.} \end{cases}$$

Intuitively, it means if all the neighborhood vertices are not in I_m , i.e., $s_1 = s_2 = \dots = s_{|N(v)|} = 0$, then v should be in I_m , counted as x_v , and if any of the neighborhood vertices is in I_m , i.e.,

$\exists i \in \{1, 2, \dots, |N(v)|\}$ s.t. $s_i = 1$, then v cannot be in I_m . As an example, for a vertex of degree 2, the resulting rank-3 tensor is

$$(4.10) \quad T(x_v) = \begin{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 1 \\ x_v & 0 \\ 0 & 0 \end{pmatrix} \end{pmatrix}.$$

With the tensors defined as $T(x_v)$, we can perform a similar computation of contracting the tensor network with the same tensor element types as described in the previous section 4.1, the result of which then produces the maximal independence polynomial.



One can see the average degree of a tensor is increase. The computational complexity of this new tensor network contraction is often greater than the one for computing the independence polynomial. However, in most sparse graphs, this tensor network contraction approach is still significantly faster than enumerating all the maximal cliques on its complement graph using the Bron-Kerbosch algorithm [8], which is the standard algorithm that we are aware of to compute the maximal independence polynomial. Let us consider the example in Sec. 3, its corresponding tensor network structure for computing maximal independent sets now becomes:

5. Maximum independent sets and its counting problem.

5.1. Tropical algebra for finding the independence number and counting MISs. In the previous section, we focused on computing the independence polynomial for a graph G of given independence number $\alpha(G)$, but we did not show how to compute this number. The method we use to compute this quantity is based on the following observations. Let $x = \infty$, the independence polynomial becomes

$$(5.1) \quad I(G, \infty) = a_{\alpha(G)} \infty^{\alpha(G)},$$

where the lower-order terms vanish. We can thus replace the polynomial type $a = (a_0, a_1, \dots, a_k)$ with $a(k) = (a_k, k)$, where the second element stores the largest exponent k and the first element stores the corresponding coefficient a_k . From this, we can define a new algebra as [ST: I've changed this, but I don't have strong feelings about this. We can certainly consider changing back. I thought this would be more consistent with the earlier notations and show how it's stored in the program as well.] [JG: I prefer the previous one, what about you @XG?]

$$(5.2) \quad \begin{aligned} a(k) \oplus a(j) &= \begin{cases} (a_k + a_j, \max(k, j)), & k = j \\ (a_j, \max(k, j)), & k < j \\ (a_k, \max(k, j)), & k > j \end{cases} \\ a(k) \odot a(j) &= (a_k a_j, k + j) \\ \mathbb{0} &= (0, -\infty) \\ \mathbb{1} &= (1, 0). \end{aligned}$$

The algebra of the exponents becomes the max-plus tropical algebra: $k \oplus j = \max(k, j)$ and $k \odot j = k + j$ [31, 34]. This algebra is the same as the one used in Liu et al. [30] to calculate

and count spin glass ground states. For independent set calculations here, the vertex tensor and edge tensor becomes:

$$(5.3) \quad W_{s_i}^{\text{tropical}} = \begin{pmatrix} 1 \\ (1, 1) \end{pmatrix}, \quad B_{s_i s_j}^{\text{tropical}} = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}.$$

5.2. Truncated polynomial algebra for counting independent sets of large size.

Instead of counting just the MISs, one may be interested in counting the independent sets of large sizes close to the MIS size. 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. (4.4):

$$(5.4) \quad \begin{aligned} a \oplus b &= (a_{\max(k_a, k_b)-1} + b_{\max(k_a, k_b)-1}, a_{\max(k_a, k_b)} + b_{\max(k_a, k_b)}), \\ a \odot b &= (a_{k_a-1} b_{k_b} + a_{k_a} b_{k_b-1}, a_{k_a} b_{k_b}), \\ \mathbb{0} &= (), [\text{ST: should this be } (0)?][\text{JG: both are fine}] \\ \mathbb{1} &= (1). \end{aligned}$$

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. As will be shown bellow, this algebra can also be extended to enumerate suboptimal solutions. [ST: can be used to enumerate suboptimal solution as well?] [JG: added some description]

6. Enumeration of configurations and enumeration bounds.

6.1. Enumeration of MIS configurations. The enumeration problems of independent sets are also interesting and has been studied extensively in the literature [8, 13, 26], including, for example, the enumeration of all independent sets, the enumeration of all maximal independent sets, or the enumeration of all MISs. The standard algorithm to enumerate all maximal independent sets is the Bron-Kerbosch algorithm [8], which, of course, includes the enumeration of all MISs and can be used to enumerate all independent sets as well. Here, we adapt the tensor element types for different enumeration problems. For example, our tensor-network based algorithm to enumerate all MISs is expectedly much faster and more space-efficient than the Bron-Kerbosch algorithm, which lists all maximal independent sets.

To enumerate all independent sets, we input a set of configurations into the tensor elements. More concretely, we design a new element type having the following algebra

$$(6.1) \quad \begin{aligned} s \oplus t &= s \cup t \\ s \odot t &= \{\sigma \vee^\circ \tau \mid \sigma \in s, \tau \in t\} \\ \mathbb{0} &= \{\} \\ \mathbb{1} &= \{0^{\otimes |V|}\}. \end{aligned}$$

where s and t are each a set of $|V|$ -bit strings and \vee° is the bitwise OR operation over two bit strings. [ST: This is the bitwise OR operation right? I can't seem to find online what you call Hadamard. Is there a definition somewhere?] [JG: bitwise OR is more often used. I think Hadamard xxx means broadcasted xxx, is this confusing?] [ST: it would be useful to give an example of the operations above, $s = \dots, t = \dots, s \oplus t = \dots, s \odot t = \dots$] [ST: do we need to define $\{\} \vee^\circ \sigma = \sigma \vee^\circ \{\} = \{\}$?] [JG: we do not need an extra definition, see my example.]

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

$$\begin{aligned}\{00001\} \oplus \{01110, 01000\} &= \{01110, 01000\} \oplus \{00001\} = \{00001, 01110, 01000\} \\ \{00001\} \oplus \{\} &= \{\}\end{aligned}$$

$$\begin{aligned}\{00001\} \odot \{01110, 01000\} &= \{01110, 01000\} \odot \{00001\} = \{01111, 01001\} \\ \{00001\} \odot \{\} &= \{\} \\ \{00001\} \odot \{00000\} &= \{00001\}\end{aligned}$$

The variable x_i in the vertex tensor is initialized to $x_i = \{e_i\}$, where e_i is the standard basis vector of size $|V|$ and having 1 at index i . The vertex and edge tensors are thus

$$(6.2) \quad W_{s_i}^{\text{enum}} = \begin{pmatrix} \mathbb{1} \\ \{e_i\} \end{pmatrix}, \quad B_{s_i s_j}^{\text{enum}} = \begin{pmatrix} \mathbb{1} & \mathbb{1} \\ \mathbb{1} & \mathbb{0} \end{pmatrix}.$$

Contraction of the tensor network enumerates all the independent sets. To enumerate only the MISs, we can combine the above algebra Eq. (6.1) with the tropical algebra in Eq. (5.2) and define $s(k) = (s_k, k)$, where the first element follows the algebra in Eq. (6.1) and the second element follows the max-plus tropical algebra. The combined operations become:

$$(6.3) \quad \begin{aligned} s(k) \oplus s(j) &= \begin{cases} (s_k \cup s_j, \max(k, j)), & k = j \\ (s_j, \max(k, j)), & k < j \\ (s_k, \max(k, j)), & k > j \end{cases} \\ s(k) \odot s(j) &= (\{\sigma \vee^\circ \tau \mid \sigma \in s_k, \tau \in s_j\}, k + j) \\ \mathbb{0} &= (\{\}, -\infty) \\ \mathbb{1} &= (\{0^{\otimes |V|}\}, 0). \end{aligned}$$

Clearly, the vertex tensor and edge tensor become

$$(6.4) \quad W_{s_i}^{\text{MISenum}} = \begin{pmatrix} \mathbb{1} \\ (\{e_i\}, 1) \end{pmatrix}, \quad B_{s_i s_j}^{\text{MISenum}} = \begin{pmatrix} \mathbb{1} & \mathbb{1} \\ \mathbb{1} & \mathbb{0} \end{pmatrix}.$$

The contraction of the corresponding tensor network yields an enumeration of all MIS configurations. 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. (6.1),

$$(6.5) \quad \begin{aligned} \sigma \oplus \tau &= \text{select}(\sigma, \tau), \\ \sigma \odot \tau &= (\sigma \vee^\circ \tau), \\ \mathbb{0} &= 1^{\otimes |V|}, [\text{ST : should be } \mathbb{0} = \{\}] \\ [\text{JG : I do not think so, in that way, we need an extra bit to represent an empty set}] \\ \mathbb{1} &= 0^{\otimes |V|}, \end{aligned}$$

where the **select** function picks one of σ and τ by some criteria to make the algebra commutative and associative, e.g. by picking one with a smaller integer value.

[ST: The zero element doesn't seem right to me. Do we need to separately define

$$a \oplus 0 = 0 \oplus a = a$$

$$a \odot 0 = 0 \odot a = 0$$

][JG: I think picking the smaller one would solve the issue.]

[ST: Can we also enumerate all maximal independent sets by combining with Eq. (4.9) or enumerate suboptimal solutions by combining with the truncated polynomial?]

6.2. Bounding the MIS enumeration space. When we use the algebra in Eq. (6.3) 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 use $\alpha(G)$ to bound the searching space. First, we compute the value of $\alpha(G)$ with tropical algebra and cache all intermediate tensors. 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. Finally, we perform masked matrix multiplication using the new element type with the above algebra, Eq. (6.3), for obtaining all 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 propagation of the gradients. To derive the back-propagation rule for 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

$$(6.6) \quad A_{ij} \odot B_{jk} \leq C_{ik}.$$

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} . Since $A_{ij} \odot B_{jk} = A_{ij} + B_{jk}$, one can move B_{jk} to the right hand side of the inequality:

$$(6.7) \quad A_{ij} \leq C_{ik} \odot B_{jk}^{\circ-1}$$

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 :

$$(6.8) \quad A_{ij} \leq \min_k (C_{ik} \odot B_{jk}^{\circ-1}) = \left(\max_k (C_{ik}^{\circ-1} \odot B_{jk}) \right)^{\circ-1} = \left(\bigoplus_k (C_{ik}^{\circ-1} \odot B_{jk}) \right)^{\circ-1} = (C^{\circ-1} B^T)_{ij}^{\circ-1}.$$

On the right hand side, we transform the operation into a tropical matrix multiplication so that we can utilize the fast tropical BLAS routines [1] [ST: do we need to cite here?][JG: would a link to github be good?]. 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 being \bar{C} , the back-propagation rule for gradient masks reads

$$(6.9) \quad \bar{A}_{ij} = \delta \left(A_{ij}, \left((C^{\circ-1} \odot \bar{C}) B^T \right)_{ij}^{\circ-1} \right),$$

where \odot is the element-wise product, boolean false is treated as the tropical number 0, and boolean true is treated as the tropical number 1. This rule defined on matrix multiplication can be easily generalized to tensor contraction by replacing the matrix multiplication between $C^{\circ-1} \odot \bar{C}$ and B^T by a tensor contraction. With the above method, one can significantly reduce the space needed to store the intermediate configurations.

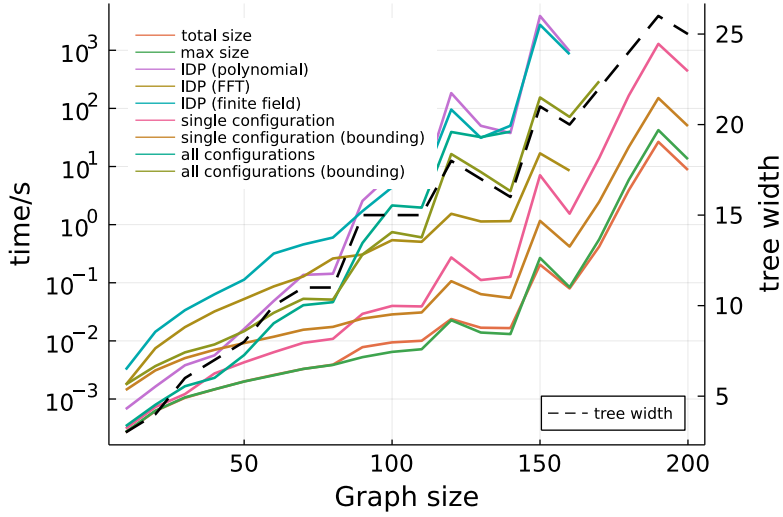


Figure 1: [ST: label x-axis as “number of vertices, $|V|$ ”] Benchmark results for computing different properties of independent sets with different tensor element types. The right axis is only for the dashed line.

[ST: split into two graphs: one with time versus number of vertices, $|V|$, and one with time versus tree width.] [ST: We also need to show/say what types of graphs is used here for benchmarking.]

7. Benchmarks and case studies.

7.1. Performance benchmarks. We run a sequential program benchmark on CPU Intel(R) Core(TM) i5-10400 CPU @ 2.90GHz, and show the results in Figure 1. When the element type is immutable, one can also run it on GPUs to speed up the computation. The graph we use are random 3 regular graphs, a typical type of sparse graph that having small tree width $tw(G) \leq |V|/6$ [16].

7.2. Example case studies. In this section, we give a few examples where the different properties of independence sets are used. In all the examples, the types of graphs we used are shown in Figure 2, where vertices are all placed on square lattices with lattice dimensions $L \times L$. The graphs include: the square grid graphs, denoted as SG; the square grid graphs with a filling factor p , denoted as $SG(p)$, where $\lfloor pL^2 \rfloor$ square grids are occupied with vertices; the King’s graphs, denoted as K; the King’s graphs with a filling factor p , denoted as $K(p)$.

7.2.1. Number of independent sets and hard-square entropy constant. 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.

7.2.2. Euler characteristics of independence complex.

7.2.3. Partition functions and finite-temperature phase transitions.

8. Discussion and conclusion. We have introduced a new approach based on tensor network contraction to compute the independence number, independence polynomial, maximal independence polynomial, and enumeration of MIS configurations. We derived the

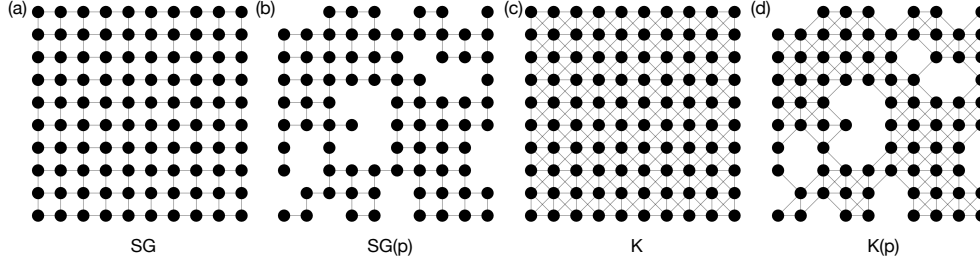


Figure 2: The types of graphs used in the benchmark and case studies. The lattice dimensions are $L \times L$. (a) Square grid graph denoted as SG. (b) Square grid graph with a filling factor $p = 0.8$, denoted as SG(0.8). (c) King’s graph denoted as K. (d) King’s graph with a filling factor $p = 0.8$, denoted as K(0.8).

backward rule for tropical tensor network to bound the search of solution space. Although many of these properties are global, we can encode them to different tensor element types as commutative semirings. The power of our tensor network approach is not only limited to the independent set problem, in Appendix C, we show how to map the matching problem and k -coloring problem to a tensor network. Here, we want to discuss more from the programming perspective. We show some of the Julia language [4] implementations in Appendix A and you will find it surprisingly short. What we need to do is just defining two operations \oplus and \odot and two special elements $\mathbb{0}$ and $\mathbb{1}$. The style that we program is called generic programming, meaning one can feed different data types into the same program, and the program will compute the result with a proper performance. In C++, one can use templates for such a purpose. We chose Julia because its just-in-time compiling is very powerful that it can generate fast code dynamically for users. Elements of fixed size, such as the finite-field algebra, truncated polynomial, tropical number and tropical number with counting or configuration field described in this paper can all be inlined in an array. Furthermore, these inlined arrays can be uploaded to GPU devices for faster computation with generic matrix multiplication implemented in CUDA.jl [3].

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REFERENCES

- [1] <https://github.com/TensorBFS/TropicalGEMM.jl>.
- [2] S. F. BARR, *Courcelle’s Theorem: Overview and Applications*, PhD thesis, Oberlin College, 2020.
- [3] T. BESARD, C. FOKET, AND B. D. SUTTER, *Effective extensible programming: Unleashing julia on gpus*, CoRR, abs/1712.03112 (2017), <http://arxiv.org/abs/1712.03112>, <https://arxiv.org/abs/1712.03112>.
- [4] J. BEZANSON, S. KARPINSKI, V. B. SHAH, AND A. EDELMAN, *Julia: A fast dynamic language for technical computing*, 2012, <https://arxiv.org/abs/1209.5145>, <https://arxiv.org/abs/1209.5145>.
- [5] J. BIAMONTE AND V. BERGHOLM, *Tensor networks in a nutshell*, 2017, <https://arxiv.org/abs/1708.00006>.
- [6] C. M. BISHOP, *Pattern Recognition and Machine Learning*, Springer, 2006.
- [7] M. BOUSQUET-MÉLOU, S. LINUSSON, AND E. NEVO, *On the independence complex of square grids*, Journal of Algebraic combinatorics, 27 (2008), pp. 423–450.

- [8] C. BRON AND J. KERBOSCH, *Algorithm 457: finding all cliques of an undirected graph*, Communications of the ACM, 16 (1973), pp. 575–577.
- [9] S. BUTENKO AND P. M. PARDALOS, *Maximum Independent Set and Related Problems, with Applications*, PhD thesis, USA, 2003. AAI3120100.
- [10] I. CIRAC, D. PEREZ-GARCIA, N. SCHUCH, AND F. VERSTRAETE, *Matrix Product States and Projected Entangled Pair States: Concepts, Symmetries, and Theorems*, arXiv e-prints, (2020), arXiv:2011.12127, p. arXiv:2011.12127, <https://arxiv.org/abs/2011.12127>.
- [11] B. COURCELLE, *The monadic second-order logic of graphs. i. recognizable sets of finite graphs*, Information and computation, 85 (1990), pp. 12–75.
- [12] J. C. DYRE, *Simple liquids’ quasiuniversality and the hard-sphere paradigm*, Journal of Physics: Condensed Matter, 28 (2016), p. 323001.
- [13] D. EPPSTEIN, M. LÖFFLER, AND D. STRASH, *Listing all maximal cliques in sparse graphs in near-optimal time*, in Algorithms and Computation, O. Cheong, K.-Y. Chwa, and K. Park, eds., Berlin, Heidelberg, 2010, Springer Berlin Heidelberg, pp. 403–414.
- [14] H. C. M. FERNANDES, J. J. ARENZON, AND Y. LEVIN, *Monte carlo simulations of two-dimensional hard core lattice gases*, The Journal of Chemical Physics, 126 (2007), p. 114508, <https://doi.org/10.1063/1.2539141>, <https://doi.org/10.1063/1.2539141>, <https://arxiv.org/abs/https://doi.org/10.1063/1.2539141>.
- [15] G. M. FERRIN, *Independence polynomials*, (2014).
- [16] F. V. FOMIN AND K. HØIE, *Pathwidth of cubic graphs and exact algorithms*, Information Processing Letters, 97 (2006), pp. 191–196.
- [17] F. V. FOMIN AND P. KASKI, *Exact exponential algorithms*, Communications of the ACM, 56 (2013), pp. 80–88.
- [18] D. GAMARNIK AND A. JAGANNATH, *The overlap gap property and approximate message passing algorithms for p-spin models*, 2019, <https://arxiv.org/abs/1911.06943>.
- [19] D. GAMARNIK AND M. SUDAN, *Limits of local algorithms over sparse random graphs*, 2013, <https://arxiv.org/abs/1304.1831>.
- [20] S. GASPERS, D. KRATSCHE, AND M. LIEDLOFF, *On independent sets and bicliques in graphs*, Algorithmica, 62 (2012), pp. 637–658, <https://doi.org/10.1007/s00453-010-9474-1>, <https://doi.org/10.1007/s00453-010-9474-1>.
- [21] G. H. GOLUB AND C. F. VAN LOAN, *Matrix computations*, vol. 3, JHU press, 2013.
- [22] J. GRAY AND S. KOURTIS, *Hyper-optimized tensor network contraction*, Quantum, 5 (2021), p. 410, <https://doi.org/10.22331/q-2021-03-15-410>, <http://dx.doi.org/10.22331/q-2021-03-15-410>.
- [23] N. J. HARVEY, P. SRIVASTAVA, AND J. VONDRÁK, *Computing the independence polynomial: from the tree threshold down to the roots*, in Proceedings of the Twenty-Ninth Annual ACM-SIAM Symposium on Discrete Algorithms, SIAM, 2018, pp. 1557–1576.
- [24] J. HASTAD, *Clique is hard to approximate within $n^{\sup 1-\epsilon}$* , in Proceedings of 37th Conference on Foundations of Computer Science, IEEE, 1996, pp. 627–636.
- [25] H. HU, T. MANSOUR, AND C. SONG, *On the maximal independence polynomial of certain graph configurations*, Rocky Mountain Journal of Mathematics, 47 (2017), pp. 2219 – 2253, <https://doi.org/10.1216/RMJ-2017-47-7-2219>, <https://doi.org/10.1216/RMJ-2017-47-7-2219>.
- [26] D. S. JOHNSON, M. YANNAKAKIS, AND C. H. PAPADIMITRIOU, *On generating all maximal independent sets*, Information Processing Letters, 27 (1988), pp. 119–123, [https://doi.org/https://doi.org/10.1016/0020-0190\(88\)90065-8](https://doi.org/https://doi.org/10.1016/0020-0190(88)90065-8), <https://www.sciencedirect.com/science/article/pii/0020019088900658>.
- [27] S. KOURTIS, C. CHAMON, E. MUCCIOLLO, AND A. RUCKENSTEIN, *Fast counting with tensor networks*, SciPost Physics, 7 (2019), <https://doi.org/10.21468/scipostphys.7.5.060>, <http://dx.doi.org/10.21468/SciPostPhys.7.5.060>.
- [28] V. E. LEVIT AND E. MANDRESCU, *The independence polynomial of a graph-a survey*, in Proceedings of the 1st International Conference on Algebraic Informatics, vol. 233254, Aristotle Univ. Thessaloniki Thessaloniki, 2005, pp. 231–252.
- [29] V. E. LEVIT AND E. MANDRESCU, *The independence polynomial of a graph at -1*, 2009, <https://arxiv.org/abs/0904.4819>.
- [30] J.-G. LIU, L. WANG, AND P. ZHANG, *Tropical tensor network for ground states of spin glasses*, Physical Review Letters, 126 (2021), <https://doi.org/10.1103/physrevlett.126.090506>, <http://dx.doi.org/10.1103/PhysRevLett.126.090506>.
- [31] D. MACLAGAN AND B. STURMFELS, *Introduction to tropical geometry*, vol. 161, American Mathematical Soc., 2015, <http://www.cs.technion.ac.il/~janos/COURSES/238900-13/Tropical/MaclaganSturmfels.pdf>.
- [32] F. MANNE AND S. SHARMIN, *Efficient counting of maximal independent sets in sparse graphs*, in International Symposium on Experimental Algorithms, Springer, 2013, pp. 103–114.
- [33] I. L. MARKOV AND Y. SHI, *Simulating quantum computation by contracting tensor networks*, SIAM Journal on Computing, 38 (2008), p. 963–981, <https://doi.org/10.1137/050644756>, <http://dx.doi.org/10.1137/050644756>.
- [34] C. MOORE AND S. MERTENS, *The nature of computation*, OUP Oxford, 2011.
- [35] R. ORÚS, *A practical introduction to tensor networks: Matrix product states and projected entangled pair*

- states, *Annals of Physics*, 349 (2014), pp. 117–158.
- [36] F. PAN AND P. ZHANG, *Simulating the sycamore quantum supremacy circuits*, 2021, <https://arxiv.org/abs/2103.03074>.
- [37] H. PICHLER, S.-T. WANG, L. ZHOU, S. CHOI, AND M. D. LUKIN, *Computational complexity of the rydberg blockade in two dimensions*, arXiv preprint arXiv:1809.04954, (2018).
- [38] J. M. ROBSON, *Algorithms for maximum independent sets*, *Journal of Algorithms*, 7 (1986), pp. 425–440.
- [39] A. SCHÖNHAGE AND V. STRASSEN, *Schnelle multiplikation grosser zahlen*, *Computing*, 7 (1971), pp. 281–292.
- [40] A. A. STEPANOV AND D. E. ROSE, *From mathematics to generic programming*, Pearson Education, 2014.
- [41] R. E. TARJAN AND A. E. TROJANOWSKI, *Finding a maximum independent set*, *SIAM Journal on Computing*, 6 (1977), pp. 537–546.
- [42] Q. WU AND J.-K. HAO, *A review on algorithms for maximum clique problems*, *European Journal of Operational Research*, 242 (2015), pp. 693–709, <https://doi.org/https://doi.org/10.1016/j.ejor.2014.09.064>, <https://www.sciencedirect.com/science/article/pii/S0377221714008030>.
- [43] M. XIAO AND H. NAGAMUCHI, *Exact algorithms for maximum independent set*, *Information and Computation*, 255 (2017), p. 126–146, <https://doi.org/10.1016/j.ic.2017.06.001>, <http://dx.doi.org/10.1016/j.ic.2017.06.001>.

Appendix A. Technical guide.

OMEinsum a package for the einsum function,

OMEinsumContractionOrders a package for finding the optimal contraction order for the einsum function

<https://github.com/Happy-Diode/OMEinsumContractionOrders.jl>,

TropicalGEMM a package for efficient tropical matrix multiplication (compatible with OMEinsum),

TropicalNumbers a package providing tropical number types and tropical algebra, one o the dependency of TropicalGEMM,

LightGraphs a package providing graph utilities, like random regular graph generator,

Polynomials a package providing polynomial algebra and polynomial fitting,

Mods and Primes packages providing finite field algebra and prime number generators.

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

```
pkg> add OMEinsum LightGraphs Mods Primes FFTW Polynomials TropicalNumbers
```

It may surprise you that the Julia implementation of algorithms introduced in the paper is so short that except the bounding and sparsity related parts, all are contained in this appendix. After installing required packages, one can open a Julia REPL and copy the following code into it.

```
using OMEinsum, OMEinsumContractionOrders
using OMEinsum: NestedEinsum, flatten, getixs
using LightGraphs
using Random

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

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

# an einsum contraction without contraction order specified is called `EinCode`,
# an einsum contraction has contraction order (specified as a tree structure) is called `
NestedEinsum`.

# assign each label a dimension-2, it will be used in contraction order optimization
# `symbols` function extracts tensor labels into a vector.
symbols(:EinCode{ixs}) where ixs = unique(Iterators.flatten(filter(x->length(x)==1,ixs)))
```



```

symbols(ne::OMEinsum.NestedEinsum) = symbols(flatten(ne))
size_dict = Dict{<code>{s=>2 for s in symbols(code)}}
# optimize the contraction order using KaHyPar + Greedy, target space complexity is 2^17
optimized_code = optimize_kahypar(code, size_dict; sc_target=17, max_group_size=40)
println("time/space complexity is $(OMEinsum.timespace_complexity(optimized_code, size_dict))")

# a function for computing independence polynomial
function independence_polynomial(x::T, code) where {T}
    xs = map(getixs(flatten(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 MAXIMUM INDEPENDENT SET SIZE AND ITS DEGENERACY #####

# using Tropical numbers to compute the MIS size and 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 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)[])")

# using fast fourier transformation to compute the independence polynomial,
# here we chose r > 1 because we care more about configurations with large independent set sizes
using FFTW
function independence_polynomial_fft(code; mis_size=Int(mis_size(code)[].n), r=3.0)
    ω = exp(-2im*π/(mis_size+1))
    xs = r .* collect(ω .^ (0:mis_size))
    ys = [independence_polynomial(x, code)[] for x in xs]
    Polynomial(ifft(ys) ./ (r .^ (0:mis_size)))
end
println("the independence polynomial (fft) is $(independence_polynomial_fft(optimized_code))")

# using finite field algebra to compute the independence polynomial
using Mods, Primes
# two patches to ensure gaussian elimination works
Base.abs(x::Mod) = x
Base.isless(x::Mod{N}, y::Mod{N}) where N = mod(x.val, N) < mod(y.val, N)

function independence_polynomial_finitefield(code; mis_size=Int(mis_size(code)[].n), max_order=1
    00)
    N = typemax(Int32) # Int32 is faster than Int.
    YS = []
    local res
    for k = 1:max_order
        N = Primes.prevprime(N-one(N)) # previous prime number
        # evaluate the polynomial on a finite field algebra of modulus `N`
        rk = _independence_polynomial(Mods.Mod{N,Int32}, code, mis_size)
        push!(YS, rk)
        if max_order==1
            return Polynomial(Mods.value.(YS[1]))
        elseif k != 1
            ra = improved_counting(YS[1:end-1])
            res = improved_counting(YS)
            ra == res && return Polynomial(res)
        end
    end
    @warn "result is potentially inconsistent."
    return Polynomial(res)
end
function _independence_polynomial(::Type{T}, code, mis_size::Int) where T

```

```

xs = 0:mis_size
ys = [independence_polynomial(T(x), code)[] for x in xs]
A = zeros(T, mis_size+1, mis_size+1)
for j=1:mis_size+1, i=1:mis_size+1
    A[j,i] = T(xs[j])^(i-1)
end
A \ T.(ys) # gaussian elimination to compute ``A^{-1} y``
end
improved_counting(sequences) = map(yi->Mods.CRT(yi...), zip(sequences...))

println("the independence polynomial (finite field) is $(independence_polynomial_finitefield(
    optimized_code))")

##### FINDING OPTIMAL CONFIGURATIONS #####

# define the config enumerator algebra
struct ConfigEnumerator{N,C}
    data::Vector{StaticBitVector{N,C}}
end
function Base.:+(x::ConfigEnumerator{N,C}, y::ConfigEnumerator{N,C}) where {N,C}
    res = ConfigEnumerator{N,C}(vcat(x.data, y.data))
    return res
end
function Base.:*(x::ConfigEnumerator{L,C}, y::ConfigEnumerator{L,C}) where {L,C}
    M, N = length(x.data), length(y.data)
    z = Vector{StaticBitVector{L,C}}(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,C}(z)
end
Base.zero(::Type{ConfigEnumerator{N,C}}) where {N,C} = ConfigEnumerator{N,C}(StaticBitVector{N,C}[])
Base.one(::Type{ConfigEnumerator{N,C}}) where {N,C} = ConfigEnumerator{N,C}([TropicalNumbers.staticfalses(StaticBitVector{N,C})])

# 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}` is a simple 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(symbols(code))]}
    N = length(vertex_index) # number of vertices
    C = TropicalNumbers.nints(N) # number of integers to store N bits
    xs = map(getixs(flatten(code))) do ix
        T = all ? CountingTropical{Float64, ConfigEnumerator{N,C}} : ConfigTropical{Float64, N,
        C}
        if length(ix) == 2
            return [one(T) one(T); one(T) zero(T)]
        else
            s = TropicalNumbers.onehot(StaticBitVector{N,C}, vertex_index[ix[1]])
            if all
                [one(T), T(1.0, ConfigEnumerator([s]))]
            else
                [one(T), T(1.0, s)]
            end
        end
    end
    return code(xs...)
end

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

# enumerating configurations directly can be very slow (~15min), please check the bounding
# version in our Github repo.
println("all optimal configurations are $(mis_config(optimized_code; all=true)[].c)")

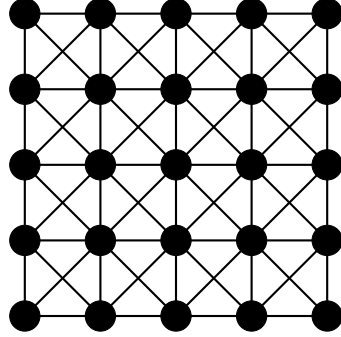
```

In the above examples, the configuration enumeration is very slow, one should use the

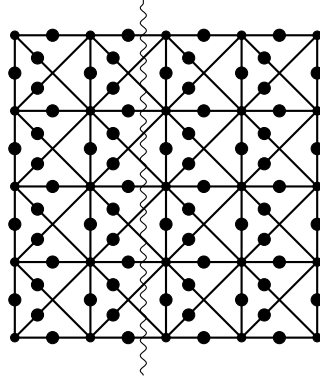
optimal MIS size for bounding as described in the main text. We will not show any example about implementing the backward rule here because it has approximately 100 lines of code. Please checkout our GitHub repository <https://github.com/Happy-Diode/NoteOnTropicalMIS>.

Appendix B. Why not introducing δ sensors.

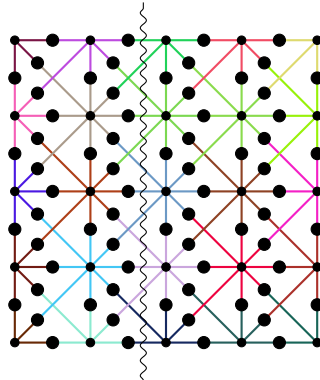
Given a graph



Its traditional tensor network representation with δ tensors is



where a small circle on an edge is a diagonal tensor. Its rank is 8 in the bulk. If we contract this tensor network in a naive column-wise order, the maximum intermediate tensor is approximately $3L$, giving a space complexity $\approx 2^{3L}$. If we treat it as the following generalized tensor network



where we use different colors to distinguish different hyperedges. Now, the vertex tensor is always rank 1. With the same naive contraction order, we can see the maximum

intermediate tensor is approximately of size 2^L by counting the colors.

Appendix C. Generalizing to other graph problems. There are some other graph problems that can be encoded in a tensor network. To understand its representation power, it is a good starting point to connect it with dynamic programming because a tensor network can be viewed as a special type of dynamic programming where its update rule can be characterized by a linear operation. Courcelle’s theorem [11, 2] states that a problem quantified by monadic second order logic (MSO) on a graph with bounded treewidth k can be solved in linear time with respect to the graph size. Dynamic programming is a traditional approach to attack a MSO problem, it can solve the maximum independent set problem in $O(2^k)n$, which is similar to the tensor network approach. We mentioned in the main text that tensor network has nice analytic property make it easier for generic programming. The cost is, the tensor network is less expressive than dynamic programming. However, there are still some other problems that can be expressed in the framework of generic tensor network.

C.1. Matching problem. A matching polynomial of a graph G is defined as

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

where k is the number of matches, and coefficients c_k are the corresponding counting.

We define a tensor of rank $d(v) = |N(v)|$ on vertex v such that,

$$(C.2) \quad W_{v \rightarrow n_1, v \rightarrow n_2, \dots, v \rightarrow n_{d(v)}} = \begin{cases} 1, & \sum_{i=1}^{d(v)} v \rightarrow n_i \leq 1, \\ 0, & \text{otherwise,} \end{cases}$$

and a tensor of rank 1 on the bond

$$(C.3) \quad B_{v \rightarrow w} = \begin{cases} 1, & v \rightarrow w = 0 \\ x, & v \rightarrow w = 1. \end{cases}$$

Here, we use bond index $v \rightarrow w$ to label tensors.

C.2. k-Coloring. Let us use 3-coloring on the vertex as an example. We can define a vertex tensor as

$$(C.4) \quad W = \begin{pmatrix} r_v \\ g_v \\ b_v \end{pmatrix},$$

and an edge tensor as

$$(C.5) \quad B = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}.$$

The number of possible coloring can be obtained by contracting this tensor network by setting vertex tensor elements r_v, g_v and b_v to 1. By designing generic types as tensor elements, one should be able to get all possible colorings. It is straight forward to define the k-coloring problem on edges hence we will not discuss the detailed construction here.

Appendix D. Discrete Fourier transform for computing the independence polynomial.

In section 4.1, we show that the independence polynomial can be obtained by solving the linear equation Eq. (4.6). 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 $\text{GF}(p)$ to circumvent overflow and round-off errors. Here, we give another method based on discrete Fourier transform. 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

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

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 ($r < 1$) or high independent set size region ($r > 1$). **[ST: is that $\omega < 1$ or $r < 1$?][JG: it is r , fixed]**

Appendix E. Integer sequences formed by the number of independent sets.

Table 2: The number of independent sets for square grid graphs of size $L \times L$. This forms the integer sequence [OEIS A006506](#).

L	square grid graphs
1	2
2	7
3	63
4	1 234
5	55 447
6	5 598 861
7	1 280 128 950
8	660 647 962 955
9	770 548 397 261 707
10	2 030 049 051 145 980 050
11	12 083 401 651 433 651 945 979
12	162 481 813 349 792 588 536 582 997
13	4 935 961 285 224 791 538 367 780 371 090
14	338 752 110 195 939 290 445 247 645 371 206 783
15	52 521 741 712 869 136 440 040 654 451 875 316 861 275
16	18 396 766 424 410 124 752 958 806 046 933 947 217 821 482 942
17	14 557 601 701 834 111 295 974 187 104 248 827 765 798 599 152 358 303
18	26 024 585 612 650 837 861 658 126 921 792 857 026 992 497 268 285 945 167 621
19	105 105 055 066 577 962 012 604 229 608 317 915 229 737 651 637 019 975 757 755 051 314
20	958 979 036 662 929 619 406 859 624 886 958 746 851 620 546 557 485 230 898 539 651 354 907 499
21	19 766 982 580 727 525 559 447 459 703 066 410 506 378 295 841 376 040 664 015 562 851 325 369 819 076 327
22	920 486 427 724 231 647 653 646 535 134 255 190 048 558 085 587 696 509 535 085 179 014 710 020 739 303 637 413 062
23	96 836 737 362 332 577 228 126 233 146 266 027 907 220 602 904 916 569 863 928 397 932 638 147 313 462 817 836 132 159 477 643
24	23 014 876 830 102 973 080 295 375 510 481 185 265 791 418 130 718 634 637 816 237 986 620 978 856 344 595 418 898 906 840 911 239 867 869
25	12 357 280 628 458 621 610 261 003 683 798 282 889 567 362 022 871 449 310 490 079 744 330 288 088 293 888 381 458 751 196 205 785 114 467 063 479 978
26	14 989 353 830 657 887 045 253 535 577 369 170 604 561 059 504 403 111 230 207 533 142 521 161 755 543 754 839 412 836 401 335 298 693 619 461 437 872 472 165 615
27	41 076 048 814 756 904 170 038 431 958 637 474 710 328 322 517 168 428 037 124 975 797 939 221 729 929 250 098 889 601 666 346 169 376 778 430 801 983 574 787 538 529 309 191
28	254 296 368 874 677 123 746 928 211 898 730 495 474 495 246 876 690 760 159 507 126 754 738 599 026 016 292 991 448 162 576 157 292 681 301 528 315 863 006 160 203 433 527 765 235 617 478
29	3 556 619 491 488 838 337 298 644 336 171 591 528 960 687 731 348 622 394 588 805 214 244 031 766 315 339 709 627 465 589 460 212 852 431 000 227 410 783 701 037 177 097 019 793 172 369 009 198 594 591
30	112 377 766 778 527 126 203 646 648 402 050 958 984 330 252 199 994 469 198 044 986 979 798 657 215 652 532 005 142 877 926 040 203 499 014 641 860 333 039 219 325 350 361 465 468 647 055 420 204 598 509 312 491 705

Table 3: The number of independent sets for King's graphs of size $L \times L$.

L	King's graphs
1	2
2	5
3	35
4	314
5	6 427
6	202 841
7	12 727 570
8	1 355 115 601
9	269 718 819 131
10	94 707 789 944 544
11	60 711 713 670 028 729
12	69 645 620 389 200 894 313
13	144 633 664 064 386 054 815 370
14	540 156 683 236 043 677 756 331 721
15	3 641 548 665 525 780 178 990 584 908 643
16	44 222 017 282 082 621 251 230 960 522 832 336
17	968 503 939 616 343 947 563 582 929 715 005 880 647
18	38 227 887 218 717 761 202 510 261 178 854 062 185 464 315
19	2 720 444 488 584 821 384 410 936 779 813 343 554 469 758 172 682
20	348 970 226 122 589 397 373 342 369 495 005 120 745 703 462 667 115 175
21	80 700 603 403 721 730 646 640 814 391 653 008 712 705 595 500 769 624 448 529
22	33 641 616 174 796 469 294 898 513 022 199 100 689 671 634 779 118 656 571 910 751 320
23	25 281 578 706 433 684 460 290 055 263 926 749 952 595 755 044 481 112 956 327 672 312 862 611
24	34 249 181 078 331 384 968 700 380 345 306 575 903 108 280 266 841 066 358 396 857 518 201 026 192 547
25	83 641 072 313 734 275 009 578 098 702 552 656 178 287 685 025 530 905 558 603 555 359 601 823 180 929 638 318
26	368 222 048 967 797 645 785 624 418 568 072 838 671 415 214 857 177 141 161 824 615 541 365 640 076 045 923 328 316 979
27	2 922 282 601 123 898 422 508 409 690 495 824 015 239 663 506 989 438 099 254 205 806 998 557 618 858 143 959 252 475 337 777 029
28	41 807 680 908 633 213 277 041 952 346 680 116 482 996 387 928 973 684 599 097 559 098 879 721 953 006 036 791 335 134 446 016 561 667 772