SOLVING THE INDEPENDENT SET PROBLEM BY GENERIC PROGRAMMING EINSUM NETWORKS *

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Abstract. This paper is about solving the independent set problem by eincoding this problem 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. We also show how to analyse the local properties of a graph by contracting an open einsum network.

Key words. maximum independent set, einsum network

AMS subject classifications. 05C31, 14N07

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 [12], 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 [23], 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 $O(2^{tw(G)} tw(G) n)$. 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 [17], but also for its close relation with physical applications like hard spheres lattice gas model [6], and Rydberg hamiltonian [20]. 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 "einsum" 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. Einsum networks.

Einstein's notation is originally proposed 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 $C_{ik} = \sum_j A_{ij} B_{jk}$. In Einstein's notation, it 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 tensor network [18]. A tensor network can be represented as a mutigraph with open edges by viewing a tensor as a vertex, a label pairing two tensors as

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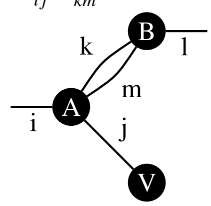
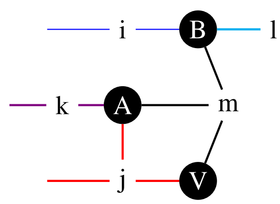
an edge, and the remaining unpaired labels as open edges.

Example 1. A tensor networks $C^l_i = A^{km}_{ij} B^l_{km} V^j$ has the following multigraph representation.



Einsum network is a generalization of tensor network 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 sum-product network or factor graph [4] in some contexts. The graphical representation of an einsum 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 an einsum 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 einsum notation rather than the tensor network notation. As a note to those who are more familiar with tensor network representation, although one can easily translate an einsum network to the equivalent 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, 11] of G to an einsum network. Independence polynomial is an important graph polynomial that contains the counting information of an independent set problem. It is defined as

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

where a_k is the number of independent sets of size k in G, and $\alpha(G)$ is the maximum independent set size. We encode this polynomial to an einsum network by placing a rank one tensor of size 2 parametrized by x_i on a vertex i

$$W(x_i)_{s_i} = \begin{pmatrix} 1 \\ x_i \end{pmatrix}_{s_i}, \tag{3.2}$$

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

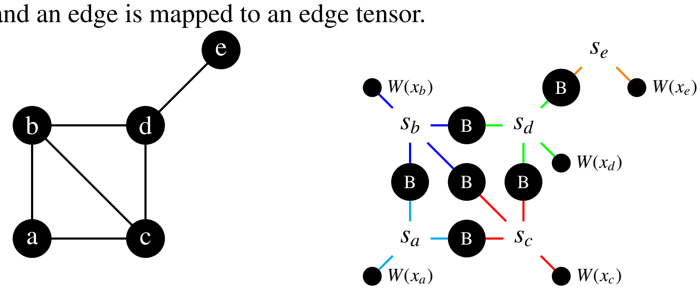
$$B_{s_i s_j} = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}_{s_i s_j}, \tag{3.3}$$

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 an einsum network gives

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

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 an einsum network is one can take the advantage of recently developed techniques in tensor network based quantum circuit simulations [10, 19], where people evaluate an einsum 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 an einsum hypergraph, while the line graph of an einsum hypergraph corresponds to the original graph G that we mapped from. [16] 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.

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



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

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

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

$$
\begin{aligned}
(a \oplus b) \oplus c = a \oplus (b \oplus c) & \qquad \triangleright \text{ commutative monoid } \oplus \text{ with identity } \mathbb{0} \\
a \oplus \mathbb{0} = \mathbb{0} \oplus a = a & \\
a \oplus b = b \oplus a & \\
\\
(a \odot b) \odot c = a \odot (b \odot c) & \qquad \triangleright \text{ commutative monoid } \odot \text{ with identity } \mathbb{1} \\
a \odot \mathbb{1} = \mathbb{1} \odot a = a & \\
a \odot b = b \odot a & \\
\\
a \odot (b \oplus c) = a \odot b + a \odot c & \qquad \triangleright \text{ left and right distributive} \\
(a \oplus b) \odot c = a \odot c \oplus b \odot c & \\
\\
a \odot \mathbb{0} = \mathbb{0} \odot a = \mathbb{0} &
\end{aligned}
$$

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 einsum network generic [22].

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 $a_0 + a_1 x + \ldots + a_k x^k$ as a vector $(a_0, a_1, \ldots, a_k) \in R^k$, 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

$$
\begin{aligned}
a \oplus b &= (a_0 + b_0, a_1 + b_1, \ldots, a_{\max(k_a, k_b)} + b_{\max(k_a, k_b)}), \\
a \odot b &= (a_0 + b_0, a_1 b_0 + a_0 b_1, \ldots, a_{k_a} b_{k_b}), \\
\mathbb{0} &= (), \\
\mathbb{1} &= (1).
\end{aligned} \tag{3.5}
$$

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 [21]. 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 einsum contraction for each $x_i \in X$ and obtain the following relations

$$\begin{aligned} a_0 + a_1 x_1 + a_1 x_1^2 + \ldots + a_m x_1^m &= y_0 \\ a_0 + a_1 x_2 + a_2 x_2^2 + \ldots + a_m x_2^m &= y_1 \\ &\ldots \\ a_0 + a_1 x_m + a_2 x_m^2 + \ldots + a_m x_m^m &= y_m \end{aligned} \tag{3.6}$$

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

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

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

$$\begin{pmatrix} 1 & r\omega & r^2\omega^2 & \ldots & r^m\omega^m \\ 1 & r\omega^2 & r^2\omega^4 & \ldots & r^m\omega^{2m} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & r\omega^m & r^2\omega^{2m} & \ldots & r^m\omega^{m^2} \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_m \end{pmatrix} = \begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_m \end{pmatrix}. \tag{3.8}$$

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 $\vec{a}_r = \mathrm{FFT}^{-1}(\omega) \cdot \vec{y}$, where $(\vec{a}_r)_j = a_j r^j$. By choosing different r, one can obtain better precision in low independent set size region ($\omega < 1$) 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 $GF(p)$

$$\begin{aligned} x \oplus y &= x + y \pmod{p}, \\ x \odot y &= xy \pmod{p}, \\ \mathbb{0} &= 0, \\ \mathbb{1} &= 1. \end{aligned} \tag{3.9}$$

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

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 $Y = (y_0, y_1, \ldots, y_m) \pmod{p}$
  $A_p = (a_0, a_1, \ldots, a_m) \pmod{p}$ = gaussian_elimination($\hat{X}, Y \pmod{p}$)
  $A_{P\times p}$ = chinese_remainder(A_P, A_p)
  if $A_P = A_{P\times p}$ **then**
    return A_P ; `// converged`
  end
  $P = P \times p$
end

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 einsum network for computing independence polynomial by adding this restriction. Instead of defining the restriction on vertices and edges, we define it on $N[v]$

$$T(x_v)_{s_1, s_2, \ldots, s_{|N(v)|}, s_v} = \begin{cases} s_v x_v & s_1 = s_2 = \ldots = s_{|N(v)|} = 0, \\ 1 - s_v & otherwise. \end{cases} \tag{3.10}$$

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

$$T(x_v) = \begin{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix} \\ \begin{pmatrix} x_v & 0 \\ 0 & 0 \end{pmatrix} \end{pmatrix}. \tag{3.11}$$

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 einsum network is often larger than the one for computing independence polynomial. However, in many sparse graphs, this einsum 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

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

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

$$
\begin{aligned}
a_x\infty^x \oplus a_y\infty^y &= \begin{cases} (a_x+a_y)\infty^{\max(x,y)}, & x=y \\ a_y\infty^{\max(x,y)}, & x<y \\ a_x\infty^{\max(x,y)}, & x>y \end{cases} \\
a_x\infty^x \odot a_y\infty^y &= a_x a_y \infty^{x+y} \\
\mathbb{0} &= 0\infty^{-\infty} \\
\mathbb{1} &= 1\infty^{0}
\end{aligned} \tag{4.2}
$$

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 [14] 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 [15, 17].

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).

$$
\begin{aligned}
a \oplus b &= (a_{\max(k_a,k_b)-1} + b_{\max(k_a,k_b)-1}, a_{\max(k_a,k_b)} + b_{\max(k_a,k_b)}), \\
a \odot b &= (a_{k_a-1}b_{k_b} + a_{k_a}b_{k_b-1}, a_{k_a}b_{k_b}), \\
\mathbb{0} &= (), \\
\mathbb{1} &= (1).
\end{aligned} \tag{4.3}
$$

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 having the following algebra

$$
\begin{aligned}
s \oplus t &= s \cup t \\
s \odot t &= \{\sigma \vee^\circ \tau | \sigma \in s, \tau \in t\} \\
\mathbb{0} &= \{\} \\
\mathbb{1} &= \{0^{\otimes n}\}
\end{aligned} \tag{5.1}
$$

where $\vee^\circ$ 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 $x_i = \{\boldsymbol{e}_i\}$, where $\boldsymbol{e}_i$ 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 einsum 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.

$$
\begin{aligned}
\sigma \oplus \tau &= \text{select}(\sigma, \tau) \\
\sigma \odot \tau &= (\sigma \vee^\circ \tau), \\
\mathbb{0} &= 1^{\otimes n}, \\
\mathbb{1} &= 0^{\otimes n},
\end{aligned} \tag{5.2}
$$

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

$$A_{ij} \odot B_{jk} \leq C_{ik}. \tag{5.3}$$

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

$$A_{ij} \leq (\oplus_k (C_{ik}^{-1} \odot B_{jk}))^{-1} \tag{5.4}$$

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

$$\overline{A}_{ij} = \delta(A_{ij}, ((C^{\circ -1} \circ \overline{C})B^T)_{ij}^{\circ -1}), \tag{5.5}$$

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 einsum by replacing the matrix multiplication between $C^{\circ -1} \circ \overline{C}$ and B^T by an einsum operation. [] [**JG: maybe add an appendix?**]

6. Tropical tensors for automated branching. [**JG:** ?] Branching rules can be automatically discovered by contracting the einsum network on a subgraph $R \subseteq G$ with tropical numbers as its element type. Let C be the set of boundary vertices defined as $C := \{u | u \in R \wedge (\exists v \in (G \backslash R) \wedge \mathrm{adj}(u, v))\}$, then the rank of the resulting tensor A is $|C|$. Here, we use $\mathrm{adj}(u, v)$ 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

$$(\sigma_a \prec \sigma_b) := (\sigma_a \neq \sigma_b) \wedge (\sigma_a \leq^\circ \sigma_b) \tag{6.1}$$

where $\leq^\circ$ is the Hadamard less or equal to operation.

Definition 6.1. *A tensors A is MIS-compact if*

$$\forall \sigma_b \neg \exists \sigma_a (\sigma_a \prec \sigma_b) \wedge (A_{\sigma_a} \geq A_{\sigma_b}). \tag{6.2}$$

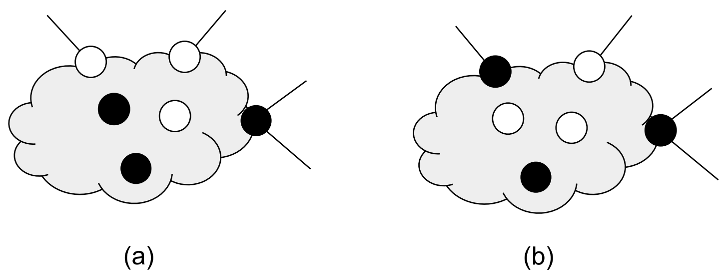
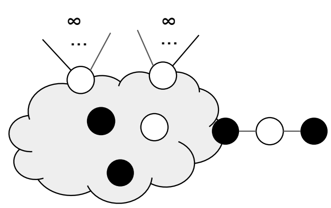


Figure 1: Two configurations with the same local independent size $A_{\sigma_a} = A_{\sigma_b} = 3$ and different boundary configurations (a) $\sigma_a = \{001\}$ and (b) $\sigma_b = \{101\}$, where black nodes are 1s (in the independent set) and white nodes are 0s (not in the independent set).

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 $u, w \in G\backslash R$ that $\mathrm{adj}(v,u) \wedge \mathrm{adj}(u,w) \wedge \neg\mathrm{adj}(v,w)$. Otherwise, we attach infinite many disconnected neighbors to v.

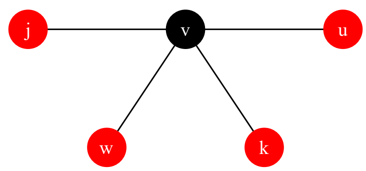


Then we have the maximum independent set size $\alpha(G,\sigma) = A_\sigma + \infty(|C| - \sum_{v=1}^{|C|} \sigma_v) + \sum_{v=1}^{|C|} 1 - \sigma_v$. Let us assume there exists another configuration τ that generating the same or better maximum independent set size $\alpha(G,\tau) \geq \alpha(G,\sigma)$.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

6.1. The einsum 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 $N[v]$ and the resulting tensor A has a rank $|N(v)|$. Each tensor entry A_σ corresponds to a locally maximized independent set size with fixed boundary configuration $\sigma \in \{0,1\}^{|N(v)|}$. If the boundary configuration is a bit string of 0s, σ_v 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

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

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

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

By studying the correlation between vertex variables, one can easily see x_v 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

$$\begin{aligned} S_{juwkv} = \{&00001, 10001, 01010, 10010, 11010, 10100, \\ &01100, 11100, 00110, 01110, 10110, 11110\}. \end{aligned} \tag{6.5}$$

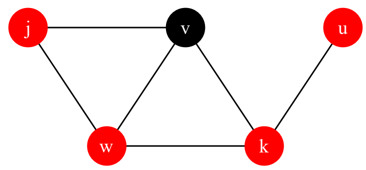
The corresponding branching vector $(1,5)$ gives a branching number $\tau(1,5) \approx 1.3247$

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

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

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 $N(v) \backslash N(w)$ 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 $N(v) \backslash N(u)$ 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

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

where entries stroked through are removed by compactification. The corresponding polynomial tensor is

$$P_{juwk} = \begin{pmatrix} \begin{pmatrix} 1 + x_v & x_u + x_u x_v \\ / & / \end{pmatrix}_{ju} & \begin{pmatrix} / & - \\ x_j x_k & - \end{pmatrix}_{ju} \\ \begin{pmatrix} / & / \\ - & - \end{pmatrix}_{ju} & \begin{pmatrix} - & - \\ - & - \end{pmatrix}_{ju} \end{pmatrix}_{wk}. \tag{6.8}$$

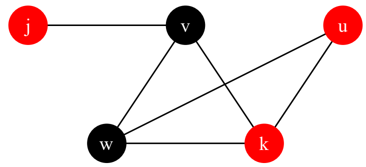
One can see w, as a mirror of v does not appear in the maximum independent set after compactification.

$$S_{juwkv} = \{00001, 01001, 10010\}. \tag{6.9}$$

Corollary 6.5 (satellite rule). *Let G be a graph, $v \in V$. A node $u \in N^2(v)$ is called satellite [13] of v, if there is some $u' \in N(v)$ such that $N[u'] \backslash N[v] = \{u\}$. 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*

$$\alpha(G) = \max\{\alpha(G \backslash \{v\}), \alpha(G \backslash N[S[v]]) + |S(v)| + 1\}. \tag{6.10}$$

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 $N[w] \backslash N[v] = \{u\}$, 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

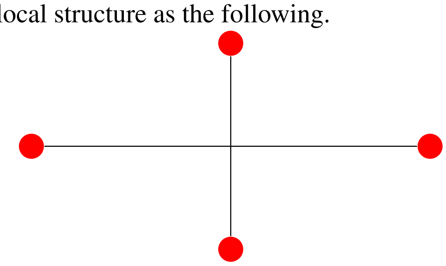
$$(6.11)\qquad P_{juk} = \begin{pmatrix} \begin{pmatrix} 1 + x_w + x_v & x_u + x_u x_v \\ x_j + x_w x_j & / \end{pmatrix}_{ju} \\ \begin{pmatrix} / & - \\ / & - \end{pmatrix}_{ju} \end{pmatrix}_k .$$

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.

$$(6.12)\qquad S_{juwkv} = \{\{00100, 00001\}, 10100, 01001\}.$$

6.2. gadget design. [**JG:** ×]

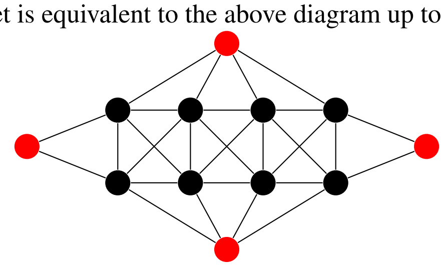
Suppose we have a local structure as the following.



Contract this local structure gives the tropical tensor

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

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



$$(6.14)\qquad \begin{pmatrix} \begin{pmatrix} 2 & 3 \\ 3 & 4 \end{pmatrix} & \begin{pmatrix} 3 & 3 \\ 4 & 4 \end{pmatrix} \\ \begin{pmatrix} 3 & 4 \\ 2 & 3 \end{pmatrix} & \begin{pmatrix} 4 & 4 \\ 3 & 4 \end{pmatrix} \end{pmatrix} \xrightarrow[\text{compactify, -2}]{} \begin{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 2 \end{pmatrix} & \begin{pmatrix} 1 & \cancel{1} \\ 2 & \cancel{2} \end{pmatrix} \\ \begin{pmatrix} 1 & 2 \\ \cancel{0} & \cancel{1} \end{pmatrix} & \begin{pmatrix} 2 & \cancel{2} \\ \cancel{1} & \cancel{2} \end{pmatrix} \end{pmatrix}$$

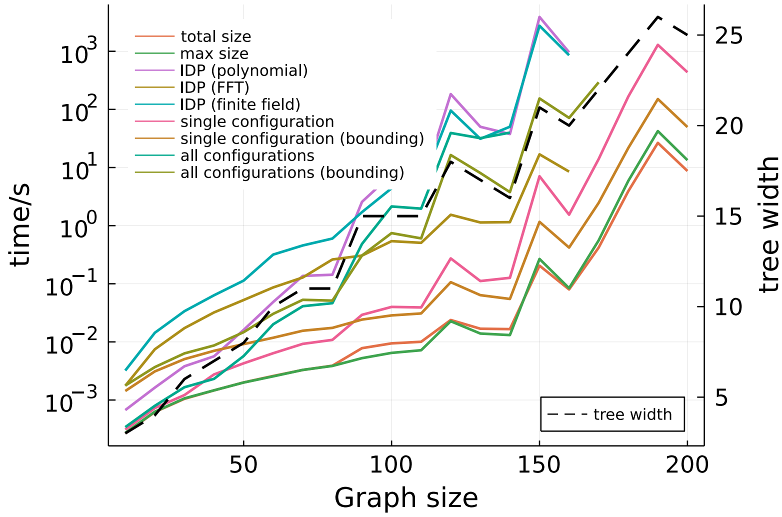


Figure 2: Benchmark results for computing different properties with different element types. The right axis is only for the dashed line.

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. Einsum 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 einsum 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 Einsum network's is not limited to the indenepent set problem, in Appendix C we show how to map matching problem and k-coloring to an einsum 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 $\oplus$ and $\odot$ and two special elements $\mathbb{0}$ and $\mathbb{1}$. The style that we program is called generic programming, meaning one can feed different data types into 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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Appendix A. Technical guide.

OMEinsum a package for einsum,

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 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.

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

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

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

# an einsum contraction without contraction order specified is called `EinCode`,
# an einsum contraction has contraction order (specified as a tree structure) is called `NestedEinsum`.
# assign each label a dimension-2, it will be used in contraction order optimization
# `symbols` function extracts tensor labels into a vector.
symbols(::EinCode{ixs}) where ixs = unique(Iterators.flatten(filter(x->length(x)==1,ixs)))
symbols(ne::OMEinsum.NestedEinsum) = symbols(flatten(ne))
size_dict = Dict([s=>2 for s in symbols(code)])
# optimize the contraction order using KaHyPar + Greedy, target space complexity is 2^17
```

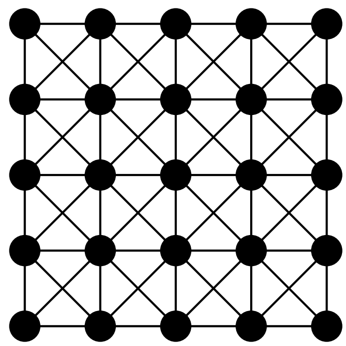
```julia
optimized_code = optimize_kahypar(code, size_dict; sc_target=17, max_group_size=40)
println("time/space complexity is $(OMEinsum.timespace_complexity(optimized_code, size_dict))")

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

########## COMPUTING MAXIMUM INDEPENDENT SET SIZE AND ITS DEGENERACY ###########

# using Tropical numbers to compute the MIS size and MIS degeneracy.
using TropicalNumbers
mis_size(code) = independence_polynomial(TropicalF64(1.0), code)[]
println("the maximum independent set size is $(mis_size(optimized_code).n)")
# A `CountingTropical` object has two fields, tropical field `n` and counting field `c`.
mis_count(code) = independence_polynomial(CountingTropical{Float64,Float64}(1.0, 1.0), code)[]
println("the degeneracy of maximum independent sets is $(mis_count(optimized_code).c)")

########## COMPUTING INDEPENDENCE POLYNOMIAL ###########

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

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

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

function independence_polynomial_finitefield(code; mis_size=Int(mis_size(code)[].n), max_order=100)
    N = typemax(Int32) # Int32 is faster than Int.
    YS = []
    local res
    for k = 1:max_order
       N = Primes.prevprime(N-one(N))  # previous prime number
        # evaluate the polynomial on a finite field algebra of modulus `N`
        rk = _independance_polynomial(Mods.Mod{N,Int32}, code, mis_size)
        push!(YS, rk)
        if max_order==1
            return Polynomial(Mods.value.(YS[1]))
        elseif k != 1
            ra = improved_counting(YS[1:end-1])
            res = improved_counting(YS)
            ra == res && return Polynomial(res)
        end
    end
    @warn "result is potentially inconsistent."
    return Polynomial(res)
end
function _independance_polynomial(::Type{T}, code, mis_size::Int) where T
   xs = 0:mis_size
   ys = [independence_polynomial(T(x), code)[] for x in xs]
   A = zeros(T, mis_size+1, mis_size+1)
```

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

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

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

# define the config enumerator algebra
struct ConfigEnumerator{N,C}
    data::Vector{StaticBitVector{N,C}}
end
function Base.:+(x::ConfigEnumerator{N,C}, y::ConfigEnumerator{N,C}) where {N,C}
    res = ConfigEnumerator{N,C}(vcat(x.data, y.data))
    return res
end
function Base.:*(x::ConfigEnumerator{L,C}, y::ConfigEnumerator{L,C}) where {L,C}
    M, N = length(x.data), length(y.data)
    z = Vector{StaticBitVector{L,C}}(undef, M*N)
    for j=1:N, i=1:M
        z[(j-1)*M+i] = x.data[i] .| y.data[j]
    end
    return ConfigEnumerator{L,C}(z)
end
Base.zero(::Type{ConfigEnumerator{N,C}}) where {N,C} = ConfigEnumerator{N,C}(StaticBitVector{N,C
    }[])
Base.one(::Type{ConfigEnumerator{N,C}}) where {N,C} = ConfigEnumerator{N,C}([TropicalNumbers.
    staticfalses(StaticBitVector{N,C})])

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

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

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

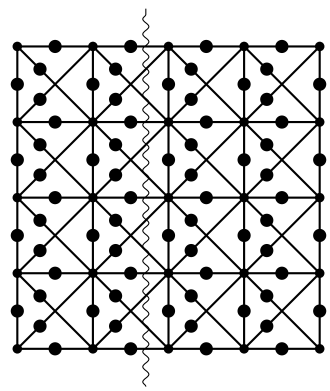
In the above examples, the configuration enumeration is very slow, one should use the optimal MIS size for bounding as decribed in the main text. We will not show any example about implementing the backward rule here because it has approximately 100 lines of code.

Please checkout our GitHub repository https://github.com/Happy-Diode/NoteOnTropicalMIS.

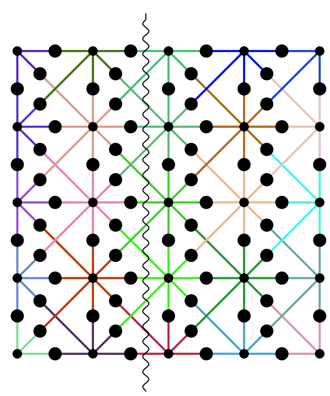
Appendix B. When a tensor network is worse than an einsum network. Given a graph



Its tensor network representation 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 einsum 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 an einsum network. To understand its representation power, it is a good starting point to connect it with dynamic programming because an einsum 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 einsum network approach. We mentioned in the main text that einsum network has nice analytic property make it easier for generic programming. The cost is, the einsum network is less expressive than dynamic programming, However, that are still some other problems that can be expressed in the framework of generic einsum network.

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

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

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,

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

and a tensor of rank 1 on the bond

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

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

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

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

and an edge tensor as

$$B = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}. \tag{C.5}$$

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