## SOLVING THE MAXIMUM INDEPENDANT SET PROBLEM BY GENERIC PROGRAMMING EINSUM NETWORKS \*

XXX<sup>†</sup> AND YYY<sup>‡</sup>

**Abstract.** Solving the maximum independent set size problem by mapping the graph to an einsum 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.

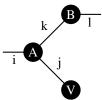
**Key words.** maximum independent set, einsum network

AMS subject classifications. 05C31, 14N07

2.1

**1. Introduction.** MIS problem is hard [7]. Branching algorithms can solve the MIS problem in  $1.1893^n n^{O(1)}$  time [16]. Previous dynamic programming approach [3] can reduce the complexity of computing to  $O(2^{tw(G)}tw(G)n)$ . A set is independent if and only if it is a clique in the graph's complement, so the two concepts are complementary. A set is independent if and only if its complement is a vertex cover. Therefore, the sum of the size of the largest independent set  $\alpha(G)$  and the size of a minimum vertex cover  $\beta(G)$  is equal to the number of vertices in the graph. It is related to hard spheres lattice gas model [1], and Rydberg hamiltonian [14].

In this work, we attack this problem by mapping it to an "einsum" network. The word "einsum" is a shorthand for Einstein's summation, however, modern einsum notation in program is actually invented by a group of programmers. Einstein's notation is originally proposed as a generalization to of multiplication between two matrices to the contraction between multiple tensors. Let A, B be two matrices, the matrix multiplication is defined as  $C_{ik} = \sum_j A_{ij} B_{jk}$ . It is denoted as  $C_i^k = A_i^j B_j^k$  in the Einstein's original notation, where the paired subscript and superscript j is a dummy index summed over. An example of tensor networks is  $C_i^l = A_{ij}^k B_k^l V^j$ . One can map a tensor network to a muti-graph with open edges by viewing a tensor in the expression on the right hand side as a vertex in a graph, a label pairing two tensors as an edge, and the remaining labels as open edges. We get the graphical notation as the following.

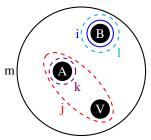


One can easily check a label in a tensor network representation appears precisely twice. Numpy programmers make a generalization to this notation by not restricting the number of times a label is used by tensors. For example,  $C_{ijk} = A_{jkm}B_{mil}V_{jm}$  is an einsum but not a tensor network. Here, all indices not appearing in the output are summed over, i.e. it represents  $C_{ijk} = \sum_{ml} A_{jkm}B_{mia}V_{jm}$ . Whether the index appear as a superscript or a subscript makes no sense now. The graphical representation of an einsum is a hypergraph, where an edge can be shared by a arbituary number of nodes.

Funding: ...

<sup>&</sup>lt;sup>†</sup>XXX (email, website).

<sup>&</sup>lt;sup>‡</sup>yyyyy (yyyy, email).



In the main text, we stick to the einsum notation rather than the tensor network notation, although one can easily translate an einsum network to the equivalent tensor network by adding  $\delta$  tensors (a generalization of identity matrix to higher order). We do not use the language of tensor network because it can sometime increase the contraction complexity of a graph. We will show an example in the appendix.

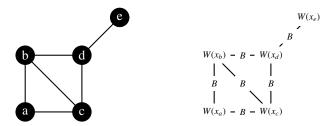


Figure 1: Mapping a graph to an einsum network.

**2. Independence polynomial.** Let us map the graph G into an einsum network, as shown in Fig. 1, by placing a rank one tensor of size 2 on vertex i

$$42 \quad (2.1) \qquad W(x_i)_{s_i} = \begin{pmatrix} 1 \\ x_i \end{pmatrix}_{s_i},$$

and a rank two tensor of size  $2 \times 2$  on edge (i, j)

35

36

38

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

- where a tensor index  $s_i$  is a boolean variable that being 1 if vertex i is in the independent set,
- 46 0 otherwise,  $x_i$  is a variable. We denote the contraction result of this einsum network as

47 (2.3) 
$$A(G,\{x_1,\ldots,x_n\}) = \sum_{s_1,s_2,\ldots,s_n=0}^{1} \prod_{i=1}^{n} W(x_i)_{s_i} \prod_{(i,j)\in E(G)} B_{s_i s_j}.$$

- 48 Here, the einsum runs over all possible vertex configurations and accumulates the product of
- 49 tensor elements to the output. Let  $x_i = x$  be the same variable, then the product over vertex
- tensors provides a factor  $x^k$ , where  $k = \sum_i s_i$  is the vertex set size, and the product over edge
- 51 tensors provides a factor 0 for configurations not being an independent set. The contraction
- of this einsum network gives the independence polynomial [2, 6] of G

53 (2.4) 
$$I(G, x) = \sum_{k=1}^{\alpha(G)} a_k x^k,$$

where  $a_k$  is the number of independent sets of size k in G, and  $\alpha(G)$  is the maximum independent set size. By mapping the independence polynomial solving problem to the einsum network contraction, one can take the advantage of recently developed techniques in tensor network based quantum circuit simulations [5, 13], 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  $O(2^{tw(G)})$ , where tw(G) is the treewidth of G. [11] The pairwise tensor contraction also makes it possible to utilize fast basic linear algebra subprograms (BLAS) functions for certain tensor element types.

Before contracting the einsum 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 relation must hold for arbitrary three elements  $a, b, c \in R$ .

```
(a \oplus b) \oplus c = a \oplus (b \oplus c)
                                                                           ▶ commutative monoid ⊕ with identity 0
70
                              a \oplus \mathbb{O} = \mathbb{O} \oplus a = a
71
                                    a \oplus b = b \oplus a
72
73
                   (a \odot b) \odot c = a \odot (b \odot c)
                                                                           ▶ commutative monoid ⊙ with identity 1
74
                              a \odot \mathbb{1} = \mathbb{1} \odot a = a
75
                                    a \odot b = b \odot a
76
77
                a \odot (b \oplus c) = a \odot b + a \odot c
                                                                           > left and right distributive
78
79
                (a \oplus b) \odot c = a \odot c \oplus b \odot c
80
                             a \odot 0 = 0 \odot a = 0
81
```

In the rest of this paper, 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 einsum network programming generic [15].

**2.1. 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  $a_0 + a_1x + \ldots + a_kx^k$  as a vector  $(a_0, a_1, \ldots, a_k) \in \mathbb{R}^k$ , 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

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

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

$$0 = (),$$

$$1 = (1).$$

By contracting the einsum 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. The only problem of this method is it suffers from a space overhead that propotional to the maximum independant 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.

**2.2.** The fitting and Fourier transformation approaches. Let  $m = \alpha(G)$  be the maximum independent set size and X be a set of m + 1 random real numbers, e.g.  $\{0, 1, 2, ..., m\}$ . We compute the einsum contraction for each  $x_i \in X$  and obtain the following relations

$$a_0 + a_1 x_1 + a_1 x_1^2 + \dots + a_m x_1^m = y_0$$

$$a_0 + a_1 x_2 + a_2 x_2^2 + \dots + a_m x_2^m = y_1$$

$$\dots$$

$$a_0 + a_1 x_m + a_2 x_m^2 + \dots + a_m x_m^m = y_m$$

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

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

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

114 (2.8) 
$$\begin{pmatrix} 1 & r\omega & r^2\omega^2 & \dots & r^m\omega^m \\ 1 & r\omega^2 & r^2\omega^4 & \dots & r^m\omega^{2m} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & r\omega^m & r^2\omega^{2m} & \dots & r^m\omega^{m^2} \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_m \end{pmatrix} = \begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_m \end{pmatrix}$$

Let us rearange the factors  $r^j$  to  $a_j$ , the matrix on left side is exactly the a descrete 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 independant set size region ( $\omega < 1$ ) and high independant set size region ( $\omega > 1$ ).

**2.3.** The finite field algebra approach. It is possible to compute the independence polynomials exactly using 64 bit integers types only, even when the factors are larger than that can be represented by 64 bit integers. We achieve this by designing a finite field algebra GF(p)

$$x \oplus y = x + y \pmod{p},$$

$$x \odot y = xy \pmod{p},$$

$$0 = 0,$$

$$126$$

$$1 = 1.$$

In a finite field algebra, we have the following observations

- 1. One can still use Gaussian elimination [4] to solve a linear equation. This is because a field has the property that the multiplicative inverse exists for any non-zero value. The multiplicative inverse here can be computed with the extended Euclidean algorithm.
- 2. Given the remainders of a larger integer x over a set of coprime 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 even though its bit width is larger than the register size.

With these observations, we developed Algorithm 2.1 to compute independent polynomial exactly without introducing space overheads. In the algorithm, except the computation of chinese remainder theorem, all computations are done with integers with fixed width W.

## Algorithm 2.1 Compute independence polynomial exactly without integer overflow

```
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 \land p \leq 2^W compute the tensor network 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{chines\_remainder}(A_P,A_p) if A_P=A_{P\times p} then \mathrm{return}\,A_P; // converged end P=P\times p
```

3. Computing maximum independent set size and its corresponding degeneracy and configurations. Obtaining the maximum independent set size and its degeneracy can be computational more efficient. Let  $x = \infty$ , then the independence polynomial becomes

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

128 129

130

131

132

133

134

135

136

137

138

139

140 141

150

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

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

$$144 \quad (3.2)$$

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

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

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

In the program, we only store the power x and the corresponding factor  $a_x$  that initialized to 1.

This algebra is consistent with the one we derived in [9] that uses the tropical tensor network for solving spin glass ground states. If one is only interested in obtaining  $\alpha(G)$ , he can drop

the factor parts, then the algebra of x becomes the max-plus tropical algebra [10, 12].

One may also want to obtain all ground state configurations, it can be achieved replacing

51 the factors  $a_x$  with a set of bit strings  $s_x$ . We design a new element type that having algebra

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

$$152 \quad (3.3)$$

$$s_{x} \infty^{x} \odot s_{y} \infty^{y} = \{\sigma + \tau | \sigma \in s_{x}, \tau \in s_{y}\} \infty^{x+y},$$

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

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

One can easily check that this replacement does not change the fact that the algebra is a commutative semiring. We first initialize the bit strings of the variable x in the vertex tensor to a vertex index i dependent onehot vector  $x_i = e_i$ , then we contract the tensor network. The resulting object will give us the set of all optimal configurations. By slightly modifying the above algebra, it can also be used to obtain just a single configuration to save computational effort. We leave this as an exercise for readers. This algorithm is parallelizable.

3.1. bounding the enumeration space. When we try to implement the above algebra for enumerating configurations, we find the space overhead is larger than than we have expected. It stores more than nessesary intermedite configurations. To speed up the computation, we use  $\alpha(G)$  that much easier to compute for bounding. 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 nonzero gradient) and boolean false otherwise. Finally, we perform masked matrix multiplication using the new element type with the above algebra for obtaining all configurations. To compute the masks, we "back propagate" the masks step by step through contraction process using the cached intermediate tensors. 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 nonzero gradi-
- ent). Let the mask for C being  $\overline{C}$ , the backward rule for gradient masks reads

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

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 the einsum of two tensors by replacing the matrix multiplication between  $C^{\circ -1} \circ \overline{C}$  and  $B^T$  by an einsum.

**4. Counting maximal independent sets.** Let us denote the neighbor 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 is no such vertex v that  $N[v] \cap I_m = \emptyset$ . Let us modify the einsum network for computing independence polynomial to count maximal independent sets. We define a tensor on N[v] to

190 capture this property

191 (4.1) 
$$T(x)_{s_1, s_2, \dots, s_{|N(v)|}, s_v} = \begin{cases} s_v x & s_1 = s_2 = \dots = s_{|N(v)|} = 0, \\ 1 - s_v & otherwise. \end{cases}$$

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

$$T(x) = \begin{pmatrix} 0 & 1 \\ 1 & 1 \\ x & 0 \\ 0 & 0 \end{pmatrix}.$$

We do the same computation as independence polynoimal, the coefficients of resulting polynomial gives the counting of maximal independent sets. In many sparse graphs, this tensor network contraction approach is much faster than computing the maximal cliques of its complement and use Bron Kerbosch algorithms for finding maximum cliques. However, the treewidth of this new tensor network is larger than the one for independence polynomial because it can not utilize some structures of the original graph, while the original tensor network can be trivially reduced to this one. We will use an example in the appendix to show why this tensor network is harder to contract.

**5. Automated branching.** Branching rules can be automatically discovered by contracting the tropical einsum network for a subgraph  $R \subseteq G$ . Let us denote the resulting tropical tensor of rank |C| as A, where C is the set of boundary vertices defined as  $C := \{c | c \in R \land c \in G \setminus R\}$  and |C| the size of C. Each tensor entry  $A_{\sigma}$  is a local maximum independant set size with a fixed boundary configuration  $\sigma \in \{0,1\}^{|C|}$  by marginalizing the inner degrees of freedom. If we are only interested in finding a single maximum independent set rather than enumerating all possible solutions, this tensor can be further "compresed" by setting some entries to tropical zero. Let us define a relation of *less restrictive* as

$$\frac{212}{213} \quad (5.1) \qquad (\sigma_a < \sigma_b) := (\sigma_a \neq \sigma_b) \land (\sigma_a \leq^{\circ} \sigma_b)$$

where  $\leq^{\circ}$  is the Hadamard less or equal operations.

Definition 5.1. A tensors A is MIS-compact if are no two nonzero entries of it that one is "better" than another, where an entry  $A_{\sigma_a}$  is "better" than  $A_{\sigma_b}$  if

$$\frac{217}{8} \quad (5.2) \qquad (\sigma_a < \sigma_b) \land (A_{\sigma_a} \ge A_{\sigma_b}).$$

If we remove such  $A_{\sigma_b}$ , the contraction over the whole graph is guaranted 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. 2 (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 set  $A_{\sigma_b}$  to tropical zero safely.

THEOREM 5.2 (). A MIS-compact tropical tensor is optimal, i.e. none of its none zero entries can be removed without accessing global information.

*Proof.* Let use prove it by showing  $\forall \sigma$  in a MIS-compact tropical tensor for a subgraph R, there exists a graph G that  $R \subseteq G$  and  $\sigma$  is the only boundary configuration that produces the maximum independent set. i.e. no tensor entry can be removed without knowledge about  $G \setminus R$ . Let A be a tropical tensor, and an entry of it being  $A_{\sigma}$ , where  $\sigma$  is the bounary configuration. Let us construct a graph G such that for a vertex  $v \in C$ , if  $\sigma_v = 1$ ,

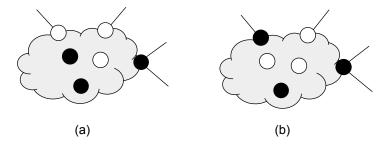
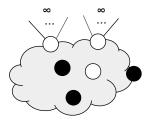


Figure 2: Two configurations with the same local independent size  $A_{\sigma_a} = A_{\sigma_b} = 3$  and different boundary configurations (a)  $\sigma_a = \{001\}$  and (b)  $\sigma_b = \{101\}$ , where black nodes are 1s (in the independent set) and white nodes are 0s (not in the independent set).

 $\alpha(N[v] \cap (G \setminus R)) = 0$ , otherwise,  $\alpha(N[v] \cap (G \setminus R)) = \infty$ , meanwhile, for any  $v, w \in C$ , 233  $N[v] \cap N[w] = \emptyset$ . The simplest construction is connecting vertices that  $\sigma_v = 0$  with infinite 234 many mutually disconnected vertices as illustrated in the following graph.



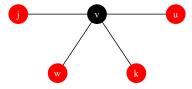
2.50

Then we have the maximum independent set size with boundary configuration  $\sigma$  being  $\alpha(G,\sigma)=\infty(|C|-|\sigma|)+A_\sigma$ , where  $|\sigma|$  is defined as the number of 1s in  $\sigma$ . Let us assume there exists another configuration  $\tau$  that generating the same or even better maximum independent set size  $\alpha(G,\tau)\geq\alpha(G,\sigma)$ . Then we have  $\tau<\sigma$ , otherwise it will suffer from infinite punishment from  $G\backslash R$ . For such a  $\tau$ , we have  $A_\tau< A_\sigma$ , otherwise  $A_\sigma< A_\tau$  contradicts with A being MIS-compact. Finally, we have  $\alpha(G,\tau)=\infty(|C|-|\sigma|)+A_\tau<\alpha(G,\sigma)$ , which contradicts with our preassumtion. Such  $\tau$  does not exist and  $\sigma$  is the only boundary configuration that  $\alpha(G)=\alpha(G,\sigma)$ .

**5.1.** The tensor network compression detects branching rules automatically. In the following, we are going to show tropical tensor networks with least restrictive principle can automatically discover branching rules. We denote the effective branching number of contracting the local degrees of freedoms as  $|\{A_{\sigma} \neq 0 | \sigma \in \{0,1\}^{|C|}\}|/2^{|R|}$ . It is the effective degree of freedoms per vertex in R.

COROLLARY 5.3. 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  $A_{\sigma}$  corresponds to a locally maximized independant set size with fixed boundary configuration  $\sigma \in \{0,1\}^{|N(\nu)|}$ . If the boundary configuration is a bit string of 0s,  $\sigma_{\nu}$  will takes value 1 to maximize the local independant set size.



After contracting N[v], v becomes an internal degree of freedom. Applying tensor com-255 pression rule Eq. (5.2), the resulting rank 4 tropical tensor is

257 (5.3) 
$$T_{juwk} = \begin{pmatrix} 1 & -\infty \\ -\infty & 2 \end{pmatrix}_{ju} & \begin{pmatrix} -\infty & 2 \\ 2 & 3 \end{pmatrix}_{ju} \\ \begin{pmatrix} -\infty & 2 \\ 2 & 3 \end{pmatrix}_{ju} & \begin{pmatrix} 2 & 3 \\ 3 & 4 \end{pmatrix}_{ju} \end{pmatrix}_{wk}.$$

2.59

261

262

263

264

266

268

269

270

271

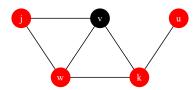
The effective branching value is  $11^{1/5} \approx 1.6154$ , which is larger than the branching number  $\tau(1,5) \approx 1.3247$ . It does not mean the tropical tensor does not find all the branches, 260 if we contract  $N^2[v]$ .

COROLLARY 5.4 (mirror rule). For some  $v \in V$ , a node  $u \in N^2(v)$  is called mirror of v, if  $N(v)\setminus N(u)$  is a clique. We denote the set of of a node v mirrors [3] by M(v). Let G=(V,E)be a graph and v a vertex of G. Then

265 (5.4) 
$$\alpha(G) = \max(1 + \alpha(G \setminus N[v]), \alpha(G \setminus (M(v) \cup \{v\})).$$

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). 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 occuppied 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.



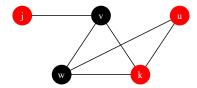
After contracting  $N[v] \cup u$ , v becomes an internal degree of freedom. Applying tensor 272 compression rule Eq. (5.2), the resulting rank 4 tropical tensor is

In this case, the effective branching number is  $3^{1/5} \approx 1.2457$ , which is smaller than the 276 branching number  $\tau(4,2) = 1.2721$  by simply applying the mirror rule. 277

Corollary 5.5 (satellite rule). Let G be agraph  $v \in V$ . A node  $u \in N^2(v)$  is called 278 satellite [8] of v, if there is some  $u' \in N(v)$  such that  $N[u'] \setminus N[v] = \{u\}$ . The set of satellites of

281 (5.6) 
$$\alpha(G) = \max\{\alpha(G\setminus\{v\}), \alpha(G\setminus N[S[v]]) + |S(v)| + 1\}.$$

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 compression rule Eq. (5.2), the resulting rank 3 tropical tensor is

286 (5.7) 
$$T_{juk} = \begin{pmatrix} \begin{pmatrix} 1 & 2 \\ 2 & -\infty \end{pmatrix}_{ju} \\ \begin{pmatrix} -\infty & -\infty \\ -\infty & -\infty \end{pmatrix}_{ju} \\ \end{pmatrix}_{k}.$$

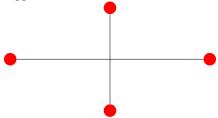
294

295

298

There are 3 nonzero entries. The internal configurations of entry T(j=1,u=0,k=0)=2 is (v=0,w=1), that of entry T(j=0,u=1,k=0)=2 is (v=1,w=0), and that of entry T(j=0,u=0,k=0)=1 is (v=1,w=0) or (v=0,w=1). For entry T(j=0,u=0,k=0)=1, we post-select the internal degree of freedom as (v=0,w=1). Then we can see the satellite rule either  $v,u\in I$  or  $v\notin I$  is satisfied. In this case, the effective branching number is  $3^{1/5}\approx 1.2457$ .

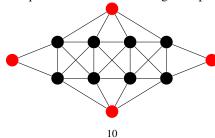
**5.2.** gadget design. Suppose we have a local structure as the following.



Contract this local structure gives the tropical tensor

296 (5.8) 
$$\begin{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 2 \end{pmatrix} & \begin{pmatrix} 1 & -\infty \\ 2 & -\infty \end{pmatrix} \\ \begin{pmatrix} 1 & 2 \\ -\infty & -\infty \end{pmatrix} & \begin{pmatrix} 2 & -\infty \\ -\infty & -\infty \end{pmatrix} \end{pmatrix}.$$

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



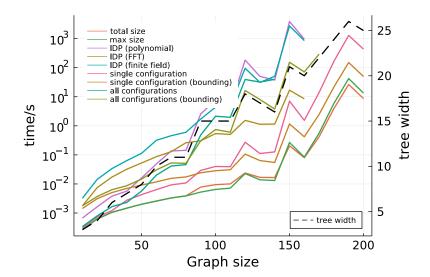


Figure 3: Benchmark results for computing different properties with different element types.

We can

301

302

303

304

305

306

307

308

309

310 311

312

313

314

315 316

317

318

319

320

**6. benchmarks.** We run a sequetial program benchmark on CPU Intel(R) Core(TM) i5-10400 CPU @ 2.90GHz, and show the results bellow.

7. discussion. We introduced in the main text how to compute the independence polynomial, maximum independent set and optimal configurations. It is interesting that although these properties are global, they can be solved by designing different element types that having two operations  $\oplus$  and  $\odot$  and two special elements  $\mathbb O$  and  $\mathbb 1$ . One thing in common is that they all defines a commutative semiring. Here, we want the  $\oplus$  and  $\odot$  operations being commutative because we do not want the contraction result of an einsum network to be sensitive to the contraction order. We show most of the implementation in Appendix A. It is supprisingly short. The style that we program is called generic programming, it is about writing a single copy of code, feeding different types into it, and the program computing the result with a proper performance. It is language dependent feature. If someone want to implement this algorithm in python, one has to rewrite the matrix multiplication for different element types in C and then export the interface to python. In C++, users can use templates for such a purpose. In our work, 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, tropical number, tropical number with counting/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.

321 REFERENCES

element type	purpose
regular number	counting all indenepent sets
tropical number	finding the maximum independent set size
tropical number with counting	finding both the maximum independent set size and its degeneracy
tropical number with configuration	finding the maximum independent set size and one of the optimal configurations
tropical number with multiple configurations	finding the maximum independent set size and all optimal configurations
polynomial	computing the indenpendence polynomials exactly
complex number	fitting the indenpendence polynomials with fast fourier transformation
finite field algebra	fitting the indenpendence polynomials exactly using number theory

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

- J. C. Dyre, Simple liquids' quasiuniversality and the hard-sphere paradigm, Journal of Physics: Condensed
   Matter, 28 (2016), p. 323001.
- 324 [2] G. M. Ferrin, Independence polynomials, (2014).

327

328

329

330 331

332

333

334

335

336

337

338

339 340

341

342 343 344

347

348

349

350

351

352

- 325 [3] F. V. Fomin and P. Kaski, Exact exponential algorithms, Communications of the ACM, 56 (2013), pp. 80–88.
- 326 [4] G. H. GOLUB AND C. F. VAN LOAN, Matrix computations, vol. 3, JHU press, 2013.
  - [5] J. Gray and S. Kourtis, Hyper-optimized tensor network contraction, Quantum, 5 (2021), p. 410, https://doi.org/10.22331/q-2021-03-15-410, https://dx.doi.org/10.22331/q-2021-03-15-410.
  - [6] N. J. A. HARVEY, P. SRIVASTAVA, AND J. VONDRÁK, Computing the independence polynomial: from the tree threshold down to the roots, 2017, https://arxiv.org/abs/1608.02282.
  - [7] J. Hastad, Clique is hard to approximate within n/sup 1-/spl epsiv, in Proceedings of 37th Conference on Foundations of Computer Science, IEEE, 1996, pp. 627–636.
  - [8] J. KNEIS, A. LANGER, AND P. ROSSMANITH, A fine-grained analysis of a simple independent set algorithm, in IARCS Annual Conference on Foundations of Software Technology and Theoretical Computer Science, Schloss Dagstuhl-Leibniz-Zentrum für Informatik, 2009.
  - [9] J.-G. Liu, L. Wang, and P. Zhang, Tropical tensor network for ground states of spin glasses, Physical Review Letters, 126 (2021), https://doi.org/10.1103/physrevlett.126.090506, http://dx.doi.org/10.1103/ PhysRevLett.126.090506.
  - [10] D. Maclagan and B. Sturmfels, Introduction to tropical geometry, vol. 161, American Mathematical Soc., 2015, http://www.cs.technion.ac.il/~janos/COURSES/238900-13/Tropical/MaclaganSturmfels.pdf.
  - [11] I. L. Markov and Y. Shi, Simulating quantum computation by contracting tensor networks, SIAM Journal on Computing, 38 (2008), p. 963–981, https://doi.org/10.1137/050644756, http://dx.doi.org/10.1137/ 050644756.
  - [12] C. Moore and S. Mertens, The nature of computation, OUP Oxford, 2011.
- [13] F. Pan and P. Zhang, Simulating the sycamore quantum supremacy circuits, 2021, https://arxiv.org/abs/2103.
   03074.
  - [14] H. PICHLER, S.-T. WANG, L. ZHOU, S. CHOI, AND M. D. LUKIN, Computational complexity of the rydberg blockade in two dimensions, arXiv preprint arXiv:1809.04954, (2018).
  - [15] A. A. Stepanov and D. E. Rose, From mathematics to generic programming, Pearson Education, 2014.
    - [16] M. XIAO AND H. NAGAMOCHI, Exact algorithms for maximum independent set, Information and Computation, 255 (2017), p. 126–146, https://doi.org/10.1016/j.ic.2017.06.001, http://dx.doi.org/10.1016/j.ic.2017.06.001.

## Appendix A. Technical guide.

**OMEinsum** a package for einsum,

353

354 355

356

357

358

359

360

361

363

364

365

366

367

370

372373

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

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

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

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

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

Polynomials a package providing polynomial algebra and polynomial fitting,

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

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

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

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

```
using OMEinsum, OMEinsumContractionOrders
          using OMEinsum: NestedEinsum, flatten, getixs
         using LightGraphs
378
          using Random
          # generate a random regular graph of size 100, degree 3
          graph = (Random.seed!(2); LightGraphs.random_regular_graph(100, 3))
383
          # generate einsum code, i.e. the labels of tensors
384
         code = EinCode(([minmax(e.src,e.dst) for e in LightGraphs.edges(graph)]..., # labels for edge
385
               tensors
386
                          [(i,) for i in LightGraphs.vertices(graph)]...), ())
                                                                                      # labels for vertex
387
               tensors
388
389
          # an einsum contraction without contraction order specified is called `EinCode`,
390
         # an einsum contraction has contraction order (specified as a tree structure) is called
391
               NestedEinsum
392
          # assign each label a dimension-2, it will be used in contraction order optimization
393
          # `symbols` function extracts tensor labels into a vector.
394
          symbols(::EinCode{ixs}) where ixs = unique(Iterators.flatten(filter(x->length(x)==1,ixs)))
395
          symbols(ne::OMEinsum.NestedEinsum) = symbols(flatten(ne))
396
          size_dict = Dict([s=>2 for s in symbols(code)])
          # optimize the contraction order using KaHyPar + Greedy, target space complexity is 2^17
397
398
          optimized_code = optimize_kahypar(code, size_dict; sc_target=17, max_group_size=40)
399
         println("time/space complexity is $(OMEinsum.timespace_complexity(optimized_code, size_dict))")
400
401
          # a function for computing independence polynomial
402
          function independence_polynomial(x::T, code) where {T}
403
             xs = map(getixs(flatten(code))) do ix
404
                  # if the tensor rank is 1, create a vertex tensor.
405
                  # otherwise the tensor rank must be 2, create a bond tensor.
406
                  length(ix)==1 ? [one(T), x] : [one(T) one(T); one(T) zero(T)]
407
              end
408
              # both `EinCode` and `NestedEinsum` are callable, inputs are tensors.
409
             code(xs...)
410
          end
411
412
          ######## COMPUTING MAXIMUM INDEPENDENT SET SIZE AND ITS DEGENERACY #########
413
414
          # using Tropical numbers to compute the MIS size and MIS degeneracy.
```

```
415
          using TropicalNumbers
416
          mis_size(code) = independence_polynomial(TropicalF64(1.0), code)[]
417
          println("the maximum independent set size is $(mis_size(optimized_code).n)")
418
          # A `CountingTropical` object has two fields, tropical field `n` and counting field `c`.
419
          \label{eq:mis_count} \verb| mis_count(code) = independence_polynomial(CountingTropical\{Float64,Float64\}(1.0,\ 1.0),\ code)[]|
420
          println("the degeneracy of maximum independent sets is $(mis_count(optimized_code).c)")
421
422
          ######### COMPUTING INDEPENDENCE POLYNOMIAL ##########
423
424
          # using Polynomial numbers to compute the polynomial directly
425
          using Polynomials
426
          println("the independence polynomial is $(independence_polynomial(Polynomial([0.0, 1.0]),
427
               optimized_code)[])")
428
429
          # using fast fourier transformation to compute the independence polynomial,
430
          \# here we chose r>1 because we care more about configurations with large independent set sizes
431
432
          using FFTW
433
          434
            \omega = \exp(-2im^*\pi/(mis\_size+1))
435
            xs = r .* collect(\omega .^ (0:mis_size))
436
            ys = [independence_polynomial(x, code)[] for x in xs]
437
            Polynomial(ifft(ys) ./ (r .^ (0:mis_size)))
438
439
          println("the independence polynomial (fft) is $(independence_polynomial_fft(optimized_code))")
440
441
          # using finite field algebra to compute the independence polynomial
442
          using Mods, Primes
443
          # two patches to ensure gaussian elimination works
444
          Base.abs(x::Mod) = x
445
          Base.isless(x::Mod{N}, y::Mod{N}) where N = mod(x.val, N) < mod(y.val, N)
446
447
          function independence_polynomial_finitefield(code; mis_size=Int(mis_size(code)[].n), max_order=1
448
449
              N = typemax(Int32) # Int32 is faster than Int.
450
             YS = []
451
             local res
452
              for k = 1:max_order
453
                N = Primes.prevprime(N-one(N)) # previous prime number
454
                  # evaluate the polynomial on a finite field algebra of modulus `N'
455
                 rk = _independance_polynomial(Mods.Mod{N,Int32}, code, mis_size)
456
                  push!(YS, rk)
457
                  if max_order==1
458
                     return Polynomial(Mods.value.(YS[1]))
459
                  elseif k != 1
460
                     ra = improved counting(YS[1:end-1])
461
                      res = improved counting(YS)
462
                      ra == res && return Polynomial(res)
463
                 end
464
              end
465
             @warn "result is potentially inconsistent."
466
             return Polynomial(res)
467
          end
468
          \label{thm:code} \textbf{function} \ \_ independance\_polynomial(::Type\{T\}, \ code, \ mis\_size::Int) \ \textbf{where} \ T
469
            xs = 0:mis_size
470
            ys = [independence_polynomial(T(x), code)[] for x in xs]
471
            A = zeros(T, mis_siz_{e+1}, mis_siz_{e+1})
472
            for j=1:mis_size+1, i=1:mis_size+1
473
               A[j,i] = T(xs[j])^{(i-1)}
474
             end
475
            A \ T.(ys) # gaussian elimination to compute ``A^{-1} y```
476
477
          improved_counting(sequences) = map(yi->Mods.CRT(yi...), zip(sequences...))
478
479
          println("the independence polynomial (finite field) is $(independence_polynomial_finitefield(
480
               optimized_code))")
481
482
          ######## FINDING OPTIMAL CONFIGURATIONS ##########
483
484
          # define the config enumerator algebra
485
          struct ConfigEnumerator{N,C}
486
             data::Vector{StaticBitVector{N,C}}
487
488
          function Base.:+(x::ConfigEnumerator{N,C}, y::ConfigEnumerator{N,C}) where {N,C}
```

```
489
              res = ConfigEnumerator{N,C}(vcat(x.data, y.data))
490
              return res
491
          end
492
          \label{thm:config} \textbf{function} \ \ \textbf{Base.:*} (x::ConfigEnumerator\{L,C\}, \ y::ConfigEnumerator\{L,C\}) \ \ \textbf{where} \ \ \{L,C\}
493
              M, N = length(x.data), length(y.data)
494
              z = Vector{StaticBitVector{L,C}}(undef, M*N)
495
              for j=1:N, i=1:M
496
                  z[(j-1)*M+i] = x.data[i] .| y.data[j]
497
              end
498
              \textbf{return} \ \texttt{ConfigEnumerator}\{\texttt{L},\texttt{C}\}(\texttt{z})
499
          end
500
          Base.zero(::Type\{ConfigEnumerator\{N,C\}\}) \ \ \textbf{where} \ \{N,C\} = ConfigEnumerator\{N,C\}(StaticBitVector\{N,C\}\}) 
501
502
          503
                staticfalses(StaticBitVector{N,C})])
504
505
          # enumerate all configurations if `all` is true, compute one otherwise.
506
          # a configuration is stored in the data type of `StaticBitVector`, it uses integers to represent
507
508
          # `ConfigTropical` is defined in `TropicalNumbers`. It has two fields, tropical number `n` and
509
               optimal configuration `config`
510
            `CountingTropical{T,<:ConfigEnumerator}` is a simple stores configurations instead of simple
                counting
512
          function mis_config(code; all=false)
513
              # map a vertex label to an integer
514
              vertex_index = Dict([s=>i for (i, s) in enumerate(symbols(code))])
515
              N = length(vertex_index) # number of vertices
516
              C = TropicalNumbers._nints(N) # number of integers to store N bits
              xs = map(getixs(flatten(code))) do ix
518
                  T = all ? CountingTropical{Float64, ConfigEnumerator{N,C}} : ConfigTropical{Float64, N,
               C}
520
                  if length(ix) == 2
521
                      return [one(T) one(T); one(T) zero(T)]
522
523
                      s = TropicalNumbers.onehot(StaticBitVector{N,C}, vertex_index[ix[1]])
524
                          [one(T), T(1.0, ConfigEnumerator([s]))]
526
                          [one(T), T(1.0, s)]
                      end
528
529
                  end
530
              end
531
             return code(xs...)
532
          end
533
534
          println("one of the optimal configurations is $(mis_config(optimized_code; all=false)[].config)"
535
536
537
          # enumerating configurations directly can be very slow (~15min), please check the bounding
538
                version in our Github repo
          println("all optimal configurations are $(mis_config(optimized_code; all=true)[].c)")
548
```

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 <a href="https://github.com/Happy-Diode/NoteOnTropicalMIS">https://github.com/Happy-Diode/NoteOnTropicalMIS</a>.

## Appendix B. When tensor network is worse than einsum network.

Given a graph

541

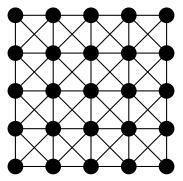
542

543

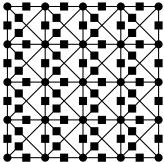
544

545

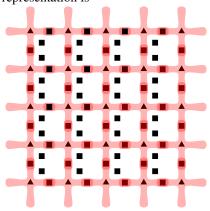
546



Its tensor network representation is



Once we represent a  $\delta$  tensor as a general tensor, the complexity of this contraction is  $\approx 2^{2L}$ . Its einsum network representation is



Appendix C. matching polynomial. One can generalize the generic einsum network for solving another #P-complete problem, the matching polynomials. A match polynomial of a graph G is defined as

554 (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.

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

558 (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

561 (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  $v \to w$  to label tensors.