Carving-width and contraction trees for tensor networks

J. Jakes-Schauer, D. Anekstein, P. Wocjan

August 30, 2019

Abstract

We study the problem of finding contraction orderings on tensor networks for physical simulations using a syncretic abstract data type, the contraction-tree, and explain its connection to temporal and spatial measures of tensor contraction computational complexity (nodes express time; arcs express space). We have implemented the Ratcatcher of Seymour and Thomas for determining the carving-width of planar networks, in order to offer experimental evidence that this measure of spatial complexity makes a generally effective heuristic for limiting their total contraction time.

1 Introduction

Tensors, for current purposes, are functionally multidimensional arrays of complex numbers. A tensor network is a factorization of a large tensor into a family of simpler tensors which tracks their interrelationships—usually graphically, as by Penrose notation—so as to make the uncompressed tensor product recoverable in principle. Good introductions are freely available (e.g. [18, 4, 6]) into the role of the tensor network in models of quantum chemistry, quantum many-body physics, and, most recently, classical approximations of quantum computation. In these simulations, the contents of the component tensors stand for superpositions of quantum particles, and their bonds for the degrees of entanglement between them. A maximally entangled system, of course, is not simplified by factorization; but the importance of locality in the systems being modeled enables it in practice. With this approach one can manipulate features of tensors whose unfactored form would require computational resources far in excess of what is physically possible, not to mention practical.

The pinch is felt when a calculation calls for the scalar equivalent of a closed network, as this requires contracting all bonds, i.e., indices; the complexity of which procedure is usually exponential in the number of component tensors. If the operation known as ‘contraction’ is the generalization of the trace of a two-dimensional tensor, then contracting two or more tensors is a generalization of matrix chain multiplication; like with matrices, the order of the pairwise contractions is irrelevant to the value obtained but highly consequential for the efficiency. Full contraction of even minimally entangled networks has been proved to be \#P-hard [28] and generally unfeasible, providing strong motivation to identify the exceptional cases. Our present preoccupation, the problem of finding a best contraction order for an existing tensor network—as opposed to incorporating different factorizations into the search—is historically known as single-term optimization, has a clean graph-theoretic analogy, and is unfortunately NP-hard [14], in contrast to the one-dimensional matrix-multiplication problem.

Optimization, for matrix multiplication or tensor contraction, generally means minimizing the total number of paired multiplication-addition operations in a multiply-nested loop, approximating, in a big-Theta sense, the time required by a single-core processor in the standard random-access machine (RAM) computation model. Any further compile-time or runtime accelerations can improve on this strategy only up to a hardware-dependent multiplicative constant. This sequential-time-complexity metric is the one used with Netcon [21], which is still, to our knowledge, the most aggressive graph-based single-term optimization algorithm, but which, by dint of its exactitude, is usable only for small to moderately sized networks of less than one hundred tensors. In fact, rather than focus primarily on contraction order, it is much more common to use lossy compression techniques [23]. An exception is the well-known MPS method [20], which is unidimensional enough that finding and executing a contraction order can be managed efficiently. However, one has only to look at the bidimensional version of MPS, PEPS [29], to see both tasks reach maximum difficulty.

Our interest is in networks with many tensors, but low average tensor dimension, for which an exact contraction result is required but an approximately minimal contraction cost is acceptable. This kind of result could be used, for instance, to validate the approximate contraction methods currently in vogue. Correspondingly, an approximation technique that minimizes the cost, not of the entire contraction, but of the most expensive part of it, leads us to carving-width, which, introduced in [25], is one of a family of “widths” researched at length by Robertson and Seymour for quantifying edge complexity of a graph. The original of these, and the most studied, is treewidth; its applicability to tensor networks was noted in an influential paper by Markov and Shi
used practically by Pednault et al. [10], and benchmarked comparatively by Dumitrescu et al. [9]. On the other hand, the relevance of carving-width to tensor networks was, to our knowledge, first remarked upon in an arXival e-print by Aharonov, Landau, and Makowsky [1], who, rediscovering it in a restricted form, knew it as ‘bubble width’; it is used in its primary sense by Oliveira Oliveira [17]. We have come to believe that its obscurity is undeserved, for several reasons:

1. The (comparatively) well-known treewidth was designed for unweighted graphs, so it only works on tensors of uniform bond dimension. This may hold for quantum circuits, but not other species of tensor networks, which is probably why it is has seen more use in circuit simulation than in the other quantum disciplines. A generalized weighted treewidth [3] is extant, but has not received the same level of attention. By contrast, carving-width works with all nonnegative real edge weights.

2. Second, because treewidth requires a vertex-weighted graph, not edge-weighted, one must take the line graph first. As shown in §3.2, finding a carving-decomposition automatically yields a tree-decomposition of the line graph.

3. Most importantly, the carving-decomposition constructed for a minimal carving-width is a binary tree and provides the basis for a datatype, explained in the next section, which best describes an arbitrary contraction order. In other words, the step between assessing the cost of a near-optimal contraction order, and finding the order itself, is short.

An obstacle to using them, even as a means to a larger end, is that carving-width [25] and treewidth (including for unweighted graphs [2]) are both NP-complete problems and must themselves be approximated. For the important class of planar graphs (drawn with no crossing edges), however, there exists the original Seymour-Thomas algorithm, rather whimsically called the ‘Ratcatcher,’ which can find the carving-width in pseudopolynomial time; whereas 2019 has passed with the existence of a comparable exploit for treewidth remaining an open problem, providing one more motivation for working with carving-width. In §4 we demonstrate how finding the carving-decomposition of a tensor network (using the Ratcatcher algorithm) can provide reasonable contraction orders for said network, provided that it is planar, and we demonstrate an application to a PEPS-like grid. §5 discusses potential extensions.

2 Graph-theoretical formulation

A tensor network is, conveniently, isomorphic to an undirected weighted graph \( G = (V, E, w) \) without self-loops or parallel edges. Vertices are identified with tensors, edges with tensor indices, and edge weights with index dimensions; the degrees of the vertices give the tensors’ orders. Edges are identified with subsets of \( V \) of cardinality 2. Parallel edges, while supportable, are disallowed, because any bundle of such edges may be replaced with a single edge, weighted with the product of their weights. Loops can similarly be eliminated by summing over the corresponding indices [21]. Importantly, these simplification operations never harm efficiency by adding to the resource requirements of contraction. Also, there is no semantic distinction between an edge with weight 1 and a nonexistent edge, meaning that they may be interchanged at will. Finally, a tensor network often has indices initially left free, to serve as model inputs. This does not a valid graph make, so we assume that free indices get bound to probability vectors and contracted preliminarily [2].

An example graph \( G \) is given in fig. 1: a ‘tensor train’ as would be part of a MPS process. We use capitals \( A, B, \ldots, F \) to label vertices and miniscules \( a, b, \ldots, g \) for edges. For instance, the index joining tensors \( A \) and \( B \), \( a \), is equivalent to the edge \( \{A, B\} \), and has dimension \( w_a = w(\{A, B\}) \), with \( w : E \to \mathbb{N}^+ \) denoting the weight function.

\[ \begin{align*} A & \quad a & B & \quad b & C \\
& c & & d & e \\
D & \quad f & E & \quad g & F \end{align*} \]

Figure 1: A \( 2 \times 3 \)-tensor network

\( A, B, \ldots, F \) to label vertices and miniscules \( a, b, \ldots, g \) for edges. For instance, the index joining tensors \( A \) and \( B \), \( a \), is equivalent to the edge \( \{A, B\} \), and has dimension \( w_a = w(\{A, B\}) \), with \( w : E \to \mathbb{N}^+ \) denoting the weight function.

2.1 Contraction

Figure 2 shows a possible contraction sequence for the graph of fig. 1.

---

1 Seymour and Thomas used natural numbers, but the extension to reals is uncomplicated, up to the imprecision of floating-point calculation.

2 The alternative, tying all the dangling edges to a new vertex and leaving them uncontracted, increases contraction time exponentially in the number of inputs.
We enumerate the tensors that arise during the contraction of a network using subsets of $V$. For any $X \subseteq V$, the tensor corresponding to $X$ is the one formed by merging all the (fundamental) tensors of $X$; that is, by contracting all edges in the induced subgraph $G[X]$. In step 2c, for example, the contraction is of tensors $X = \{A, B\}$ and $X' = \{D, E\}$, outputting $X \cup X' = ABDE$. Clearly, due to the distributive law the output of a sequence of contractions does not depend on the order of combination.

However, the cost, in terms of computational complexity, does. To illustrate this we need the concept of a ‘cut’, which is a separation of $G$ into disconnected subgraphs by the removal of a subset of $E$.

**Definition 1 (2-cut).** A 2-cut, edge-cut, or just cut is a bipartition of $E$. For $X, X' \subseteq V$ with $X \cap X' = \emptyset$, define the cut-set $\delta(X, X')$ as the set of edges needed to disconnect $G[X]$ from $G[X']$:

$$\delta(X, X') = \{(A, B) \in E \mid A \in X, B \in X'\}$$

(1)

In other words, $\delta(X, X')$ is the set of edges having one endpoint in $X$ and one in $X'$.

This generalizes easily to the idea of a multiway $m$-cut $\delta(X_1, \ldots, X_m)$; but the only other case we will specifically need is $m = 3$:

**Definition 2 (3-cut).** For $X, X', X'' \subseteq V$ with $X \cap X' = \emptyset, X \cap X'' = \emptyset, X' \cap X'' = \emptyset$, define

$$\delta(X, X', X'') = \delta(X, X') \cup \delta(X, X'') \cup \delta(X', X'')$$

(2)

For subsets of edges $F \subseteq E$, it useful to define the weight of $F$ to be the product of the weights of the edges in $F$, that is,

$$w(F) = \prod_{e \in F} w_e.$$

This makes possible:

**Definition 3 (Cut-weight).** For $X_1, \ldots, X_m$ with $\bigcup_i X_i = V$, the cut-weight, $w(X_1, \ldots, X_m)$, is given by

$$w(X_1, \ldots, X_m) = w(\delta(X_1, \ldots, X_m)),$$

with obvious applicability to 2- and 3-cuts.

To motivate use of these definitions, we first need to refine the meaning of ‘contraction sequence.’ We start the contraction sequence $S$ with the $|V|$ fundamental tensors as input, identifying each of which with a singleton subset of $V$. For every contraction step in the sequence, we always select two tensors $X$ and $Y$ and contract them to a new tensor $Z = XY$. In total, we create $|V| - 1$ new tensors by pairwise contractions, with the last one being the scalar value of the fully contracted network. Each tensor created along the way corresponds to the union of the preceding subsets of $V$—mapping, in turn, to tensors earlier in the sequence. We now have a list of $2|V| - 1$ subsets of $V$, with the second half describing the contractions. E.g., for fig. 2

$$S = \left\{ \{A\}^1, \{B\}^2, \{C\}^3, \{D\}^4, \{E\}^5, \{F\}^6, \{A, B\}^7, \{C, F\}^8, \{D, E\}^9, \{A, B, D, E\}^{10}, \{A, B, C, D, E, F\}^{11} \right\}.$$
with positional IDs added as superscripts. Each contractive step \(i \in [|V|..2|V|-1] \) can also be associated with a minor of \(G\), that is, a partially contracted graph, as follows. Let \(P(i)\) be the partition of \(V\) formed by taking the first \(i\) elements of the sequence, removing any member which is a subset of another. \(P(i)\) is homomorphic to the minor \(G_{P(i)} = (P(i),E_{P(i)},w_{P(i)})\), where, for all \(X,Y \in P(i)\),
\[
w_{P(i)}(X,Y) = w_G(X,Y) = w(\delta_G(X,Y));
\]
while \(E_{P(i)}\) is simply the set of vertex pairs for which \(w_{P(i)}\) is not 1.

Generalizing these precedential relationships, we see that each \(P(i)\) is a layer in a join-semilattice. More specifically, a contraction order can be described by a binary tree \(T\) with an injective map \(\phi : [1..(2|V|-1)] \to V_T\). This \(\phi\) must satisfy the so-called max-heap property: the ID of each internal node has to be greater than the IDs of both its children. Intuitively, an ID marks the point in \(S\) at which the corresponding tensor is produced, and it makes sense that its two constituent tensors must have been created first. Thus the vertices of \(G\) map to \(T\)'s leaves.

Formally:

**Definition 4 (Rooted contraction tree).** A rooted contraction tree \(T_r\) of the weighted graph \(G = (V,E,w)\) is a rooted, labeled, unordered, full binary tree with each external node identified with a unique \(v \in V\). This tree type was used earlier in [7], though the labeling offered there differs somewhat from ours. We label both nodes and arcs\(^5\) as follows:

- The removal of an arc \(a\) partitions the leaves into the two disjoint sets \(X_a\) and \(\overline{X}_a\); the label of arc \(a\) is
  \[
  \delta_a = \delta(X_a,\overline{X}_a).
  \]
- The removal of an internal node \(n\) partitions the leaves into the three mutually disjoint sets \(X_n, Y_n,\) and \(X_n \overline{Y}_n\); the label of node \(n\) is
  \[
  \delta_n = \delta(X_n, Y_n, \overline{X_n Y_n}).
  \]

For the special case of the root node, one of these sets is empty, making it a de facto 2-cut. The other internal nodes are all 3-cuts.
- The label of an external node \(v\) is

  \[
  \delta_v = \{ e \in E \mid v \in e \},
  \]

  that is, all edges incident at \(v\). Note that \(\delta_v\) is equal to \(\delta_a\), where \(a\) is the unique arc connecting the leaf node to the rest of the contraction tree. Due to the redundancy, labels of this sort will be omitted from figures, such as fig. 3.

**Remark.** It is important to observe that the nodes \(n\) of the rooted contraction tree \(T_r\) could be naturally identified with subsets of \(V\). However, we do not make this identification a required part of the definition because—as we shall shortly see—it will be very useful to consider ‘free’ contraction trees with which such identification is no longer possible.

It should be clear that many contraction sequences give rise to the same \(T_r\), per the variability of the \(\phi\) mapping. The benefit of using 2- and 3-cuts (definitions [3] and [2]), is that they provide a complexity measure which abstracts away unnecessary information.

\[^5\]To reduce ambiguity, we call components vertices and edges when referring to the network \(G\) and nodes and arcs only with contraction trees—a small abuse of terminology for undirected trees.
Definition 5 (Tensor space complexity). The number of bytes needed to store tensor $X$, up to a multiplicative constant, is the cut-weight

$$w(X, X),$$

and for a contraction tree arc $a$ with $\delta_a = \delta(X_a, X_a)$,

$$w_a = w(\delta_a) = w(X_a, X_a).$$

Definition 6 (Contraction time complexity). Symmetrically, the number of primitive operations in contracting tensors $X$ and $Y$ to get $XY = X \oplus Y$ is, up to a multiplicative constant, the cut-weight

$$w(X, Y, XY).$$

For a contraction tree node $n$,

$$w_n = w(\delta_n) = w(X, Y, XY).$$

Definition 7 (Space bottleneck). Define the space bottleneck, $B^s_{Tr}$, of a contraction tree as the maximum over all arcs:

$$B^s_{Tr} = \max_a \{w_a\}.$$

Definition 8 (Time bottleneck). Symmetrically, define the time bottleneck, $B^t_{Tr}$, as the maximum over all nodes:

$$B^t_{Tr} = \max_n \{w_n\}.$$

For unweighted graphs, this reduces to the contraction complexity of Markov and Shi [16].

Definition 9 (Total time). Finally, define the total time complexity, $C^t_{Tr}$, the sum over all internal nodes:

$$C^t_{Tr} = \sum_n w_n.$$

It is trivially true that $B^s \leq B^t \leq C^t$, a relationship we will examine further in the next section. For now, note that given the root $r$ with incident arcs $a$ and $a'$, then $\delta_r = \delta_a = \delta_{a'}$. This means that the root node never determines $B^s$ or $B^t$, suggesting that we consider a homeomorphic rootless tree.

Definition 10 ([Free] contraction tree). An unrooted or free contraction tree (in future, just contraction tree) $T$ of the weighted graph $G = (V, E, w)$ is a free, unordered binary tree with leaves mapped bijectively to $V$ and nodes and arcs labeled as in definition [4] save, of course, the root $r$. Any $T_r$ can be converted to a $T$ by removing the root and splicing its arcs together so as to make its children neighbors. $B^s$ and $B^t$ are the same for $T$ and $T_r$, while $C^t_T = C^t_{T_r} + w_r$. A contraction sequence can only be built from a rooted tree; however, because we can always “re-root” $T$ optimally (and efficiently; see §4.4), the contribution made by $r$ to the time complexity is asymptotically negligible. Hence we will treat all contraction trees as free by default.

3 Space vs. time optimization

$B^s$, $B^t$, and $C^t$ for contraction trees measure local optima; their definitions can be made global with respect to a given $G$ simply by minimizing over all possible contraction trees. There are $(2|V| - 3)!!$ such $T$. The Netcon

---

6I.e., the number of free, unordered, terminally-labeled binary trees [26]. The rooted kind has $(2|V| - 5)!!$. 

---
algorithm of Pfeifer, Haegeman, and Verstraete uses branch-and-bound techniques to construct \( \arg \min \ C_T \) directly; however, it turns out that \( B_C \) and \( B'_C \) also are the targets of existing algorithmic methods. The choice of labels for the contraction tree was made to match this intuition: informally, arc labels denote space complexity, and node labels, time; and either can be obtained from its counterpart. §3.1 and §3.2 provide the formal details as to how the contraction tree encodes, respectively, treewidth and carving-width, while §3.3 offers some simple bounds.

### 3.1 Weighted treewidth and \( B^3 \)

A tree-decomposition of a graph, also known as a junction tree, is formed by grouping the vertices of that graph into sets, or ‘bags,’ according to a triad of rules—which are reviewed below—so that these bags form the nodes of a tree. The object is to keep the bags as small as possible, because the width of the tree-decomposition is determined by the cardinality of the largest bag; the treewidth, or \( tw(G) \), is the smallest width of any tree-decomposition feasible; and a variety of algorithms that are NP-hard for arbitrary graphs—tensor networks, for example—are exponential merely in the treewidth, becoming tractable when that is provably bounded. For decomposition feasible; and a variety of algorithms that are NP-hard for arbitrary graphs—tensor networks, treewidth

\[ A \]

\[ B \]

\[ 3.1 \]

\[ \text{Weighted treewidth and } B^3 \]

The weighted treewidth of the line graph, \( wtw(L) \), is the smallest width of any tree-decomposition of \( L \).

**Definition 11 (Weighted tree-decomposition of \( L \)).** The weighted tree-decomposition \( T_0 \) of the line graph \( L \) of \( G = (V, E, w) \) is a tree whose nodes \( n \) are labeled by subsets \( b(n) \) of \( E \), together satisfying the following properties:

1. For each index \( i \in E \), there exists at least one node \( n \) with \( i \in b(n) \).
2. For each pair of indices \( i' \) and \( i'' \) incident on the same vertex \( v \in V \), there exists at least one node \( n \) with \( \{i', i''\} \subseteq b(n) \).
3. For each index \( i \in E \), the subgraph induced by the subset of nodes \( \{n \mid i \in b(n)\} \) is connected. In the machine-learning literature this is known as the running intersection property.

The weighted width of the tree-decomposition \( T_0 \) is

\[ \text{ww}(T_0) = \max_n \left\{ w(b(n)) \right\}, \]

where the maximum is taken over all nodes of the tree \( T_0 \).

The weighted treewidth of the line graph, \( wtw(L) \), is the minimal weighted width

\[ \text{wtw}(L) = \min_{T_0} \left\{ \text{ww}(T_0) \right\}, \]

taken over all admissible tree-decompositions of \( L \).

Instead of counting the bags’ contents, one multiplies the associated weights. The original application was to Bayesian networks, where the weight \( w_C(i) \) measured the domain of some random variable; here we use it as the range of a tensor index.

**Theorem 1 (Contraction tree \( \mapsto \) tree-decomposition).** An arbitrary contraction tree \( T \), modulo its 2-cuts \( \delta_a \), forms a tree-decomposition of the line graph \( L \) having width \( B^3_T \).

**Proof.** Let \( e = \{v, v'\} \) be any index in \( E \). By construction of the labels of the leaf nodes, we have \( e \in \delta_v \) and also \( e \in \delta_{v'} \). Properties \( 1 \) and \( 2 \) follow immediately.

This leaves the running intersection property:

**Lemma 1 (RIP).** Let \( T \) be an arbitrary free contraction tree. For any \( e \in E \), the subgraph induced by the subset of nodes \( \{n \mid e \in \delta_n\} \) is a path.

**Proof.** Begin with a version of \( T \) which is “bare,” having leaf nodes still mapped to \( V \) but being otherwise unlabeled. Then construct an alternative labeling \( \hat{\delta} \) using the desired property and show that the resulting tree \( \hat{T} \) is equivalent to \( T \). The alternative labeling \( \hat{\delta}_n \) of the nodes and \( \hat{\delta}_e \) of the arcs is defined thus:

- For every leaf node \( v \), set \( \hat{\delta}_v = \text{edges}(v) \).

\(^7\text{Stripping the leaf nodes is optional. They will never contribute to the treewidth.}\)
Theorem 2 (Tree-decomposition → contraction tree). Let $\mathcal{T}_d$ be an arbitrary tree-decomposition of the line graph $L$ of $G$. Then, $\mathcal{T}_d$ can always be efficiently transformed to a new tree-decomposition $\mathcal{T}'_d$ such that $\text{ww}(\mathcal{T}_d) \leq \text{ww}(\mathcal{T}'_d)$ and $\mathcal{T}'_d$ forms a free contraction tree.

Proof. Use the following three-step algorithm to meet the specific structural requirements of a contraction tree (degree-3 internal nodes, and so on):

1. As before, take the bare version of $\mathcal{T}_d$ from which all but the leaf labels have been struck. Grow the tree by attaching some $|V|$ new leaf nodes identified with $v \in V$. The attachment point for each $v$ may be an arbitrary $n$ such that $\text{edges}(v) \subseteq b(n)$; for example, the lexicographic minimum. Calling this new tree $\hat{\mathcal{T}}_d$, empty all its internal nodes’ bags entirely and refill them from $V$ based on the alternative labeling used in lemma 1 that is, by putting $e = \{v, v'\}$ into the path between $v$ and $v'$. Label the arcs correspondingly. $\hat{\mathcal{T}}_d$ with bags $\hat{\delta}_n$ at this point defines a valid tree-decomposition of $L$; properties 1 and 2 are trivially satisfied by the leaf nodes $v$, where we have $\hat{\delta}_v = \text{edges}(v)$. Property 3 is satisfied because the labeling $\hat{\delta}_n$ meets the stronger condition that the subgraph $\hat{\mathcal{T}}_d \{v \mid e \in \hat{\delta}_n\}$ induced, for any edge $e \in E$, is a path. Moreover, because $\hat{\delta}_n \subseteq b(n)$, thanks to the RIP, we know that the weighted width, $\text{ww}(\hat{\mathcal{T}}_d)$, cannot have grown.

All nodes left with empty bags should be contracted into their neighbors—as should nodes with degree 2. (This sub-step is unnecessary if we can stipulate from the start that no bag in $\mathcal{T}_d$ is a subset of another, a condition known in e.g. [8] as reduced form.) Any remaining degree-1 node must be one of the newly added leaves.

2. Label arcs using eq. 3. $\hat{\mathcal{T}}_d$ is now a free contraction tree, except that its internal nodes may not be—indeed, likely are not—ternary.

3. Each node with more than three arcs now gets split, with the process repeated until all that remain have degree 3. Let $n$ be an offending node, and let $a', a''$ be any two of its arcs. We split $n$ into two nodes $m', m''$ and connect them with a new arc $a'''$ so that

\[
\text{edges}(m') = \{a', a'', a'''\}
\]
\[
\text{edges}(m'') = \{a'''\} \cup (\text{edges}(n) \setminus \{a, a'\})
\]
with labels
\[
\hat{\delta}_{m'} = \hat{\delta}_a \cup \hat{\delta}_a',
\]
\[
\hat{\delta}_{m''} = \hat{\delta}_a \cup \hat{\delta}_a''.
\]

Note that this is the same labeling scheme used in lemma 1. Clearly, the widths of the bags of \( m' \) and \( m'' \) cannot be larger than that of \( n; \ |\text{edges}(m')| = 3 \) and \( |\text{edges}(m'')| = |\text{edges}(n)| - 1 \).

Remark. If desired, it is always possible to find a split of \( n \) so that at least one of \( m' \) or \( m'' \) has strictly smaller width. In nontrivial cases, that is, unless \( \exists v \in V \) such that \( \hat{\delta}_n = \text{edges}(v) \), the splitting process can be used as an opportunity to shrink both child nodes.

At this point, we have a free binary tree with \( |V(\hat{T}_d)| = 2|V| - 2 \) whose external nodes correspond one-to-one to the sets \( \{\text{edges}(v) \mid v \in V\} \). The resulting node- and arc-labeled tree forms a contraction tree, up to epimorphism. The entire process of trimming and relabeling can be done with, na"ıvely, time complexity in \( \mathcal{O}(|V| \cdot |E|) \).

\[\square\]

3.2 Carving-width and \( B^* \)

Introduced by Seymour and Thomas \([25]\) as an ancilla to a third tree-based metric, branchwidth, carving-width is the least well known of the three. Weighted-graph branchwidth and carving-width are notable for their own merit in addressing the ‘call-routing problem’ for telecoms. We will omit branchwidth from the discussion and proceed directly to carving-width. One prompt advantage over treewidth is that the edges-to-vertices interchange is fairly tight: the isomorphism between weights is merely a matter of transferring between the groups \((\mathbb{N}, +)\) and \((\mathbb{R}^*, \times)\).

**Theorem 3** (Free contraction tree \( \cong \) carving-decomposition). An arbitrary contraction tree \( T \), modulo its 3-cuts \( \delta_a \), is isomorphic to a carving-decomposition. \( B^*_T \) is equal, up to logarithmic concavity, to the carving-width:
\[
\text{carw}(G) = \log B^*_G.
\]

**Proof.** Straightforwardly, the 2-cuts of the contraction tree duplicate, by design, the branch structure of a carving-decomposition. The isomorphism between weights is merely a matter of transferring between the groups \((\mathbb{N}, +)\) and \((\mathbb{R}^*, \times)\). \[\square\]

3.3 \( B^*, B^t, \) and \( C^t \) united

**Theorem 4.** The asymptotic relationship between \( B^* \), \( B^t \), and \( C^t \) is fairly tight:
\[
B^* \leq B^t \leq (B^t)^{1.5}
\]
\[
B^t + 4(|V| - 3) \leq C^t \leq (|V| - 2)B^t
\]
whether taken with respect to a given contraction tree or its graph.

**Proof.** The left inequality of eq. 5, \( B^* \leq B^t \), is trivial. For the right, use the following lemma:

**Lemma 2.** For any internal node \( n \) in a free contraction tree with adjacent arcs \( a, a', a'' \),
\[
w_n = \sqrt{w_a w_{a'} w_{a''}}.
\]

**Proof.** By the inclusion-exclusion principle of measure theory,
\[
w_n = w_a w_{a'} w_{a''} \div \left( \prod_{e \in \delta_a \cap \delta_{a'}} w_e \cdot \prod_{e \in \delta_a \cap \delta_{a''}} w_e \cdot \prod_{e \in \delta_{a'} \cap \delta_{a''}} w_e \right) \times \prod_{e \in \delta_a \cap \delta_{a'} \cap \delta_{a''}} w_e.
\]

\[\text{The frankly more appealing } \text{cw}(G) \text{ is often seen, but that abbreviation can also mean cut-width, another tree complexity measure.}\]
Because our networks are not hypergraphs, the three-way intersection $\delta \cap \delta_{a'} \cap \delta_{a''}$ is always empty. Using set algebra, we can rewrite the large product that is the middle expression as

$$\prod \{ w_e \mid e \in (\delta_a \cap \delta_{a'}) \cup (\delta_a \cap \delta_{a''}) \cup (\delta_{a'} \cap \delta_{a''}) \}$$

$$\prod \{ w_e \mid e \in [\delta_a \cap (\delta_{a'} \cup \delta_{a''})] \cup [\delta_{a'} \cap (\delta_a \cup \delta_{a''})] \cup [\delta_{a''} \cap (\delta_a \cup \delta_{a'})] \}.$$ 

Recalling that $\delta_{a'} \cup \delta_{a''} = \delta_a \cup \delta_{a''} = \delta_a \cup \delta_{a'} = \delta_n$, from eq. 4 this reduces to

$$\prod \{ w_e \mid e \in (\delta_a \cap \delta_{a'}) \cup (\delta_{a'} \cap \delta_{a''}) \cap \delta_n \}$$

which is simply $w_n$. Thus $w_n = w_a w_{a'} w_{a''} / w_n$ as was intended.

Now assume $w_n = B_T$. Knowing that $a, a'$, and $a''$ cannot exceed $B_T$, then in the worst case we have $B_T = \sqrt{(B_T^G)^3}$, which finishes eq. 5. The same is true for $B_G$ and $B_D^T$ because $B_T$ cannot be worse than $(B_T^G)^{1.5}$ for the $T'$ with the best possible carving-width.

The inequalities of eq. 6 are merely the minimum and maximum possible when summing over all $|V| - 2$ contractions. In the case of the lower bound, the minimal $c'$-value for an individual contraction is 4. This is because, in order for $G$ to be connected, at most one out of the three 2-cuts which form $\delta(n)$ may be empty, with cut-weights $\geq 2$ for the other two.

Remark. It is not guaranteed that a $B^*$-optimal contraction tree should be $B^t$-optimal, or conversely. Figure 5 shows a simple $K_4$ graph for which the contraction tree indicated by $\{AB, CD\}$ is $B^*$-optimal, but that of $\{AC, BD\}$ is $B^t$-optimal.

![Figure 5: $B^*$ and $B^t$ uncorrelated. Edge labels are bond dimensions.](image)

4 Efficient computation of contraction orders for planar tensor networks

4.1 ‘Ratcon’

The Ratcatcher algorithm, which gets its name from a game theory analogy the authors of [25] use in their verification proof, addresses what is referred to as the call-routing problem: given a collection of calls made between a set of locations, design a network to route these calls such that the maximum network congestion is minimized. Provided the graph representing calls between locations is planar, Seymour and Thomas demonstrated that the decision problem of whether the maximum congestion, the carving-width, is less than some integer $k$ can be solved in polynomial time. The Ratcatcher is used as a subroutine in incrementally constructing a carving-decomposition for an input graph. Knowing that carving-width and $B^*$ are analogues under the isomorphism outlined in theorem 5, it is possible to find the minimal $B^*$ and a corresponding free contraction tree for a planar tensor network in polynomial time. In this section we review our implementation of the Ratcatcher algorithm and its use in constructing a rooted contraction tree with the corresponding carving-width, from which a space-optimal contraction order is derived. We will refer to the entire process as Ratcon.
4.2 Generation of sample planar tensor networks for experimentation

We describe now how we chose the tensor networks used to evaluate the performance of the Ratcon algorithm. We wanted our tensor networks to resemble those that occur naturally when describing and simulating interesting quantum many-body systems.

Matrix product states (MPS; e.g. [20]) play a popular role in simulating one-dimensional quantum systems. Because the network graph of such a system is a path, a MPS tensor can be contracted very efficiently by treating all contractions as matrix multiplications. Projected entangled pair states (PEPS; e.g. [29]) are a two-dimensional generalization of MPS whose subsystems correspond to the vertices of triangular, square, or hexagonal grids. Unfortunately, PEPS tensor networks cannot be contracted efficiently, and it is typically necessary to perform approximate instead of exact contractions when faced with simulating a system of more than several dozens of tensors. Singular value decomposition is the tool employed in these ‘truncation’ methods to reduce the bond dimensions of tensors that grow too large [23]. The goal of the present paper is understanding the computational cost when the contraction phase, at least, is as exact as possible. We would like to have an efficient algorithm for computing a close-to-optimal contraction ordering for PEPS networks, in order to bring the cost of exactitude down to the realm of the possibility for instances containing hundreds of tensors.

Figure 6: Ket tensor network for a PEPS state.

Figure 7: Bra-ket tensor network for a PEPS state.

Figure 6 shows a PEPS two-dimensional quantum state consisting of qubits arranged on a $5 \times 5$ grid. The perpendicular edges are free indices of weight 2 (because the state space of a qubit is a two-dimensional Hilbert space). The weights of the horizontal edges correspond to so-called bond dimensions and are in general nonuniform. Figure 7 shows a tensor network of a shape that often needs contracting to compute some interesting physical quantity, such as the expected value of an observable.

It is clear that this “bra-ket” graph is not planar and, thus, that it is not possible to directly apply the Ratcon algorithm. Naive ways of planarizing these graphs, such as “squashing” the upper and lower grids by prioritizing contraction of the vertical edges, tend to produce highly objectionable scores, because the dimensions of the virtual bonds get squared. To test the performance of the Ratcon algorithm, then, we have settled for considering half-graphs, that is, square grids that look like the graph in fig. 6 but without the free edges. Tests on the full PEPS forms are deferred until such time as an approximation extension into three dimensions can be found.

4.2.1 Lognormal prior

To find a domain which produces challenging, but not impossible, samples, we begin with square grid graphs—because of the relation to PEPS, and because of their high genera, with which they are naturally complex—and apply independent bond dimensions as edge weights, subject to acceptance-rejection testing. We wish to make as few assumptions about prior probabilities as possible. To restrict the space to “realistic” sizes, we reject any sample graph which would require more than 5TiB of working memory, assuming 16-byte complex-valued
A plain uniform distribution being useless under these restrictions, we use instead a normal prior—or rather lognormal, because every sample thereof can be rounded to a positive integer, and which should better reflect the exponential growth that occurs over the course of, for example, imaginary time evolution. The mean μ for the lognormal distribution, or rather \( \exp(\mu) \), varies with \( L \), set to the largest value for which a uniform grid would be contractible within the aforestated memory bounds. The standard deviation \( \sigma \) is allowed to vary from edge to edge, as a uniform, continuous, i.i.d. random variable. Maxima for \( \sigma \) are determined, for each \((L, \mu)\) pair in turn, by estimating, through a simple examination of a graphical plot of many candidates' \( B^* \) scores, where the probability of finding a graph meeting the feasibility criteria would drop, effectively, to zero. Only an upper bound is needed.

The object for this sample population, as filtered through the rejection criteria, is to represent graphs at the extreme of what can be done practically and without loss, where the contraction order will make the greatest difference.

### 4.3 Pre-processing of tensor networks

Once a tensor network for a given \( L \) has had its bond dimensions generated, the logarithmic mapping described in theorem
\footnote{The precise value they report is \( 2^{42} \) bytes.} is applied to the network. Unlike the original integral formulation of carving-width for the Ratcatcher, we now have real-valued, or rather floating-point, weights. This reduces the accuracy of the carving-width representation according to the arithmetic constraints of the architecture used.

Following the logarithmic mapping, the carving-width of the input graph is calculated using a modified binary search: the lower bound of this search begins at the largest fundamental bond dimension, and the upper bound is determined by incrementally and exponentially scaling a value \( k \) until the Ratcatcher reports that it has exceeded the carving-width. A conventional binary search is then conducted on the interval \([\frac{L}{2}, k]\) until the carving-width is found. The time complexity of the Ratcatcher component, which solves the decision problem at each iteration, is \( O(|V|^2) \) \footnote{Our colleagues provide in \cite{24} a more detailed explanation of ITE applied to PEPS, and how it motivated the search for better contraction heuristics.}.* The Ratcatcher is called \( \Theta(\log_2 B_G^*) \) times in this binary search and so runs in \( O(|V|^2 \cdot \log B_G^*) \) time. The algorithm is pseudopolynomial due to the dependency of carving-width on the total weight of the graph, and not the number of edges. Importantly, this proportionality to \( \text{carw}(G) = \log_2 B_G^* \) should only pose a problem when \( C^t \) is so large as to prohibit contraction—in which case the whole exercise would be pointless in practice.

With the carving-width now available, a carving-decomposition \footnote{As \( G \) is planar, \( E_G \in \Theta(V_G) \).} can be constructed using what is called by Hicks \footnote{Actually a ‘carving’, a set-theory isomorph of the carving-decomposition.} the edge-contraction algorithm, which incrementally locates eligible edges of the partially-contracted graph: an edge is eligible if its weight is no more than the carving-width of the current minor; if its contraction results in a minor that is also biconnected; and if this new minor has carving-width no more than that of the original \( G \).

To improve contraction total time, the edge-contraction procedure must be done more than once, because a typical graph supports many \( B^* \)-optimal contraction trees with widely varying \( C^t \) values. A simple compensation is to perform many random edge contractions and keep the best one. This makes the time complexity for this phase of processing \( O(N \cdot |V|^4 \cdot \log B_G^*) \), where \( N \) is chosen for the edge-contraction sample size.

### 4.4 Post-processing of carving-decompositions

The carving-decomposition returned by the edge-contraction phase is next used to generate a space-efficient contraction order. This step can be broken into two: rooting the carving-decomposition (free contraction tree) to yield a rooted contraction tree, which provides a contraction template with a locally-optimal time bottleneck, and then deriving a contraction order from that template. When rooting a free contraction tree, the goal is to minimize the resulting \( C^r \). Finding a location to root the tree is slightly dependent on whether the tensor network will be contracted sequentially or in parallel, i.e., whether multiple contractions can be done simultaneously.

Here we treat only the most straightforward case of a sequential time-optimal strategy, which means inserting a root node \( r \) into \( T \) so that \( C^r_T \) is minimized. Since \( C^t_T - C^r_T = w_r \), we have only to minimize the complexity \( w_r \) itself, which we can do very quickly by splitting the edge

\[
\arg \min_{e \in E_T} w_e
\]

and naming that new node as the root.
An always-optimal algorithm is described by Lam et al. [15]. and that the multiplicands and their product must be stored separately. This is not strictly optimal, because it reclaimed as soon as that tensor has been contracted with another, but not before the contraction has finished, node if cone else cost of contracting the left subtree first $\text{Contract left subtree first}$ seq = lseq + rseq + [contraction] return (seq, max \{c^*(n), lfirst\}, c^*(n)) else seq = rseq + lseq + [first] return (seq, max \{c^*(n), rfirst\}, c^*(n)) end if end if end procedure

Secondarily, we conserve memory in the process of generating a contraction sequence. We can now offer a measure of space complexity $C^*_G$, pursuant to the assumption that the resources for storing a tensor may be reclaimed as soon as that tensor has been contracted with another, but not before the contraction has finished, and that the multiplicands and their product must be stored separately. This is not strictly optimal, because it always fully contracts one of the subtrees before attending to the other, but is adequate for a proof of concept.

Let $T_r$ be a rooted contraction tree. For convenience, define $c^*(n)$ for every node. If $n$ is an endpoint of arc $a = \{n, n'\}$, where $n$ is farther from the root—deeper—than $n'$, then let

$$c^*(n) = w_a$$

with $c^*(r) = 1$. If $n$ is an internal node, we designate its child nodes as $n_l$ and $n_r$. Then

$$C^*(T_r) = C^*(r)$$

using the recursive definition

$$C^*(n) = \begin{cases} w_n & \text{if } n \in V_G \\ \max \left\{ \min \left\{ C^*(n_l) + c^*(n_r), c^*(n_l) + C^*(n_r) \right\} \right\} & \text{otherwise.} \end{cases} \quad (8)$$

Other post-processing optimization formulæ are possible if, for example, one wishes to trade space for time and attempt true simultaneous contractions. We have not taken that route, in part for simplicity, and in part because the concurrent element can be delegated to software libraries such as the Cyclops Tensor Framework [27].

The memory-conservation function $C^*(\cdot)$ is realized in algorithm [1] which constructs a concomitant concrete contraction sequence and returns it as a list of edges. If $w(\cdot)$ and $c^*(\cdot)$ are appropriately preempted, the time complexity of algorithm [1] remains $\Theta(|V|)$, which leaves Ratcon at $O(|V|^4 \cdot \log B_G^2)$. From the output sequence we may calculate $C^*$ in linear time.

### 4.5 Hardware

All tests have been conducted on AWS EC2 c5.large instances running Ubuntu 16.04 [10]. Ratcon-related processes are implemented in Python 3.6 and byte-compiled using PyPy 3.6 v7.1.0, approximately doubling their performance as compared to basic CPython. For Netcon, we use the authors’ original C++ backend [21], compiled through GCC 5.4.0 with -O3 optimization. There is also a MATLAB frontend which we have adapted to GNU Octave, but the C++ component accounts for more than 98% of the execution time. Our implementation of the Ratcatcher incorporates some, but not all, of the optimizations described in the $A_1$ implementation by Bian, Gu, and Zhu [5].

---

13 An always-optimal algorithm is described by Lam et al. [15].
Table 1: Results. All times presented are in seconds. \( \tau = \frac{\text{Ratcon time}}{\text{Netcon time}}, \rho = \frac{\text{Ratcon } C^t}{\text{Netcon } C^t}. \)

4.6 Experimental results

Table 1 summarizes the statistics after running both Netcon and Ratcon on 30 sample graphs per \( L \) value, with edge-contraction sample size \( N = 100, \) for \( L \in [5,10]. \) We use this range simply because for \( L < 5 \) the single-term optimization problem is too easy, and for \( L > 10 \) Netcon is too slow.

The ‘\( \text{carw()} \) time’ column records the time spent by the Ratcatcher solving the initial pseudopolynomial function problem, i.e., finding \( \text{carw}(G) = \log_2 B_G. \) ‘Ratcon time’ is this value plus the cumulative EC (edge contraction) time; ‘Average EC time’ is the mean iteration time thereof. ‘Ratcon \( C^t \)’ reflects the best contraction trees found for each graph.

For each graph Netcon was used to find the optimum \( C^t, \) unless its running time, given in the ‘Netcon time’ column, exceeded a predefined limit of 7200 seconds, or two hours, in which case it got prematurely terminated. This occurred for one \( L = 9 \) sample and fully sixteen out of thirty \( L = 10 \) graphs as Netcon reached its operational limits. Cells in the tables marked with an asterisk had these incomplete samples excluded from their calculation. \( \tau \) is the ratio of the running times on a graph-by-graph basis. Ratcon underperforms for small \( L, \) where the time lost in repeated ECs dominates, then becomes exponentially faster at \( L = 9 \) or 10. The last column, \( \rho, \) is the error factor in the total time estimation. For example, the mean 3.92 for \( L = 6 \) indicates that if a full tensor-network contraction were performed on one of these 36-vertex graphs, it could be expected to take four times as long using a Ratcon-derived contraction order as the best possible. The \( L = 9 \) mean is skewed, by an order of magnitude, due to a single outlier boasting an error factor of 249. We never obtained an \( \rho \) less than 30 for this particular graph, even after trying thousands of edge-contractions; we have to infer that this is one of the graphs for which the \( B^t \) approximation seldom or never results in a fast contraction order.

5 Conclusions and directions for future work

One way of applying these results is as follows. A tensor contraction requires taking an equal number of sums as products, nearly; for complex numbers, addition and multiplication use 2 and 6 floating-point operations, respectively; therefore \( 8 \cdot C^t_G \) gives a good lower bound on the number of arithmetic instructions to run a full contraction sequence. Referring to the statistics for the (completed) \( L = 10 \) experiments, we can say that if a contraction sequence takes 0.09 times as long to find with Ratcon but 3.36 times as long to execute, then the
tipping-even point is found by

\[
(3.36 - 1) \cdot \frac{8 \times 1.06 \cdot 10^{14}}{\text{FLOPS}} \leq (1 - 0.09) \times 4.25 \cdot 10^3
\]

\[
\text{FLOPS} \geq 5.17 \cdot 10^{11},
\]
suggesting that Ratcon would be the more efficient on a computer capable of 500 GFLOPS or better. In practice, we would recommend that the researcher always hedge her bets by running a Netcon search in parallel with contraction of a Ratcon-derived sequence. If Netcon comes up with a stronger sequence, she can restart the contraction and be none the worse.

Note that the times given are not intended as true benchmarks. Their purpose is mainly to demonstrate how the relative error remains small and at the same order of magnitude as grid size increases. Our Ratcatcher implementation is not especially heavily optimized and would be faster if it were rewritten in a statically-typed language such as C++, and included the rest of the enhancements proposed in [5, 11, 12]. The heuristic from algorithm [4] could be replaced by the algorithm from [13].

The greatest shortcoming of the Ratcatcher, obviously, is its planarity limitation. Extending \(B^s\)-optimization to general tensor networks would mean introducing another degree of approximation. Khuller, Raghavachari, and Young [13], for example, provide for an error factor of \(O(\log |V|)\) on the carving-width; however, in moving to the multiplicative ring, this would translate to a space bottleneck of \((B^s)^{O(\log |V|)}\).

The exponential bloat would apply equally if we preferred to switch to treewidth. \(B^t\) is intuitively closer than \(B^s\) to \(C_t\), and Dumitrescu et al. [3] report some (exact!) treewidth algorithms outperforming Netcon in speed. As previously mentioned, these apply only to unweighted graphs; we would need to adapt them to weighted treewidth [3], then use some form of the edge-contraction process to form a contraction tree.

Finally, inasmuch as the primary goal of this paper is to highlight the contraction tree datatype itself, there is no reason not to apply ML or other metaheuristic techniques directly to the construction of these trees. We have made a step in this direction with a simple genetic algorithm for evolving contraction sequences, included with the rest of the Ratcon source code, which may be found at https://github.com/TensorCon.

Acknowledgments

We would like to thank Illya Hicks for letting us use his Ratcatcher source code as a reference point for our own implementation; Robert Pfeifer and the American Physical Society for giving permission to redistribute Netcon; and Eduardo Mucciolo for sharing the graphics of figs. 6 and 7, as well as the term ‘bottleneck.’

This work was supported by National Science Foundation grant CCF-1525943.

References

[1] D. Aharonov, Z. Landau, and J. Makowsky. “The quantum FFT can be classically simulated”. In: eprint arXiv:quant-ph/0611156 (Nov. 2006). eprint: quant-ph/0611156.

[2] Stefan Arnborg, Derek G. Corneil, and Andrzej Proskurowski. “Complexity of finding embeddings in a k-tree”. In: SIAM JOURNAL OF DISCRETE MATHEMATICS 8.2 (1987), pp. 277–284.

[3] Emgad Bachoore and Hans L. Bodlaender. “Weighted Treewidth: Algorithmic Techniques and Results”. In: Algorithms and Computation: 18th International Symposium, ISAAC 2007, Sendai, Japan, December 17-19, 2007. Proceedings. Ed. by Takeshi Tokuyama. Berlin, Heidelberg: Springer Berlin Heidelberg, 2007, pp. 893–903. ISBN: 978-3-540-77120-3. DOI: 10.1007/978-3-540-77120-3_77. URL: https://doi.org/10.1007/978-3-540-77120-3_77.

[4] J. Biamonte and V. Bergholm. “Tensor Networks in a Nutshell”. In: ArXiv e-prints (July 2017). arXiv: 1708.00006 [quant-ph].

[5] Zhengbing Bian, Qian-Ping Gu, and Mingzhe Zhu. “Practical algorithms for branch-decompositions of planar graphs”. In: Discrete Applied Mathematics 199 (2016), pp. 156–171.

[6] Jacob C Bridgeman and Christopher T Chubb. “Hand-waving and interpretive dance: an introductory course on tensor networks”. In: Journal of Physics A: Mathematical and Theoretical 50.22 (2017), p. 223001. URL: http://stacks.iop.org/1751-8121/50/i=22/a=223001.

[7] M. de Oliveira Oliveira. “On the Satisfiability of Quantum Circuits of Small Treewidth”. In: ArXiv e-prints (Apr. 2014). arXiv: 1404.5565 [cs.CC].
[27] Edgar Solomonik et al. “A massively parallel tensor contraction framework for coupled-cluster computations”. In: Journal of Parallel and Distributed Computing 74.12 (2014). Domain-Specific Languages and High-Level Frameworks for High-Performance Computing, pp. 3176–3190. ISSN: 0743-7315. DOI: https://doi.org/10.1016/j.jpdc.2014.06.002 URL: http://www.sciencedirect.com/science/article/pii/S074373151400104X

[28] M. Van den Nest. “Classical simulation of quantum computation, the Gottesman-Knill theorem, and slightly beyond”. In: ArXiv e-prints (Nov. 2008). arXiv: 0811.0898 [quant-ph]

[29] F. Verstraete and J. I. Cirac. “Renormalization algorithms for quantum-many body systems in two and higher dimensions”. In: (2004). arXiv: cond-mat/0407066 [cond-mat]