COMPUTING PROPERTIES OF INDEPENDENT SETS BY GENERIC PROGRAMMING TENSOR NETWORKS *

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Abstract. We introduce a method of using generic programming tensor network to compute various properties of independent sets, which include, for example, the size of the maximum independent sets and the number and 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. Our framework can be easily extended to compute properties of other problems such as the cut size, coloring, and maximal cliques, 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.

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

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1. Introduction.

In graph theory and combinatorial optimization, there are many interesting and hard computational problems concerning various properties of independent sets. For an undirected graph $G = (V, E)$, an independent set $I \subseteq V$ is a set of vertices that for any vertex pair $u, v \in I$, $(u, v) \notin E$. One of the paradigmatic independent set *properties* is the maximum independent set (MIS) and the size of the MIS, $\alpha(G) \equiv \max_I |I|$. There is widespread interest in this MIS problem not only because it is a well-known NP-complete problem [29] that can be mapped from many other important combinatorial optimization problems in polynomial time such as the 3-satisfiability problem, the maximum clique problem, and the minimum vertex cover problem [42], but also because it has a wide range of applications in scheduling, logistics, wireless networks and telecommunication, and computer vision, etc. [12, 51]. Some other properties, such as the number and enumeration of independent sets or maximal independent sets of a given size, are equally interesting, if not more important, in many practical applications. These other properties can be found in physics applications such as in the hard-core lattice gas model [16, 19] in statistical mechanics and the Rydberg hamiltonian with neutral atoms [46, 17] [**ST: replace with experiment paper when ready**]; they can, for example, be used to understand phase transitions [16, 19], to identify harder graphs in an ensemble of graphs [17] and to analyze the presence of the overlap gap property [24, 23]. Meanwhile, finding the number of independent sets of a given size is equivalent to computing the coefficients of the independence polynomial [28, 20]. which is a useful graph characteristic related to, for example, the partition functions [35, 52] and Euler characteristics of the independence complex [10, 37]. However, there is a lack of general and versatile tool to compute the different properties of independent sets.

In this paper, we introduce a generic programming tensor-network framework to compute a number of different independent set properties. We map the computation of these properties into generic tensor network contraction with specially designed tensor element algebra. It is different from the standard tensor network methods in that the tensor elements

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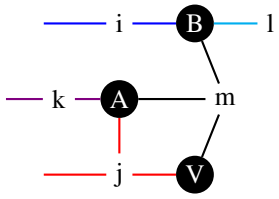
are not restricted to standard number types such as floating point numbers and integers. Traditional algorithms for finding the MIS size include the branching algorithms [50, 47] and dynamic programming based algorithms [15, 22]. The complexity of our tensor-network based algorithms is similar to that of dynamic programming algorithms [15, 22], which have a complexity scaling exponentially with the treewidth, tw(G), of the graph; for sparse graphs, the treewidth is usually much smaller than the number of vertices [21]. Our algorithms, on the other hand, are much more versatile than traditional methods and can be used to compute many other properties than just the MIS size. We benchmark our algorithms in Sec. 7 by computing a number of independent set properties of certain sparse graphs on central processing units (CPUs) and graphics processing units (GPUs) and show its good performance. The high performance benefits from recent advances in random tensor-network contraction for the purposes of quantum circuit simulations [27, 44, 33], where efficient heuristic algorithms have been developed to optimize the contraction order for tensor networks up to thousands of vertices. For cases where the tensors are too large to fit into a GPU, slicing techniques can be used to further reduce the space consumption. Lastly, we provide a few examples and demonstrate the versatility of our tool by 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. Our method can also be used to find "maximal" independent set properties; a maximal independent set is an independent set that is not a subset of any other independent set, but its size may not be the maximum. We show how to compute properties related to maximal independent sets and properties for other combinatorial optimization problems in Appendix C.

2. Tensor networks. Tensor network [14, 43] is also known as einsum, factor graph or sum-product network [9] 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. 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 because one can easily translate a generalized tensor network to the standard notation by adding δ tensors, a high dimensional equivalence of the identity matrix. However, introducing δ tensors may significantly increase the complexity of the tensor contraction. We illustrate this subtle point in Appendix B.

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. In previous works relating tensor networks and combinatoric problems [34, 8], the elements in the tensor networks are limited to standard number types such as floating point numbers and integers. Owning to the development of modern compiling technology, we no longer need to limit our imagination to standard number types. One of the key concepts that push the technology forward is called generic programming:

Definition 3.1 (Generic programming [49]). *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.*

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 [7]. 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 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 [6].

This motivates us to think about what is the most general 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

element type	**property to compute**
$\mathbb{R}$	the number of independent sets
Polynomial (Eq. (4.5: PN))	independence polynomial
Tropical (Eq. (5.3: T))	MIS size
Polynomial truncated to highest order (Eq. (5.2: P1))	MIS size and the number of MISs
Polynomial truncated to 2nd highest order (Eq. (5.5: P2))	the number of MISs and independent sets of size $\alpha(G) - 1$
Set (Eq. (6.1: SN))	enumeration of independent sets
Bit string (Eq. (6.5: S1))	one independent set
Polynomial truncated to highest order combined with Bit string	MIS size and one MIS
Polynomial truncated to highest order combined with Set (Eq. (6.3: P1+SN))	MIS size and all MISs

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

must hold for any arbitrary three elements $a, b, c \in R$.

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

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

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

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

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 program [49]. The Table 1 summarizes those properties that can be computed by various tensor element types.

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

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

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 $I(G, 1)$. To compute this polynomial, we map this expression to a tensor network contraction. We map a vertex $i \in V$ to a label $s_i \in \{0, 1\}$ 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_i, we defined a parametrized rank-one vertex tensor $W(x_i)$ as

$$W(x_i) = \begin{pmatrix} 1 \\ x_i \end{pmatrix}. \tag{4.2}$$

We use subscripts to index tensor elements, e.g. $W(x_i)_0 = 1$ is the first element associated with $s_i = 0$ and $W(x_i)_1 = x_i$ 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

$$B = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}. \tag{4.3}$$

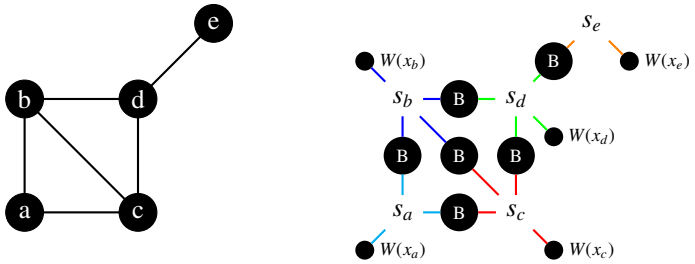
The corresponding tensor network contraction gives

$$P(G, \{x_1, x_2, \ldots, x_{|V|}\}) = \sum_{s_1, s_2, \ldots, s_{|V|}=0}^{1} \prod_{i=1}^{|V|} W(x_i)_{s_i} \prod_{(i,j)\in E(G)} B_{s_i s_j}, \tag{4.4}$$

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 2 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). 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. The summation counts the number of independent sets of size k.

To evaluate Eq. (4.4), directly summing up the $2^{|V|}$ product terms is computationally inefficient. 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 to $O(2^{\mathrm{tw}(G)})$ [41], while requiring a space at the same order of magnitude to store intermediate contraction results. 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 2. 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. We attach a vertex tensor on each hyperedge and an edge tensor between two hyperedges if vertices of the two hyperedges are connected in the original graph.



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

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

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. 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

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

Here, the multiplication operation can be evaluated efficiently using the convolution theorem [48]. 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

(4.6)
$$
W^{\mathrm{PN}} = \begin{pmatrix} \mathbb{1} \\ (0, 1) \end{pmatrix}, \qquad B^{\mathrm{PN}} = \begin{pmatrix} \mathbb{1} & \mathbb{1} \\ \mathbb{1} & \mathbb{0} \end{pmatrix}.
$$

By contracting the tensor network with the polynomial type, we have the exact representation of the independence polynomial. However, 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. Here, 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:

$$\begin{pmatrix} 1 & x_0 & x_0^2 & \dots & x_0^{\alpha(G)} \\ 1 & x_1 & x_1^2 & \dots & x_1^{\alpha(G)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{\alpha(G)} & x_{\alpha(G)}^2 & \dots & x_{\alpha(G)}^{\alpha(G)} \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_{\alpha(G)} \end{pmatrix} = \begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_{\alpha(G)} \end{pmatrix}. \tag{4.7}$$

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):

$$\begin{aligned} x \oplus y &= x + y \pmod p, \\ x \odot y &= xy \pmod p, \\ \mathbb{0} &= 0, \\ \mathbb{1} &= 1. \end{aligned} \tag{4.8: GF(p)}$$

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

1. One can use Gaussian elimination [26] to solve the linear equation Eq. (4.7) 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. 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 $\chi = (x_0, x_1, \dots, x_{\alpha(G)})$ on GF(p) and denote the outputs as $(y_0, y_1, \dots, y_{\alpha(G)}) \pmod p$. Then we solve Eq. (4.7) using Gaussian elimination on GF(p) to find the coefficient modulo p, $A_p \equiv (a_0, a_1, \dots, a_{\alpha(G)}) \pmod p$. 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. In Appendix D, we provide another method to solve the linear equation using discrete Fourier transformation.

5. Maximum independent sets and its counting.

5.1. Tropical algebra for finding the MIS size and counting MISs. In the previous section, we focused on computing the independence polynomial for a graph G of a given MIS size $\alpha(G)$, 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

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

Algorithm 4.1 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

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. From this, we can define a new algebra as

$$
\begin{aligned}
a_x\infty^x \oplus a_y\infty^y &= \begin{cases} (a_x + a_y)\infty^{\max(x,y)}, & x = y \\ a_y\infty^{\max(x,y)}, & x < y \\ a_x\infty^{\max(x,y)}, & x > y \end{cases} , \\
a_x\infty^x \odot a_y\infty^y &= a_x a_y \infty^{x+y} \\
\mathbb{0} &= 0\infty^{-\infty} \\
\mathbb{1} &= 1\infty^0 .
\end{aligned}
\tag{5.2: P1}
$$

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 [39, 42]:

$$
\begin{aligned}
x \oplus y &= \max(x, y) \\
x \odot y &= x + y \\
\mathbb{0} &= -\infty \\
\mathbb{1} &= 0 .
\end{aligned}
\tag{5.3: T}
$$

This algebra is the same as the one used in Liu et al. [38] to calculate and count spin glass ground states. For independent set calculations here, the vertex tensor and edge tensor becomes:

$$
W^{\mathrm{T}} = \begin{pmatrix} \mathbb{1} \\ \infty \end{pmatrix}, \qquad B^{\mathrm{T}} = \begin{pmatrix} \mathbb{1} & \mathbb{1} \\ \mathbb{1} & \mathbb{0} \end{pmatrix}.
\tag{5.4}
$$

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. (4.5: PN) as:

$$
\begin{aligned}
a \oplus b &= (a_{\max(k_a,k_b)-1} + b_{\max(k_a,k_b)-1}, a_{\max(k_a,k_b)} + b_{\max(k_a,k_b)}),\\
a \odot b &= (a_{k_a-1} b_{k_b} + a_{k_a} b_{k_b-1}, a_{k_a} b_{k_b}),\\
\mathbb{0} &= (),\\
\mathbb{1} &= (1).
\end{aligned}
\tag{5.5: P2}
$$

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. As will be shown below, this algebra can also be extended to enumerate those large-size independent sets.

6. Enumeration of independent sets.

6.1. Set algebra for configuration enumeration. The enumeration problems of independent sets are also interesting and has been studied extensively in the literature [11, 18, 32], including, for example, the enumeration of all independent sets, the enumeration of all maximal independent sets, or the enumeration of all MISs. To enumerate all independent sets, we designed an algebra defined on sets of bitstrings:

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

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 3. 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

$$
W^{\mathrm{SN}}(\{\boldsymbol{e}_i\}) = \begin{pmatrix} \mathbb{1} \\ \{\boldsymbol{e}_i\} \end{pmatrix}, \qquad B^{\mathrm{SN}} = \begin{pmatrix} \mathbb{1} & \mathbb{1} \\ \mathbb{1} & \mathbb{0} \end{pmatrix}.
\tag{6.2}
$$

This set algebra can serve as the coefficients in Eq. (4.5: PN) to enumerate independent sets of all different sizes, Eq. (5.2: P1) to enumerate all MISs, or Eq. (5.5: 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

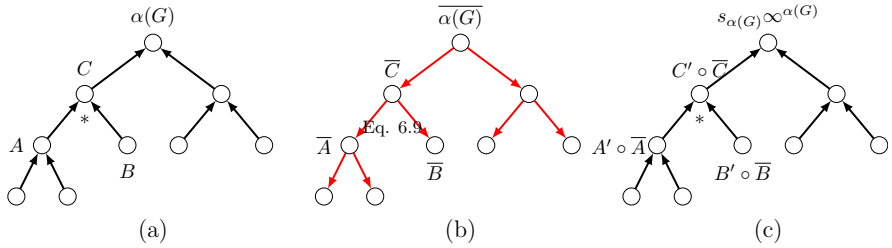


Figure 1: Bounded enumeration of maximum independent sets. In these graphs, a circle is a tensor, an arrow specifies execution direction of a function and $\circ$ is the Hadamard (element-wise) multiplication. $\overline{A}$ means the boolean mask of A. (a) is the forward pass with algebra Eq. (5.3: 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. (6.3: P1+SN) for enumerating configurations.

$s_k\infty^k$, where the coefficients follow the algebra in Eq. (6.1: SN) and the orders (exponents) follow the max-plus tropical algebra. The combined operations become:

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

Clearly, the vertex tensor and edge tensor become

(6.4)
$$W^{\text{P1+SN}}(\{\boldsymbol{e}_i\infty^1\}) = \begin{pmatrix} \mathbb{1} \\ \{\boldsymbol{e}_i\}\infty^1 \end{pmatrix}, \qquad B^{\text{P1+SN}} = \begin{pmatrix} \mathbb{1} & \mathbb{1} \\ \mathbb{1} & \mathbb{0} \end{pmatrix}.$$

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: SN),

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

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

6.2. Bounding the MIS enumeration space. When we use the algebra in Eq. (6.3: 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. 1, (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. (6.3: 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

$$A_{ij} \odot B_{jk} \leq C_{ik}. \tag{6.6}$$

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 [1] 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:

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

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

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]. 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

$$\overline{A}_{ij} = \delta \left(A_{ij}, \left(\left(C^{\circ -1} \circ \overline{C} \right) B^{\mathsf{T}} \right)_{ij}^{\circ -1} \right), \tag{6.9}$$

where δ 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^{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.

7. Benchmarks and case studies.

7.1. 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 2. 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 $|V|/6$ [21].

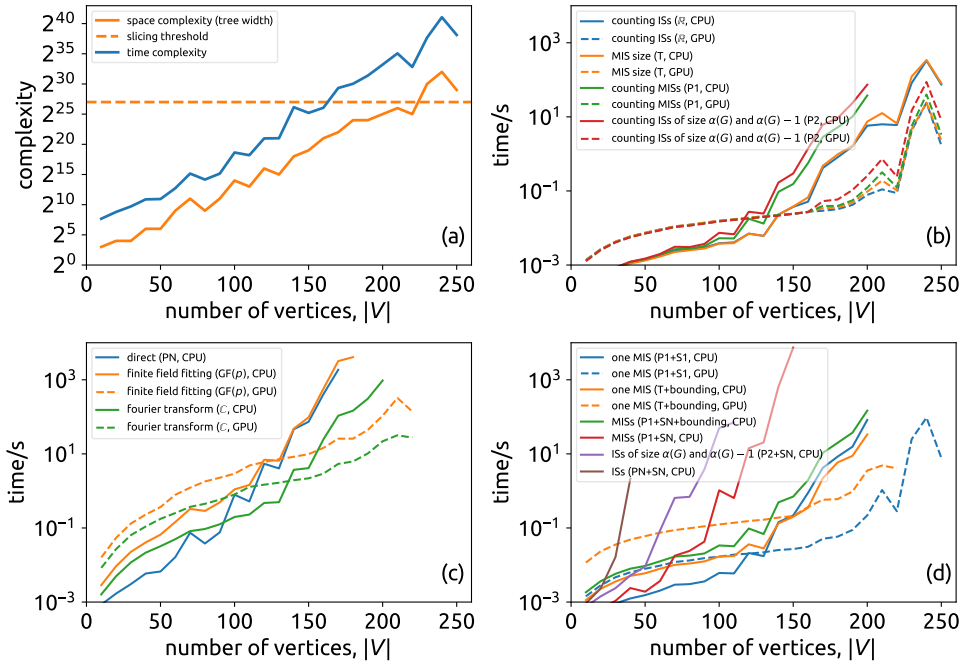


Figure 2: Benchmark results for computing different properties of independent sets of a random three regular graph with different tensor element types. The time in these plots only includes tensor network contraction, without taking the contraction order finding and just-in-time compiling time into account. Legends are properties, algebra and devices that we used in the computation; one can find the corresponding computed 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, and the number of independent sets having size $\alpha(G)$ and $\alpha(G) - 1$. (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 $\alpha(G) - 1$, with or without bounding the enumeration space.

Figure (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. The contraction order is obtained using the local search algorithm in Ref. [33]. In practice, slicing technique 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 (b), (c) and (d) have a strong correlation with the treewidth. Among these benchmarks, computational tasks with data types `T (CPU)`, $\mathbb{R}$ `(CPU)`, $\mathbb{R}$ `(GPU)`, $\mathbb{C}$ `(CPU)`, $\mathbb{C}$ `(GPU)` and `T+bounding (CPU)` can utilize fast BLAS functions to evaluate tensor contractions, hence are much faster comparing to non-BLAS element types in the same category. 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 GPU, except those requiring dynamic

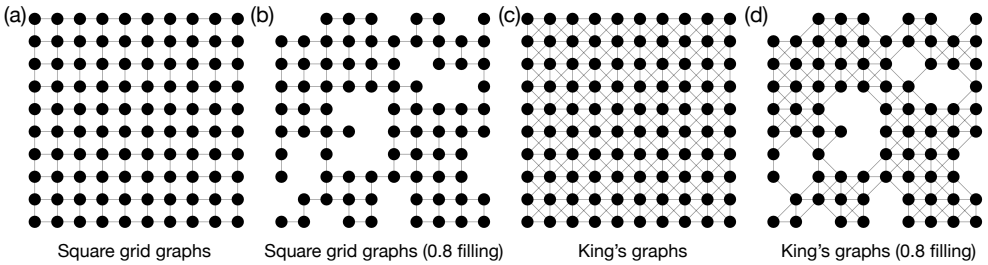


Figure 3: The types of graphs used in the case study in section 7.2.1. The lattice dimensions are $L \times L$. (a) Square grid graphs. (b) Square grid graphs with a filling factor $p = 0.8$. (c) King's graphs. (d) King's graphs with a filling factor $p = 0.8$.

sized structures, i.e. `PN` and `SN`. In figure (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. 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 (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 ~ 150 on a device with 32GB main memory.

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

7.2.1. 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 3, where vertices are all placed on square lattices with lattice dimensions $L \times L$. The types of graphs include: the square grid graphs (Figure 3(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 3(b)); the King's graphs (Figure 3(c)); the King's graphs with a filling factor $p = 0.8$ (Figure 3(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 useful number that can be computed using the number of independent sets is the entropy constant for the hardcore lattice gases on these graphs. 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 [5, 45] 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. 4, 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 3. 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.

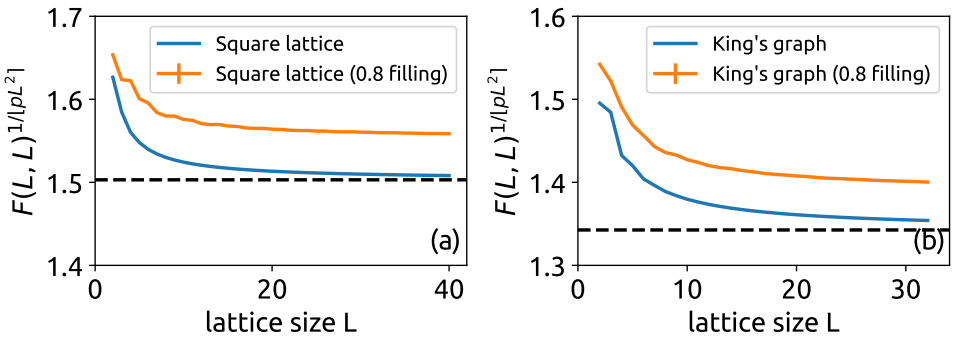


Figure 4: Mean entropy for lattice gases on graphs defined in Fig. 3. We sampled 1000 instances for $p = 0.8$ lattices and the error bar is too small to be visible. The horizontal black dashed lines are for $\lim_{L\to\infty} F(L,L)^{1/L^2}$ for the corresponding non-disordered square grid and King's graphs.

7.2.2. 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 [24, 23]. 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 [24, 23]. Here, we use the computed configurations of large independent sets to investigate the presence or absence of the overlap gap property. In particular, in Fig. 5, we enumerated all ISs of size $\geq \alpha(G) - 1$ for two random three regular graph instances of size 100 and show the pairwise Hamming distance statistics for the enumerated configurations. In Fig. 5(a), we observed the multiple peak structure for the pairwise Hamming distance for one of the 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.

8. Discussion and conclusion. In this paper, we introduce a method to use generic programming tensor networks to compute a number of different independent set properties, including the size of the MISs and the number and enumeration of independent sets of a given size. For each property, we design an algebra of a commutative semiring with a particular element type and map the computation of the property to the contraction of a tensor network with such an element type. The data types introduced in the main text can be represented in the following diagram, where we use overlap to represent two algebras that can be combined to create a new algebra.

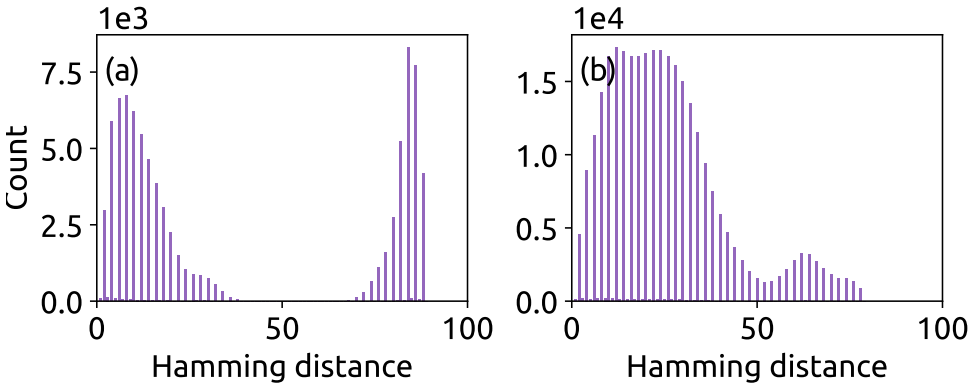
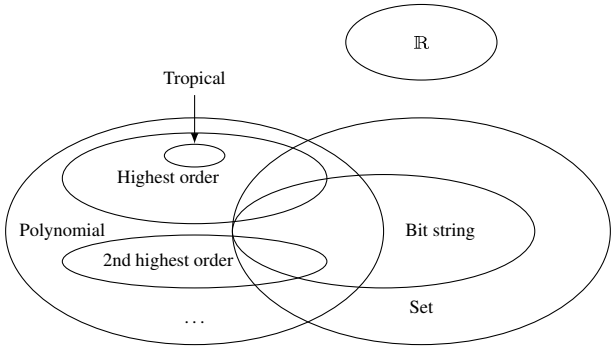


Figure 5: The distribution of pairwise Hamming distances between every two independent sets of size $\geq \alpha(G) - 1$ for two random three regular graph instances of size 100.



Other than the the case with real numbers, we have polynomials and truncated polynomials as algebra types. We combine them with the set algebra and the bitstring algebra for set enumeration and sampling. This approach to use generic tensor networks can be easily extended 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 [36], the clique polynomial [30], 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 A. A complete implementation can be found in our Github repository [2]. We expect our tool can be used to understand and study many interesting applications of independent sets and beyond. This approach of generic tensor networks should also inspire future works on tensor network computations.

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TropicalGEMM.jl. We would also like to thank a number of open-source software developers, including Roger Luo, Time Besard, and Katharine Hyatt, for solving some implementation issues voluntarily. [**JG: funding information**]

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Appendix A. Technical guide. This project depends on multiple open source packages in Julia ecosystem. We list the Julia packages playing 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 art algorithms for finding the optimal contraction order for the an tensor network, including the KaHypar+Greedy [27, 44] and local transformation based approaches [33],

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
```

It may surprise you that the Julia implementation of algorithms introduced in the paper is so short that except the bounding algorithm, 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 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 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
# `uniquelabels` function extracts tensor labels into a vector.
size_dict = Dict([s=>2 for s in uniquelabels(code)])
# optimize the contraction order using the `TreeSA` method, 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 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 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 = _independance_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 _independance_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 set algebra
struct ConfigEnumerator{N}
    # NOTE: BitVector is dynamic, 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`, maybe using random sampler is better.
    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}` 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(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)"
     )

# enumerating configurations directly 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 performance reason, we still 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. Here is a short introduction to the functionalities in this package.

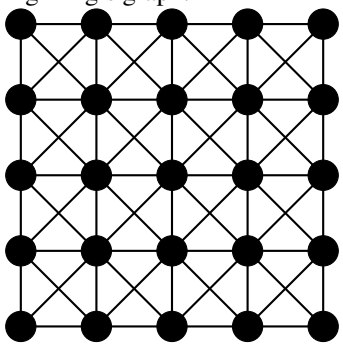
```
julia> using GraphTensorNetworks, Random, Graphs

julia> graph = (Random.seed!(2); Graphs.smallgraph(:petersen))
{10, 15} undirected simple Int64 graph

julia> problem = Independence(graph; optimizer=TreeSA(sc_target=0, sc_weight=1.0, ntrials=10, βs=
     0.01:0.1:15.0, niters=20, rw_weight=0.2));
┌ Warning: target space complexity not found, got: 4.0, with time complexity 7.965784284662087,
     read-right complexity 8.661778097771988.
└ @ OMEinsumContractionOrders ~/.julia/dev/OMEinsumContractionOrders/src/treesa.jl:71
time/space complexity is (7.965784284662086, 4.0)

# maximum independent set size
julia> solve(problem, "size max")
0-dimensional Array{TropicalNumbers.TropicalF64, 0}:
4.0ₜ
```

```
# all independent sets
julia> solve(problem, "counting sum")
0-dimensional Array{Float64, 0}:
76.0

# counting maximum independent sets
julia> solve(problem, "counting max")
0-dimensional Array{TropicalNumbers.CountingTropicalF64, 0}:
(4.0, 5.0)ₜ

# counting independent sets of max two sizes
julia> solve(problem, "counting max2")
0-dimensional Array{Max2Poly{Float64, Float64}, 0}:
30.0*x^3 + 5.0*x^4

# using `Polynomial` type
julia> solve(problem, "counting all")
0-dimensional Array{Polynomial{Float64, :x}, 0}:
Polynomial(1.0 + 10.0*x + 30.0*x^2 + 30.0*x^3 + 5.0*x^4)

# using the finitefield approach
julia> solve(problem, "counting all (finitefield)")
0-dimensional Array{Polynomial{BigInt, :x}, 0}:
Polynomial(1 + 10*x + 30*x^2 + 30*x^3 + 5*x^4)

# using the fourier approach
julia> solve(problem, "counting all (fft)", r=1.0)
0-dimensional Array{Polynomial{ComplexF64, :x}, 0}:
Polynomial(1.0000000000000029 + 2.6645352591003376e-16im + (10.000000000000004 - 1.95124353988574
     92e-16im)x + (30.0 - 1.9622216671393801e-16im)x^2 + (30.0 + 1.1553104311877194e-15im)x^3 +
     (5.0 - 1.030417436395244e-15im)x^4)

# one of MISs
julia> solve(problem, "config max")
0-dimensional Array{CountingTropical{Float64, ConfigSampler{10, 1, 1}}, 0}:
(4.0, ConfigSampler{10, 1, 1}(1010000011))ₜ

julia> solve(problem, "config max (bounded)")
0-dimensional Array{CountingTropical{Float64, ConfigSampler{10, 1, 1}}, 0}:
(4.0, ConfigSampler{10, 1, 1}(1010000011))ₜ

# enumerate all MISs
julia> solve(problem, "configs max")  # not recommended
0-dimensional Array{CountingTropical{Float64, ConfigEnumerator{10, 1, 1}}, 0}:
(4.0, {1010000011, 0100100110, 1001001100, 0010111000, 0101010001})ₜ

julia> solve(problem, "configs max (bounded)")
0-dimensional Array{CountingTropical{Int64, ConfigEnumerator{10, 1, 1}}, 0}:
(4, {1010000011, 0100100110, 1001001100, 0010111000, 0101010001})ₜ

# enumerate all MIS and MIS-1 configurations
julia> solve(problem, "configs max2")
0-dimensional Array{Max2Poly{ConfigEnumerator{10, 1, 1}, Float64}, 0}:
{0010101000, 0101000001, 0100100010, 0010100010, 0100000011, 0010000011, 1001001000, 1010001000,
      1001000001, 1010000001, 1010000010, 1000000011, 0100100100, 0000101100, 0101000100, 000100
     1100, 0000100110, 0100000110, 1001000100, 1000001100, 1000000110, 0100110000, 0000111000, 0
     101010000, 0001011000, 0010110000, 0010011000, 0001010001, 0100010001, 0010010001}*x^3 + {1
     010000011, 0100100110, 1001001100, 0010111000, 0101010001}*x^4

# enumerate all IS configurations
julia> solve(problem, "configs all")
0-dimensional Array{Polynomial{ConfigEnumerator{10, 1, 1}, :x}, 0}:
Polynomial({0000000000} + {0010000000, 0000100000, 0001000000, 0100000000, 0000001000, 000000000
     1, 0000000010, 1000000000, 0000000100, 0000010000}*x + {1000000010, 0010100000, 0010001000,
      0100100000, 0000101000, 0101000000, 0001001000, 0001000001, 0100000001, 0010000001, 000010
     0010, 0100000010, 0010000010, 0000000011, 1001000000, 1000001000, 1010000000, 1000000001, 0
     000000110, 0000100100, 0001000100, 0100000100, 0000001100, 1000000100, 0010010000, 00001100
     00, 0001010000, 0100010000, 0000011000, 0000010001}*x^2 + {1010000010, 1000000011, 00101010
     00, 0101000001, 0100100010, 0010100010, 0100000011, 0010000011, 1001001000, 1010001000, 100
     1000001, 1010000001, 0000100110, 0100000110, 0100100100, 0000101100, 0101000100, 0001001100
     , 1001000100, 1000001100, 1000000110, 0010110000, 0010011000, 0100110000, 0000111000, 01010
     10000, 0001011000, 0001010001, 0100010001, 0010010001}*x^3 + {1010000011, 0100100110, 10010
     01100, 0010111000, 0101010001}*x^4)
```

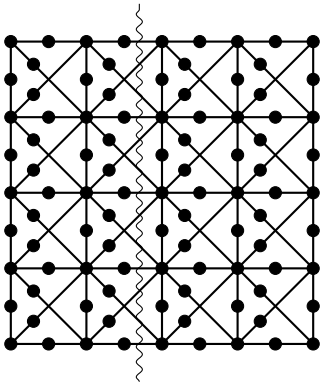
Appendix B. The reason to not using the standard tensor network notations. As we have mentioned in the main text, a standard tensor network notation is equivalent to the generalized tensor network by introducing δ tensors, where a δ tensor of rank d is defined as

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

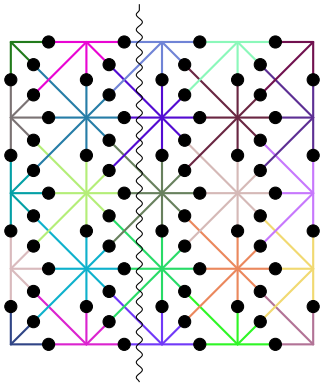
Let us consider the following King's graph.



By mapping the independent set problem to a standard tensor network, we have the following graphical representation.



In this diagram, the circle on each vertex in the original graph is a δ tensor of rank 8. 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 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. Again, if we contract this tensor network in the column-wise order, the maximum intermediate tensor rank is $\sim L$, which can be see by counting the number of colors.

Appendix C. Generalizing to other graph problems.

C.1. Maximal independent sets and maximal cliques. Finding maximal independent sets of a graph is equivalent to finding the maximal cliques of its complement graph, so in the following we mainly discuss how to find maximal independent sets. 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 $v \in V$ such that $I_m \cap N[v] = \emptyset$. Similar to the independence polynomial, the maximal independence polynomial counts the number of maximal independent sets of various sizes [31], which can help us understand why the program for solving MIS is trapped in a local minimum. Concretely, it is defined as

$$I_{\max}(G, x) = \sum_{k=0}^{\alpha(G)} b_k x^k, \tag{C.1}$$

where b_k is the number of maximal independent sets of size k in graph $G = (V, E)$. Comparing with the independence polynomial in Eq. (4.1), we have $b_k \leq a_k$ and $b_{\alpha(G)} = a_{\alpha(G)}$. $I_{\max}(G, 1)$ counts the total number of maximal independent sets [25, 40], where the fastest algorithm currently has a runtime of $O(1.3642^{|V|})$ [25]. If we want to find an 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 [31].

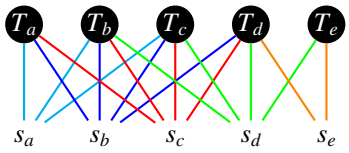
We can modify the tensor network for computing the independence polynomial to include this restriction. Instead of defining the restriction on vertices and edges, it is more natural to define it on $N[v]$:

$$T(x_v)_{s_1,s_2,\ldots,s_{|N(v)|},s_v} = \begin{cases} s_v x_v & s_1 = s_2 = \ldots = s_{|N(v)|} = 0, \\ 1 - s_v & \text{otherwise.} \end{cases} \tag{C.2}$$

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

$$T(x_v) = \begin{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix} \\ \begin{pmatrix} x_v & 0 \\ 0 & 0 \end{pmatrix} \end{pmatrix}. \tag{C.3}$$

By contracting this tensor network with generic element type, we can compute the maximum independent set properties such as maximal independence polynomial, enumerating maximal independent sets. Let us consider the example in Sec. 2: its corresponding tensor network structure for computing the maximal independent polynomial becomes



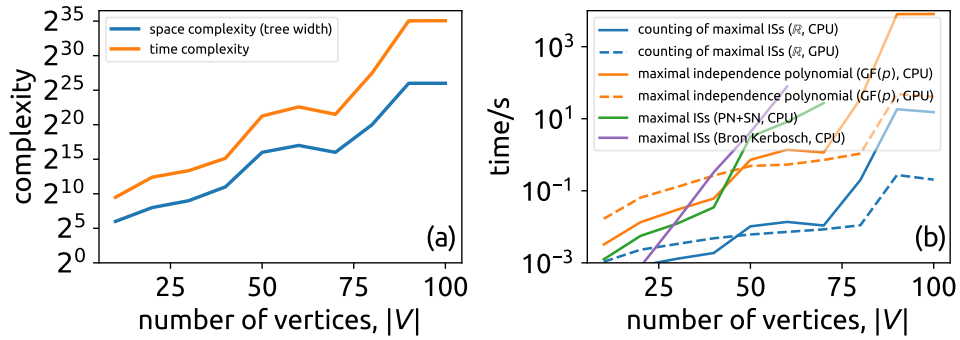


Figure 6: Benchmark results for computing different properties of maximal independent sets on a random three regular graph with different tensor element types. (a) treewidth versus the number of vertices for the benchmarked graphs. (b) The computing time for calculating the number of independent sets and enumerate all MISs.

One can see that the average degree 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. However, for most sparse graphs, this tensor network contraction approach is still much faster than enumerating all the maximal cliques on its complement graph using the Bron-Kerbosch algorithm [11], which is the standard algorithm that we are aware of to compute the maximal independence polynomial. We show the benchmark of computing the maximal independent set properties in Fig. 6, including a comparison to the Bron-Kerbosch algorithm from Julia package Graphs [3]. the treewidth of this tensor network is significantly larger, hence only small graphs can be benchmarked. 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 stops working at size 70 and above.

C.2. Matching problem. A matching polynomial of a graph G is defined as

$$M(G, x) = \sum_{k=1}^{|V|/2} c_k x^k, \tag{C.4}$$

where k is the number of matches, and coefficients c_k are the corresponding counting. We map an edge $(u, v) \in E$ to a label $\langle u, v\rangle \in \{0, 1\}$ in a tensor network, where 1 means two vertices of an edge are matched, 0 means otherwise. Then we define a tensor of rank $d(v) = |N(v)|$ on vertex v such that,

$$W_{\langle v,n_1\rangle,\langle v,n_2\rangle,\ldots,\langle v,n_{d(v)}\rangle} = \begin{cases} 1, & \sum_{i=1}^{d(v)} \langle v, n_i\rangle \leq 1, \\ 0, & \text{otherwise}, \end{cases} \tag{C.5}$$

and a tensor of rank 1 on the bond

$$B_{\langle v,w\rangle} = \begin{cases} 1, & \langle v, w\rangle = 0 \\ x, & \langle v, w\rangle = 1, \end{cases} \tag{C.6}$$

where label $\langle v, w\rangle$ is equivalent to $\langle w, v\rangle$. Here, a vertex tensor specifies the restriction that a vertex can not be in two matched edges, while an edge tensor contributes the variable in the polynomial.

C.3. k-Colouring. Let us use 3-colouring problem defined on vertices as an example. For a vertex v, we define the degree of freedoms $c_v \in \{1, 2, 3\}$ and a vertex tensor labelled by it as

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

For an edge (u, v), we define an edge tensor as a matrix labelled by (c_u, c_v) to specify the constraint

$$B = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}. \tag{C.8}$$

The number of possible colouring 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 can get other properties. Similarly, one can define the k-colouring problem on edges too by switching the roles of edges and vertices.

C.4. Max cut problem. Max cut problem is also known as the boolean spin glass problem. For a vertex $v \in V$, we define a boolean degree of freedom $s_v \in \{0, 1\}$. Then the max cut problem can be encoded to tensor networks by mapping an edge $(i, j) \in E$ to an edge matrix labelled by $s_i s_j$

$$B(x_{\langle i,j\rangle}) = \begin{pmatrix} 1 & x_{\langle i,j\rangle} \\ x_{\langle i,j\rangle} & 1 \end{pmatrix}, \tag{C.9}$$

where variable $x_{\langle i,j\rangle}$ represents a cut on edge (i, j) or a domain wall of an Ising spin glass. Similar to other problems, we can define a polynomial about edges variables by setting $x_{\langle i,j\rangle} = x$, where its kth coefficient is two times the number of configurations of cut size k.

C.5. 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 just remove the rank 2 restriction of the edge tensor in Eq. (4.3)

$$B_{v,w,\ldots,z} = \begin{cases} 1, & v + w + \ldots + z \leq 1, \\ 0, & \text{otherwise.} \end{cases} \tag{C.10}$$

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

In section 4, we show that the independence polynomial can be obtained by solving the linear equation Eq. (4.7). 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

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

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 $\vec{a}_r = \mathrm{FFT}^{-1}(\omega)\cdot\vec{y}$, 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 E. Integer sequences 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 on GPUs. The tensor element type is finite field algebra so that we can reach arbitrary precision. We also computed independence polynomial rigorously for these lattices 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 show two updated entries for $L = 38, 39$, which to our knowledge, has not been computed before. [13]

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