SOLVING THE INDEPENDENT SET PROBLEM BY GENERIC PROGRAMMING TENSOR NETWORKS *

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Abstract. This paper is about solving the independent set problem by eincoding this problem to a tensor network. We show how to obtain the maximum independent set size, the independence polynomial and optimal configurations of a graph by engineering the tensor element algebra. We also show how to analyse the local properties of a graph by contracting an open tensor network.

Key words. maximum independent set, tensor network

AMS subject classifications. 05C31, 14N07

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1. Introduction. In this work, we introduce a tensor based framework to study the famous graph problem of finding independent sets. 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 the maximum independent set (MIS) size $\alpha(G) \equiv \max_{I} |I|$ belongs to the complexity class NP-complete [13], which is unlikely to be decided in polynomial time. It is hard to even approximate this size in polynomial time within a factor $|V|^{1-\epsilon}$ for an arbitrarily small positive ϵ . The exhaustive search for a solution costs time $2^{|V|}$. More efficient algorithms to compute the MIS size exactly includes the branching algorithm and dynamic programming. Without changing the fact of exponential scaling in computing time, the branching algorithm gives a smaller base. For example, in [24], a sophisticated branching algorithm has a time complexity $1.1893^n n^{O(1)}$. The dynamic programming approach [5, 8] works better for graphs with small tree width tw(G), it gives an algorithms of complexity $O(2^{hv(G)}tw(G)n)$. People are interested in solving the independent set problem better not only because it is an NP-complete problem that directly related to other NP-complete problems like maximal cliques and vertex cover [18], but also for its close relation with physical applications like hard spheres lattice gas model [6], and Rydberg hamiltonian [21]. However, in these applications, knowing the MIS size and one of the optimum solutions is not the only goal. People often ask different questions about independent sets in order to understand the landscape of their models better. These questions includes but not limited to, counting all independent sets, obtaining all independent sets of size $\alpha(G)$ and $\alpha(G) - 1$, counting the number of (maximal) independent sets of different sizes, and understanding the effect of a local gadget. In this work, we attack this problem by mapping it to an generic tensor network. It does not give a better time complexity comparing to dynamic programming, but is versatile enough to answer the above questions by engineering the tensor elements with minimum effort.

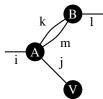
2. Tensor networks. A tensor network can be viewed as a generalization to of binary matrix multiplication to n-ary tensor contraction. Let A, B be two matrices, the matrix multiplication is defined as $C_{ik} = \sum_j A_{ij} B_{jk}$. A traditional tensor network refers to the Einstein's notation. In this notation, the matrix multiplication is denoted as $C_i^k = A_i^j B_j^k$, where the paired subscript and superscript j is a dummy index summed over, hence each index appears precisely twice. When we have multiple tensors doing the above sum-product operation, we get a traditional tensor network [19]. A traditional tensor network can be

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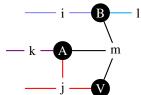
[‡]yyyyy (yyyy, email).

- represented as a mutigraph 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 traditional tensor network $C_i^l = A_{ij}^{km} B_{km}^l V^j$ has the following multigraph representation.



Here, we want to use a generalized tensor network notation by not restricting the number of times a label appears in the notation, hence whether an index is a superscript or a subscript makes no sense now. It is also called einsum, sum-product network or factor graph [4] in some contexts. The graphical representation of a tensor network 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, it represents $C_{ijk} = \sum_{ml}A_{jkm}B_{mia}V_{jm}$. Its hypergraph representation is as the following, where we use different color to annotate different hyperedges.



In the main text, we stick to the our generalized tensor network notation rather than the traditional notation. As a note to those who are more familiar with the traditional tensor network representation, although one can easily translate a generalized tensor network to the equivalent traditional tensor network by adding δ tensors (a generalization of identity matrix to higher order). It can sometime increase the contraction complexity of a graph. We have an example demonstrating this point in Appendix B.

3. Independence polynomial. One can encode the independence polynomial [7, 12] of G to a tensor network. Independence polynomial is an important graph polynomial that contains the counting information of an independent set problem. It is defined as

63 (3.1)
$$I(G, x) = \sum_{k=1}^{\alpha(G)} a_k x^k,$$

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where a_k is the number of independent sets of size k in G, and $\alpha(G)$ is the maximum independent set size. The problem of computing independence polynomial belongs to the complexity class #P-hard. A traditional approach to compute independence polynomial rigorusly requires a computing time $O(1.442^n)$ [7][JG: I am not sure about this complexity, this is baed on the naive analysis of theorem 2.2 in [7]]. There are some interests in approximating this polynomial efficiently [11], but here, we focus on the rigorous approaches. We encode this polynomial to a tensor network by placing a rank one tensor of size 2 parametrized by x_i on a vertex i

$$W(x_i)_{s_i} = \begin{pmatrix} 1 \\ x_i \end{pmatrix}_{s_i},$$

and a rank two tensor of size 2×2 on an edge (i, j)

$$B_{s_i s_j} = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}_{s_i s_j},$$

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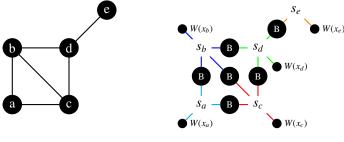
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where a tensor index s_i is a boolean variable that having the meaning of being 1 if vertex i is in the independent set, 0 otherwise. It corresponds to a hyperedge in the hypergraph. The contraction of such a tensor network gives

78 (3.4)
$$P(G, \{x_1, \dots, x_n\}) = \sum_{s_1, s_2, \dots, s_n = 0}^{1} \prod_{i=1}^{n} W(x_i)_{s_i} \prod_{(i, j) \in E(G)} B_{s_i s_j},$$

where the summation runs over all vertex configurations $\{s_1, \ldots, s_n\}$ and accumulates the product of tensor elements to the scalar output P. We can see an edge tensor represents the restriction on an edge that if both vertices connected by it are included in the set, then such configuration has no contribution to the output. When we set $x_i = x$, the contraction result corresponds to the independence polynomial. One can see the connection from the fact that the product over vertex tensor elements gives 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, 0 otherwise. One directly benefit of mapping the independent set problem to a tensor network is one can take the advantage of recently developed techniques in tensor network based quantum circuit simulations [10, 20], where people evaluate a tensor network by pairwise contracting tensors in a heuristic order. A good contraction order can reduce the time complexity significantly, at the cost of having a space overhead of $O(2^{tw(G)})$. Here tw(G) is the tree width of the line graph of a tensor network hypergraph, while the line graph of a tensor network hypergraph corresponds to the original graph G that we mapped from. [17] The pairwise tensor contraction also makes it possible to utilize basic linear algebra subprograms (BLAS) functions to speed up our computation for certain tensor element types.

95 **Example 3.** Mapping a graph (left) to a tensor network, the resulting tensor network is 96 shown in the right panel. In the generalize tensor network's graphical representation, a vertex 97 is mapped to a hyperedge, and an edge is mapped to an edge tensor.



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

 $a, b, c \in R$.

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$$\sum_{s_{a}, s_{b}, s_{c}, s_{d}, s_{e}} W(x_{a})_{s_{a}} W(x_{b})_{s_{b}} W(x_{c})_{s_{c}} W(x_{d})_{s_{d}} W(x_{e})_{s_{e}} B_{s_{a}s_{b}} B_{s_{b}s_{d}} B_{s_{a}s_{c}} B_{s_{b}s_{c}} B_{s_{d}s_{e}}.$$
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$$= \sum_{s_{b}, s_{c}} \left(\sum_{s_{d}} \left(\left(\left(\sum_{s_{e}} B_{s_{d}s_{e}} W(x_{e})_{s_{e}} \right) W(x_{d})_{s_{d}} \right) (B_{s_{b}s_{d}} W(x_{b})_{s_{b}}) \right) (B_{s_{c}s_{d}} W(x_{c})_{s_{c}}) \right)$$
101
$$\left(B_{s_{b}s_{c}} \left(\sum_{s_{a}} B_{s_{a}s_{b}} \left(B_{s_{a}s_{c}} W(x_{a})_{s_{a}} \right) \right) \right)$$
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$$= 1 + x_{a} + x_{b} + x_{c} + x_{d} + x_{e} + x_{a}x_{d} + x_{a}x_{e} + x_{c}x_{e} + x_{b}x_{e}$$

$$= 1 + 5x + 4x^{2}$$

Before contracting the tensor network and evaluating the independence polynomial numerically, let us first give up thinking 0s and 1s in tensors W(x) and B as regular computer numbers such as integers and floating point numbers. Instead, we treat them as the additive identity and multiplicative identity of a commutative semiring. A semiring is a ring without additive inverse, while a commutative semiring is a semiring that multiplication commutative. To define a commutative semiring with addition algebra \oplus and multiplication algebra \odot on a set R, the following relations must hold for arbitrary three elements

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$$(a \oplus b) \oplus c = a \oplus (b \oplus c)$$
 > commutative monoid \oplus with identity 0

115 $a \oplus 0 = 0 \oplus a = a$

116 $a \oplus b = b \oplus a$

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118 $(a \odot b) \odot c = a \odot (b \odot c)$ > commutative monoid \odot with identity 1

119 $a \odot 1 = 1 \odot a = a$

120 $a \odot b = b \odot a$

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122 $a \odot (b \oplus c) = a \odot b + a \odot c$

123 $(a \oplus b) \odot c = a \odot c \oplus b \odot c$

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126 $a \odot 0 = 0 \odot a = 0$

The property of being commutative is required here because we want the contraction result independent of the contraction order. In the following, we show how to obtain the independence polynomial, the maximum independent set size and optimal configurations of a general graph G by designing tensor element types as commutative semirings, i.e. making the tensor network generic [23].

3.1. The polynomial approach. A straight forward approach to evaluate the independence polynomial is treating the tensor elements as polynomials, and evaluate the polynomial directly. Let us create a polynomial type, and represent a polynomial $a_0 + a_1x + ... + a_kx^k$ as a vector $(a_0, a_1, ..., a_k) \in \mathbb{R}^k$, 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

$$a \oplus b = (a_0 + b_0, a_1 + b_1, \dots, a_{\max(k_a, k_b)} + b_{\max(k_a, k_b)}),$$

$$a \odot b = (a_0 + b_0, a_1 b_0 + a_0 b_1, \dots, a_{k_a} b_{k_b}),$$

$$0 = (),$$

$$138$$

$$1 = (1).$$

By contracting the tensor network with polynomial type, the final result is the exact representation of the independence polynomial. In the program, the multiplication can be evaluated efficiently with the convolution theorem [22]. The only problem of this method is it suffers from a space overhead that proportional to the maximum independent set size because each polynomial requires a vector of such size to store the factors. In the following subsections, we managed to solve this problem.

3.2. The fitting and Fourier transformation approaches. Let $m = \alpha(G)$ be the maximum independent set size and X be a set of real numbers of cardinality m + 1. We compute the tensor network contraction for each $x_i \in X$ and obtain the following relations

$$a_{0} + a_{1}x_{1} + a_{1}x_{1}^{2} + \dots + a_{m}x_{1}^{m} = y_{0}$$

$$a_{0} + a_{1}x_{2} + a_{2}x_{2}^{2} + \dots + a_{m}x_{2}^{m} = y_{1}$$

$$\dots$$

$$a_{0} + a_{1}x_{m} + a_{2}x_{m}^{2} + \dots + a_{m}x_{m}^{m} = y_{m}$$

$$a_{0} + a_{1}x_{m} + a_{2}x_{m}^{2} + \dots + a_{m}x_{m}^{m} = y_{m}$$

The polynomial fitting between X and $Y = \{y_0, y_1, \dots, y_m\}$ gives us the factors. The polynomial fitting is essentially about solving the following linear equation

152 (3.7)
$$\begin{pmatrix} 1 & x_1 & x_1^2 & \dots & x_1^m \\ 1 & x_2 & x_2^2 & \dots & x_2^m \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_m & x_m^2 & \dots & x_m^m \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_m \end{pmatrix} = \begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_m \end{pmatrix}.$$

In practise, the fitting can suffer from the non-negligible round off errors of floating point operations and produce unreliable results. This is because the factors of independence polynomial can be different in magnitude by many orders. Instead of choosing X as a set of random real numbers, we make it form a geometric sequence in the complex domain $x_j = r\omega^j$, where $r \in \mathbb{R}$ and $\omega = e^{-2\pi i/(m+1)}$. The above linear equation becomes

$$\begin{pmatrix}
1 & r\omega & r^2\omega^2 & \dots & r^m\omega^m \\
1 & r\omega^2 & r^2\omega^4 & \dots & r^m\omega^{2m} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
1 & r\omega^m & r^2\omega^{2m} & \dots & r^m\omega^{m^2}
\end{pmatrix}
\begin{pmatrix}
a_0 \\ a_1 \\ \vdots \\ a_m
\end{pmatrix} = \begin{pmatrix}
y_0 \\ y_1 \\ \vdots \\ y_m
\end{pmatrix}$$

Let us rearrange the factors r^j to a_j , the matrix on left side is exactly the a discrete Fourier transformation (DFT) matrix. Then we can obtain the factors using the inverse Fourier transformation $\vec{a}_r = \text{FFT}^{-1}(\omega) \cdot \vec{y}$, where $(\vec{a}_r)_j = a_j r^j$. By choosing different r, one can obtain better precision in low independent set size region ($\omega < 1$) and high independent set size region ($\omega > 1$).

3.3. The finite field algebra approach. It is possible but not trivial to compute the independence polynomial rigorously using integer number types only. The hardness originates from the practical consideration of computing speed and precision. Fixed width integer types are often too small to store the counting, while big integer with varying width can be very slow and incompatible with graphic processing units (GPU) devices. This problem can be solved by introducing finite field algebra GF(p)

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x \oplus y = x + y \pmod{p},
x \odot y = xy \pmod{p},
0 = 0,
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1 = 1.
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In a finite field algebra, we have the following observations

- 1. One can use Gaussian elimination [9] to solve a linear equation Eq. (3.7) because it is a generic function 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 unkown integer x over a set of co-prime integers $\{p_1, p_2, \ldots, p_n\}$, $x \pmod{p_1 \times p_2 \times \ldots \times p_n}$ can be computed using the Chinese remainder theorem. With this, one can infer big integers from small integers.

With these observations, we developed Algorithm 3.1 to compute independence polynomial exactly without introducing space overheads. In the algorithm, except the computation of Chinese remainder theorem, all computations are done with integers of fixed width W.

Algorithm 3.1 Compute independence polynomial exactly without integer overflow

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Let P=1, vector X=(0,1,2,\ldots,m), matrix \hat{X}_{ij}=X_i^j, where i,j=0,1,\ldots m while true do compute the largest prime p that \gcd(p,P)=1 and p\leq 2^W compute the tensor contraction on GF(p) and obtain Y=(y_0,y_1,\ldots,y_m)\pmod p A_p=(a_0,a_1,\ldots,a_m)\pmod p=\mathrm{gaussian\_elimination}(\hat{X},Y\pmod p) A_{P\times p}=\mathrm{chinese\_remainder}(A_P,A_p) if A_P=A_{P\times p} then return A_P; // converged end P=P\times p
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3.4. Maximal independence polynomial. Some times people are interested in knowing maximal solutions to understand why their program is trapped in a local minimal. Then they might want to compute the maximal independence polynomial. Let us denote the neighbour of a vertex v as N(v) and $N[v] = N(v) \cup \{v\}$. A maximal independent set I_m is an independent sets that there does not exist a vertex v that $N[v] \cap I_m = \emptyset$. Let us modify the tensor network for computing independence polynomial by adding this restriction. Instead of defining the restriction on vertices and edges, we define it on N[v]

192 (3.10)
$$T(x_{\nu})_{s_{1},s_{2},\dots,s_{|N(\nu)|},s_{\nu}} = \begin{cases} s_{\nu}x_{\nu} & s_{1} = s_{2} = \dots = s_{|N(\nu)|} = 0, \\ 1 - s_{\nu} & otherwise. \end{cases}$$

194 As an example, for a vertex of degree 2, the resulting rank 3 tensor is

195 (3.11)
$$T(x_{\nu}) = \begin{pmatrix} 0 & 1 \\ 1 & 1 \\ x_{\nu} & 0 \\ 0 & 0 \end{pmatrix}.$$

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We do the same computation as independence polynomial, the coefficients of resulting polynomial gives the counting of maximal independent sets, or the maximal independence polynomial. The computational complexity of this new tensor network is often larger than the one for computing independence polynomial. However, in many sparse graphs, this tensor network contraction approach is still much faster than computing the maximal cliques on its complement by applying the Bron-Kerbosch algorithm.

4. Maximum independent sets and its counting problem. In the previous section, we focused on computing independence polynomial for a given maximum independent set size $\alpha(G)$, but we didn't mention 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

208 (4.1)
$$I(G, \infty) = a_k \infty^{\alpha(G)},$$

09 where the lower orders terms disappear automatically. We can define a new algebra as

$$a_{x} \infty^{x} \oplus a_{y} \infty^{y} = \begin{cases} (a_{x} + a_{y}) \infty^{\max(x,y)}, & x = y \\ a_{y} \infty^{\max(x,y)}, & x < y \\ a_{x} \infty^{\max(x,y)}, & x > y \end{cases}$$

$$a_{x} \infty^{x} \odot a_{y} \infty^{y} = a_{x} a_{y} \infty^{x+y}$$

$$0 = 0 \infty^{-\infty}$$

$$1 = 1 \infty^{0}$$

- In the program, we only store the power x and the corresponding factor a_x that initialized to 1. This algebra is the same as the one in [15] for counting spin glass ground states. If one is only interested in obtaining $\alpha(G)$, he can drop the factor parts, then the new algebra becomes the max-plus tropical algebra [16, 18].
 - **4.1. Sub-optimal solutions.** Some times people are interested in finding sub-optimal solutions efficiently. We define a truncated polynomial algebra by keeping only largest two factors in the polynomial in Eq. (3.5).

$$a \oplus b = (a_{\max(k_a, k_b) - 1} + b_{\max(k_a, k_b) - 1}, a_{\max(k_a, k_b)} + b_{\max(k_a, k_b)}),$$

$$a \odot b = (a_{k_a - 1}b_{k_b} + a_{k_a}b_{k_b - 1}, a_{k_a}b_{k_b}),$$

$$0 = (),$$

$$1 = (1).$$

- In the program, we need a data structure that contains three fields, the largest order k and factors for two largest orders a_k and a_{k-1} .
- 5. Enumerating configurations. One may also want to obtain all solutions, it can be achieved replacing the factors a_x with a set of bit strings s_x , We design a new element type

225 having the following algebra

$$s \oplus t = s \cup t$$

$$s \odot t = \{\sigma \lor^{\circ} \tau | \sigma \in s, \tau \in t\}$$

$$0 = \{\}$$

$$1 = \{0^{\otimes n}\}$$

where \vee° is the Hadamard logic or operation over two bit strings, which means joining of two local configurations. The variable x in the vertex tensor is initialized to $x_i = \{e_i\}$, where e_i is a one hot vector of size |G|. One can easily check this algebra is a commutative semiring. When we use the above algebra as factors of independence polynomials, the resulting algebra is also a commutative semiring. With this new element type, the tensor network contraction will give all solutions rather than just a number for counting. By slightly modifying the above algebra, it can also be used to obtain just a single configuration to save the computational effort.

$$\sigma \oplus \tau = \operatorname{select}(\sigma, \tau)$$

$$\sigma \odot \tau = (\sigma \vee^{\circ} \tau),$$

$$0 = 1^{\otimes n},$$

$$1 = 0^{\otimes n},$$

where the select function picks one of σ_x and σ_y by some criteria to make the algebra commutative and associative, e.g. by their integer values. In practise, one can just pick randomly from them, then the program will output one of the configurations randomly.

5.1. Bounding the enumeration space. When one uses the set algebra in Eq. (5.1) to represent the factors in Eq. (4.2) for enumerating all optimum configurations, he will find the program stores more than necessary intermediate configurations and cause significant overheads in space. To speed up the computation, we use $\alpha(G)$ to bound the searching space. We first compute the value of $\alpha(G)$ with tropical numbers and cache all intermediate tensors. Then we compute a boolean masks for each cached tensor, where we use a boolean true to represent a tensor element having contribution to the maximum independent set (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 for obtaining all configurations. Notice that these masks are in fact tensor elements with non-zero gradients with respect to MIS size, we compute these masks by back propagating gradients. To derive the backward rule, we consider a tropical matrix multiplication C = AB, we have the following inequality

$$A_{ij} \odot B_{jk} \le C_{ik}.$$

Moving B_{ik} to the right hand side, we have

$$A_{ij} \le (\oplus_k (C_{ik}^{-1} \odot B_{jk}))^{-1}$$

where the tropical multiplicative inverse is defined as the additive inverse of the regular algebra. The equality holds if and only if element A_{ij} contributions to C (i.e. has non-zero gradient). Let the mask for C being \overline{C} , the backward rule for "gradient" masks reads

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

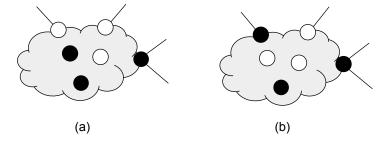


Figure 1: Two configurations with the same local independent size $A_{\sigma_a} = A_{\sigma_b} = 3$ and different boundary configurations (a) $\sigma_a = \{001\}$ and (b) $\sigma_b = \{101\}$, where black nodes are 1s (in the independent set) and white nodes are 0s (not in the independent set).

where $^{\circ -1}$ is the Hadamard inverse, \circ is the Hadamard product, boolean false is treated as tropical zero and boolean true is treated as tropical one. 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. [] [JG: maybe add an appendix?]

6. Tropical tensors for automated branching. [JG: ?] Branching rules can be automatically discovered by contracting the tensor network on a subgraph $R \subseteq G$ with tropical numbers as its element type. Let C be the set of boundary vertices defined as $C := \{u | u \in R \land (\exists v \in (G \backslash R) \land \operatorname{adj}(u, v))\}$, then the rank of the resulting tensor A is |C|. Here, we use $\operatorname{adj}(u, v)$ to denote two vertices u and v are adjacent to each other. Each tensor entry A_{σ} is a local maximum independent set size for the fixed boundary configuration $\sigma \in \{0, 1\}^{|C|}$. Suppose our goal is to find the maximum independent set size, then this tensor can be further "compactified" by removing some entries. To determine which entry can be removed, let us define a relation of *less restrictive* as

$$(\sigma_a \prec \sigma_b) := (\sigma_a \neq \sigma_b) \land (\sigma_a \leq^{\circ} \sigma_b)$$

where \leq° is the Hadamard less or equal to operation.

Definition 6.1. A tensors A is MIS-compact if

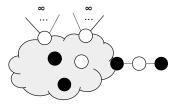
$$\forall \sigma_b \neg \exists \sigma_a (\sigma_a < \sigma_b) \land (A_{\sigma_a} \ge A_{\sigma_b}).$$

If we remove such A_{σ_b} , the contraction over the whole graph is guaranteed to give the same maximum independent set size. It can be seen by considering two entries with the same local maximum independent set sizes and different boundary configurations as shown in Fig. 1 (a) and (b). If we have $\sigma_b \cup \overline{\sigma_b}$ being one of the solutions for maximum independent sets in G, then $\sigma_a \cup \overline{\sigma_b}$ is another solution giving the same $\alpha(G)$. Hence, we can remove entry A_{σ_b} safely.

Theorem 6.2. A MIS-compact tropical tensor can not be further reduce without gloal information, i.e. any of its non-zero entries can produce the only global optimal solution given a proper environment.

Proof. Let us prove it by showing for any σ in a MIS-compact tropical tensor of a subgraph R, there exists a parent graph G that $R \subseteq G$ and σ is the boundary configuration

that gives the only maximum independent set. Let A be a tropical tensor, and an entry of it being A_{σ} , where σ is the boundary configuration. Let us construct a graph G such that for a vertex $v \in C$, if $\sigma_v = 1$, we connect it with two vertices $u, w \in G \setminus R$ that adj $(v, u) \land \operatorname{adj}(u, w) \land \neg \operatorname{adj}(v, w)$. Otherwise, we attach infinite many disconnected neighbors to v.



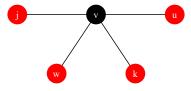
Then we have the maximum independent set size $\alpha(G,\sigma) = A_{\sigma} + \infty(|C| - \sum_{\nu=1}^{|C|} \sigma_{\nu}) + \sum_{\nu=1}^{|C|} 1 - \sigma_{\nu}$. Let us assume there exists another configuration τ that generating the same or better maximum independent set size $\alpha(G,\tau) \geq \alpha(G,\sigma)$. Then we have $\tau < \sigma$, otherwise it will loss infinite contribution from the environment. For such a τ , we have $A_{\tau} < A_{\sigma}$, otherwise $A_{\sigma} < A_{\tau}$ contradicts with A being MIS-compact. Finally, we have $\alpha(G,\tau) = \infty(|C| - |\sigma|) + A_{\tau} + \sum_{\nu=1}^{|C|} 1 - \sigma_{\nu} < \alpha(G,\sigma)$, hence σ is the only boundary configuration that gives the maximum independent set for this graph.

6.1. The tensor network compactification detects branching rules automatically.

Almost all branching rules are based on the same idea of analysing a local subgraph induced by a vertex v by including its neighbourhoods, and keep only the configurations that has the potential to produce the only maximum independent set. Since an MIS-compact tensor is optimal, by analysing the correlation of vertex configurations on the resulting tensor for the k-th neighbourhood $N^k[v]$, one can discover the optimal branching vector automatically. In the following, we are going to introduce several important rules for branching in the literature and show how it is connected to our tensor formulation.

COROLLARY 6.3. If a vertex v is in an independent set I, then none of its Neighbors can be in I. On the other hand, if I is a maximum (and thus maximal) independent set, and thus if v is not in I then at least one of its Neighbors is in I.

Contract $N[\nu]$ and the resulting tensor A has a rank $|N(\nu)|$. Each tensor entry A_{σ} corresponds to a locally maximized independent set size with fixed boundary configuration $\sigma \in \{0,1\}^{|N(\nu)|}$. If the boundary configuration is a bit string of 0s, σ_{ν} will takes value 1 to maximize the local independent set size.



After contracting N[v], v becomes an internal degree of freedom. Applying tensor compactification rule Eq. (6.2), the resulting rank 4 tropical tensor is

323 (6.3)
$$T_{juwk} = \begin{pmatrix} 1 & -\infty & 2 \\ -\infty & 2 \end{pmatrix}_{ju} \begin{pmatrix} -\infty & 2 \\ 2 & 3 \end{pmatrix}_{ju} \\ \begin{pmatrix} -\infty & 2 \\ 2 & 3 \end{pmatrix}_{ju} \begin{pmatrix} 2 & 3 \\ 3 & 4 \end{pmatrix}_{ju} \end{pmatrix}_{wk},$$

where we use "-" to denote an entry is forbidden. If we use sets for counting, one can check all configurations too. The resulting polynomial tensor is

327 (6.4)
$$P_{juwk} = \begin{pmatrix} 1 + x_v & - \\ - & x_j x_u \end{pmatrix}_{ju} \begin{pmatrix} - & x_u x_k \\ x_j x_k & x_u x_j x_k \end{pmatrix}_{ju} \\ \begin{pmatrix} - & x_w x_u \\ x_w x_j & x_w x_j x_u \end{pmatrix}_{ju} \begin{pmatrix} x_w x_k & x_w x_k x_u \\ x_w x_k x_j & x_j x_u x_w x_k \end{pmatrix}_{ju} \end{pmatrix}_{wk}.$$

By studying the correlation between vertex variables, one can easily see x_{ν} does not co-exist with other vertex variables. These anti-correlation determines possible branching vectors in the maximum independent set problem. It is easier to see if we list the set of optimal solutions as

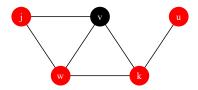
333 (6.5)
$$S_{juwkv} = \{00001, 10001, 01010, 10010, 11010, 10100, 01100, 11100, 00110, 01110, 10110, 11110\}.$$

335 The branching vector (1, 5) gives a branching number $\tau(1, 5) \approx 1.3247$

COROLLARY 6.4 (mirror rule). For some $v \in V$, a node $u \in N^2(v)$ is called mirror of v, if $N(v)\backslash N(u)$ is a clique. We denote the set of of a node v mirrors [8] by M(v). Let G = (V, E) be a graph and v a vertex of G. Then

339 (6.6)
$$\alpha(G) = \max(1 + \alpha(G \setminus N[v]), \alpha(G \setminus (M(v) \cup \{v\})).$$

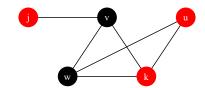
This rule states that if v is not in M, there exists an MIS I that $M(v) \notin I$. otherwise, there must be one of N(v) in the MIS ($local\ maximum\ rule$). Although this statement involves N(u), however, deriving this rule only requires information upto second neighbourhood of v. If w is in I, then none of $N(v) \cap N(w)$ is in I, then there must be one of node in the clique $N(v) \setminus N(w)$ in I ($local\ maximum\ rule$), since clique has at most one node in the MIS, by moving the occupied node to the interior, we obtain a "better" solution. In the following example, since $u \in N^2(v)$ and $N(v) \setminus N(u)$ is a clique, u is a mirror of v.



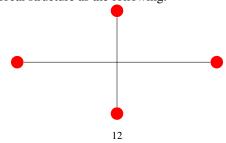
After contracting $N[v] \cup u$, v becomes an internal degree of freedom. Applying tensor compactification rule Eq. (6.2), the resulting rank 4 tropical tensor is

349 (6.7)
$$T_{juwk} = \begin{pmatrix} \begin{pmatrix} 1 & 2 \\ \cancel{1} & \cancel{2} \end{pmatrix}_{ju} & \begin{pmatrix} \cancel{1} & -\infty \\ 2 & -\infty \end{pmatrix}_{ju} \\ \begin{pmatrix} \cancel{1} & \cancel{2} \\ -\infty & -\infty \end{pmatrix}_{ju} & \begin{pmatrix} -\infty & -\infty \\ -\infty & -\infty \end{pmatrix}_{ju} \end{pmatrix}_{wk},$$

- where entries stroked through are removed by compactification. The corresponding polynomial tensor is
- 353 (6.8) $P_{juwk} = \begin{pmatrix} 1 + x_v & x_u + x_u x_v \\ / & / \end{pmatrix}_{ju} \begin{pmatrix} / & \\ x_j x_k & \end{pmatrix}_{ju} \\ \begin{pmatrix} / & \\ & \end{pmatrix}_{ju} \begin{pmatrix} & \\ & \end{pmatrix}_{ju} \\ w_k \end{pmatrix}.$
- One can see w, as a mirror of v does not appear in the maximum independent set after compactification.
- $S_{juwkv} = \{00001, 01001, 10010\}.$
- COROLLARY 6.5 (satellite rule). Let G be a graph, $v \in V$. A node $u \in N^2(v)$ is called satellite [14] of v, if there is some $u' \in N(v)$ such that $N[u'] \setminus N[v] = \{u\}$. The set of satellites of a node v is denoted by S(v), and we also use the notation $S[v] := S(v) \cup v$. Then
- 362 (6.10) $\alpha(G) = \max\{\alpha(G\setminus\{v\}), \alpha(G\setminus N[S[v]]) + |S(v)| + 1\}.$
- This rule can be capture by contracting $N[v] \cup S(v)$. In the following example, since $u \in N^2(v)$ and $w \in N(v)$ satisfies $N[w] \setminus N[v] = \{u\}$, u is a satellite of v.



- After contracting $N[v] \cup u$, both v and w become internal degrees of freedoms. Applying tensor compactification rule Eq. (6.2), the resulting rank 3 polynomial tensor is
- 367 (6.11) $P_{juk} = \begin{pmatrix} 1 + x_w + x_v & x_u + x_u x_v \\ x_j + x_w x_j & / \\ / & \\ / & \end{pmatrix}_{ju} .$
- By choosing one of the optimal configurations in each entry, we can see the satellite rule of either $v, u \in I$ or $v \notin I$ is satisfied.
- $371 \atop 372$ (6.12) $S_{juwkv} = \{\{00100, 00001\}, 10100, 01001\}.$
- 373 **6.2. gadget design.** $[JG: \times]$
- Suppose we have a local structure as the following.



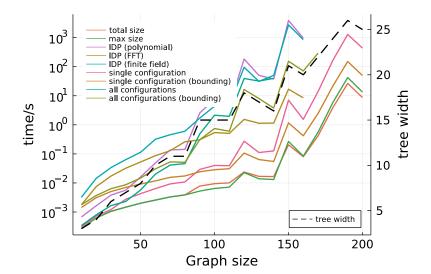


Figure 2: Benchmark results for computing different properties with different element types. The right axis is only for the dashed line.

Contract this local structure gives the tropical tensor

376 (6.13)
$$\begin{pmatrix} 0 & 1 \\ 1 & 2 \end{pmatrix} & \begin{pmatrix} 1 & -\infty \\ 2 & -\infty \end{pmatrix} \\ \begin{pmatrix} 1 & 2 \\ -\infty & -\infty \end{pmatrix} & \begin{pmatrix} 2 & -\infty \\ -\infty & -\infty \end{pmatrix}$$

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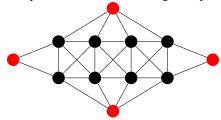
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385 386 The following gadget is equivalent to the above diagram up to a constant 2.



$$\begin{pmatrix}
\begin{pmatrix}
2 & 3 \\
3 & 4
\end{pmatrix} & \begin{pmatrix}
3 & 3 \\
4 & 4
\end{pmatrix} \\
\begin{pmatrix}
3 & 4 \\
2 & 3
\end{pmatrix} & \begin{pmatrix}
4 & 4 \\
3 & 4
\end{pmatrix}
\end{pmatrix}
\xrightarrow{\text{compactify, -2}}
\begin{pmatrix}
\begin{pmatrix}
0 & 1 \\
1 & 2
\end{pmatrix} & \begin{pmatrix}
1 & \cancel{1} \\
2 & \cancel{2}
\end{pmatrix}$$

We can see these two subgraphs produce exactly the same compact tensor. When we replace the original tensor with this gadget, the solution.

7. Benchmarks and case study. We run a sequetial program benchmark on CPU Intel(R) Core(TM) i5-10400 CPU @ 2.90GHz, and show the results bellow. Tensor network contraction is parallelizable. When the element type is immutable, one can just upload the data to GPU to enjoy the speed up.

8. Discussion. We introduced in the main text how to compute the independence polynomial, maximum independent set and optimal configurations, derived the backward rule for tropical tensor network to bound the search of solution space. Although many of these properties are global, we can encode it to different tensor element types as commutative semirings. The power of tensor network's is not limited to the indenepent set problem, in Appendix C we show how to map matching problem and k-coloring to a tensor network. Here, we want to discuss more from the programming perspective. We show some of the Julia language [3] implementations in Appendix A, you will find it being surprisingly short. What we need to do is just defining two operations ⊕ and ⊙ and two special elements 0 and 1. The style that we program is called generic programming, meaning one can feed different data types into a same program, and the program will compute the result with a proper performance. In C++, users 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 used in the main text can be inlined in an array. Furthermore, these inlined arrays can be upload to GPU devices for faster generic matrix multiplication implemented in CUDA.jl [2].

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element type	purpose
regular number	counting all indenepent sets
tropical number (Eq. (4.2))	finding the maximum independent set size
tropical number with counting (Eq. (4.2))	finding both the maximum independent set size and its degeneracy
tropical number with configurations (Eq. (5.2))	finding the maximum independent set size and one of the optimal configurations
tropical number with sets (Eq. (5.1))	finding the maximum independent set size and all optimal configurations
polynomial (Eq. (3.5))	computing the indenpendence polynomials exactly
truncated polynomial (Eq. (4.3))	counting the suboptimal independent sets
complex number	fitting the indenpendence polynomials with fast fourier transformation
finite field algebra Eq. (3.9)	fitting the indenpendence polynomials exactly using number theory

Table 1: Tensor element types used in the main text and their purposes.

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 449 001.

Appendix A. Technical guide.

- **OMEinsum** a package for the einsum function,
- 452 **OMEinsumContractionOrders** a package for finding the optimal contraction order for the 453 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,
- 459 **LightGraphs** a package providing graph utilities, like random regular graph generator,
- 460 **Polynomials** a package providing polynomial algebra and polynomial fitting,
- 461 **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.

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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
473
          using OMEinsum: NestedEinsum, flatten, getixs
474
         using LightGraphs
475
         using Random
476
477
          # generate a random regular graph of size 100, degree 3
478
          graph = (Random.seed!(2); LightGraphs.random_regular_graph(100, 3))
479
480
          # generate einsum code, i.e. the labels of tensors
481
          code = EinCode(([minmax(e.src,e.dst) for e in LightGraphs.edges(graph)]..., # labels for edge
482
               tensors
483
                          [(i,) for i in LightGraphs.vertices(graph)]...), ())
                                                                                       # labels for vertex
484
485
486
          # an einsum contraction without contraction order specified is called `EinCode`.
487
          \# an einsum contraction has contraction order (specified as a tree structure) is called `
488
489
          # assign each label a dimension-2, it will be used in contraction order optimization
490
          # `symbols` function extracts tensor labels into a vector.
491
          symbols(::EinCode{ixs}) where ixs = unique(Iterators.flatten(filter(x->length(x)==1,ixs)))
492
          symbols(ne::OMEinsum.NestedEinsum) = symbols(flatten(ne))
493
          size_dict = Dict([s=>2 for s in symbols(code)])
494
          # optimize the contraction order using KaHyPar + Greedy, target space complexity is 2^17
495
          optimized_code = optimize_kahypar(code, size_dict; sc_target=17, max_group_size=40)
496
         println("time/space complexity is $(OMEinsum.timespace_complexity(optimized_code, size_dict))")
497
498
          # a function for computing independence polynomial
499
         function independence_polynomial(x::T, code) where {T}
500
            xs = map(getixs(flatten(code))) do ix
501
                  # if the tensor rank is 1, create a vertex tensor.
502
                  # otherwise the tensor rank must be 2, create a bond tensor.
503
                 length(ix)==1 ? [one(T), x] : [one(T) one(T); one(T) zero(T)]
504
505
              # both `EinCode` and `NestedEinsum` are callable, inputs are tensors.
506
            code(xs...)
507
508
509
          ######## COMPUTING MAXIMUM INDEPENDENT SET SIZE AND ITS DEGENERACY ##########
510
511
          # using Tropical numbers to compute the MIS size and MIS degeneracy.
512
          using TropicalNumbers
513
         mis_size(code) = independence_polynomial(TropicalF64(1.0), code)[]
514
         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`.
515
516
517
          \verb|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)")
518
519
          ######## COMPUTING INDEPENDENCE POLYNOMIAL #########
520
521
          # using Polynomial numbers to compute the polynomial directly
522
          using Polynomials
523
         println("the independence polynomial is $(independence_polynomial(Polynomial([0.0, 1.0]),
524
525
               optimized_code)[])")
526
527
          # 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
528
529
530
         function independence_polynomial_fft(code; mis_size=Int(mis_size(code)[].n), r=3.0)
531
            \omega = \exp(-2im^*\pi/(mis\_size+1))
532
                     * collect(\omega .^ (0:mis_size))
533
             ys = [independence_polynomial(x, code)[] for x in xs]
          Polynomial(ifft(ys) ./ (r .^ (0:mis_size)))
```

```
535
536
          println("the independence polynomial (fft) is $(independence_polynomial_fft(optimized_code))")
537
538
          # using finite field algebra to compute the independence polynomial
539
          using Mods, Primes
540
          # two patches to ensure gaussian elimination works
541
          Base.abs(x::Mod) = x
542
         Base.isless(x::Mod{N}, y::Mod{N}) where N = mod(x.val, N) < mod(y.val, N)
543
544
          function independence_polynomial_finitefield(code; mis_size=Int(mis_size(code)[].n), max_order=1
545
546
             N = typemax(Int32) \# Int32 is faster than Int.
547
              YS = []
548
             local res
549
              for k = 1:max_order
550
                N = Primes.prevprime(N-one(N)) # previous prime number
551
                 # evaluate the polynomial on a finite field algebra of modulus `N'
552
                 rk = \_independance\_polynomial(Mods.Mod{N,Int32}, code, mis\_size)
553
                 push!(YS, rk)
554
                  if max_order==1
555
                     return Polynomial(Mods.value.(YS[1]))
556
                  elseif k != 1
557
                     ra = improved_counting(YS[1:end-1])
558
                      res = improved_counting(YS)
559
                     ra == res && return Polynomial(res)
560
                 end
561
              end
562
              @warn "result is potentially inconsistent."
563
             return Polynomial(res)
564
565
          function _independance_polynomial(::Type{T}, code, mis_size::Int) where T
566
            xs = 0:mis_size
567
            ys = [independence_polynomial(T(x), code)[] for x in xs]
568
             A = zeros(T, mis_size+1, mis_size+1)
569
             for j=1:mis_size+1, i=1:mis_size+1
570
               A[j,i] = T(xs[j])^{(i-1)}
             end
572
            A \ T.(ys) # gaussian elimination to compute ``A^{-1} y```
573
          end
574
          improved_counting(sequences) = map(yi->Mods.CRT(yi...), zip(sequences...))
575
576
         println("the independence polynomial (finite field) is $(independence_polynomial_finitefield())
577
               optimized code))")
578
579
          ######## FINDING OPTIMAL CONFIGURATIONS #########
580
581
          # define the config enumerator algebra
582
          struct ConfigEnumerator{N,C}
583
             data::Vector{StaticBitVector{N.C}}
584
          end
585
          \textbf{function} \ \ \text{Base.:+(x::ConfigEnumerator\{N,C\}, y::ConfigEnumerator\{N,C\})} \ \ \textbf{where} \ \ \{N,C\}
586
             res = ConfigEnumerator{N,C}(vcat(x.data, y.data))
587
              return res
588
          end
589
          \label{thm:config} \textbf{function} \ \ \textbf{Base.:*} (x::ConfigEnumerator\{L,C\}, \ y::ConfigEnumerator\{L,C\}) \ \ \textbf{where} \ \ \{L,C\}
590
             M. N = length(x.data). length(v.data)
591
              z = Vector{StaticBitVector{L,C}}(undef, M*N)
592
              for j=1:N, i=1:M
593
                 z[(j-1)*M+i] = x.data[i] .| y.data[j]
594
             end
595
             \textbf{return} \ \texttt{ConfigEnumerator}\{\texttt{L},\texttt{C}\}(\texttt{z})
596
          end
597
          598
599
          600
               staticfalses(StaticBitVector{N,C})])
601
602
          # enumerate all configurations if `all` is true, compute one otherwise.
603
          # a configuration is stored in the data type of `StaticBitVector`, it uses integers to represent
604
                bit strings.
605
          # `ConfigTropical` is defined in `TropicalNumbers`. It has two fields, tropical number `n` and
606
               optimal configuration `config`
607
          # `CountingTropical{T,<:ConfigEnumerator}` is a simple stores configurations instead of simple
608
```

```
609
          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))])
610
611
612
              N = length(vertex_index) # number of vertices
613
              C = TropicalNumbers._nints(N) # number of integers to store N bits
614
              xs = map(getixs(flatten(code))) do ix
615
                  T = all ? CountingTropical{Float64, ConfigEnumerator{N,C}} : ConfigTropical{Float64, N,
616
                C}
                   if length(ix) == 2
617
618
                       return [one(T) one(T); one(T) zero(T)]
619
                         = \mbox{TropicalNumbers.onehot(StaticBitVector{N,C}, vertex\_index[ix[{\color{red}1}]])}
620
621
622
623
                           [one(T), T(1.0, ConfigEnumerator([s]))]
                       else
624
                            [one(T), T(1.0, s)]
625
                       end
626
627
              end
628
             return code(xs...)
629
630
631
          println("one of the optimal configurations is $(mis_config(optimized_code; all=false)[].config)"
632
633
634
          \# enumerating configurations directly can be very slow (~15min), please check the bounding
635
639
          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 decribed 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 tensors.

Given a graph

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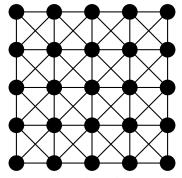
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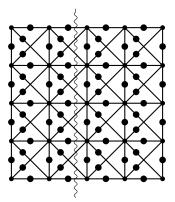
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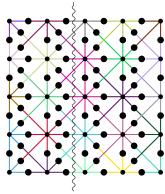
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Its traditional tensor network representation with δ tensors is



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 [5, 1] states that a problem quantified by monadic second order logic (MSO) on a graph with bounded tree width 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, that 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

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

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

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

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

and a tensor of rank 1 on the bond

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

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

C.2. k-Colouring. Let us use 3-colouring on the vertex as an example. We can define a 676 677 vertex tensor as

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

and an edge tensor as 680

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

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The number of possible colouring can be obtained by contracting this tensor network by 683 setting vertex tensor elements r_{ν} , g_{ν} and b_{ν} to 1. By designing generic types as tensor 684 elements, one should be able to get all possible colourings. It is straight forward to define 685

the k-colouring problem on edges hence we will not discuss the detailed construction here. 686