Evaluating the Jones polynomial with tensor networks

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We introduce tensor network contraction algorithms for the evaluation of the Jones polynomial of arbitrary knots. The value of the Jones polynomial of a knot maps to the partition function of a \(q\)-state Potts model defined as a planar graph with weighted edges that corresponds to the knot. For any integer \(q\), we cast this partition function into tensor network form and employ fast tensor network contraction protocols to obtain the exact tensor trace, and thus the value of the Jones polynomial. By sampling random knots via a grid-walk procedure and computing the full tensor trace, we demonstrate numerically that the Jones polynomial can be evaluated in time that scales subexponentially with the number of crossings in the typical case. This allows us to evaluate the Jones polynomial of knots that are too complex to be treated with other available methods. Our results establish tensor network methods as a practical tool for the study of knots.

Knot theory is immensely interdisciplinary, with results and open questions spanning many fields of science, such as physics \cite{1–8}, quantum computation \cite{9, 10}, quantum cryptography \cite{11, 12}, chemistry and biology \cite{13–16}, study of every day life knotting of strands \cite{17}, and complexity theory \cite{18–21}. A key notion in knot theory is that of a knot \textit{invariant} — a quantity extracted from a knot which changes only under topology non-preserving knot operations, such as passing the knot through itself or cutting and recombing its strand. The Jones polynomial \(V_K(t)\) \cite{22} — a Laurent polynomial in \(t \in \mathbb{C}\) — is such one invariant that pervades knot theory. Knots \(K, K'\) are distinct if \(V_K(t) \neq V_{K'}(t)\). The Jones polynomial is thus pertinent to questions related to knottedness, such as the unknotting problem, a decision problem which is known to be in NP but unknown whether it lies in P \cite{23}. Hence, in addition to being central to the aforementioned applications of knot theory, evaluating the Jones polynomial is also a fundamental computational problem.

Exact evaluation of the Jones polynomial is generally a \#P-hard problem: computing \(V_K(t)\) takes time that is expected to scale exponentially with the number of crossings in a knot. Exceptions to this occur for \(t\) restricted to certain roots of unity, where \(V_K(t)\) corresponds to quantum amplitudes of a quantum field theory \cite{2}, understood as braiding of anyons \cite{24}. In particular, for \(t = \pm 1, \pm i, \pm e^{2\pi i/3}, \pm (e^{2\pi i/3})^2\), \(V_K(t)\) can be evaluated efficiently \cite{25}. Moreover, quantum algorithms can efficiently approximate the Jones polynomial at principal roots of unity in both the conventional quantum circuit model \cite{26, 27} and the setting of topological quantum computation \cite{28}. On the other hand, exponential classical algorithms that yield the \textit{full} expression for the Jones polynomial \cite{29–33} in the general case have been implemented and are readily usable, but have a relatively small reach (up to \(\sim 20\) crossings).

Many knot invariants are intimately connected to statistical mechanical models \cite{34}. The Jones polynomial, in particular, is related to the \(q\)-state Potts model \cite{35, 36}. Remarkably, the partition function \(Z(q)\) of a Potts model defined on a planar graph whose structure is defined by the topology of a knot \(K\) is essentially \(V_K(t(q))\) at

\[
t(q) = \frac{1}{2}(q + \sqrt{q(t^2 - 4)}),
\]

up to a normalization. Partition functions of classical models are of great interest in condensed matter physics and powerful algorithms have been developed to compute them, albeit mostly on graphs with periodic structure. Tensor network methods are an especially successful class of such techniques, which typically employ the renormalization-group procedure to efficiently approximate partition functions of classical lattice models very accurately \cite{37–43}. Recently, it was demonstrated that tensor network contraction schemes can also be very fast in obtaining the partition function of classical models \textit{exactly}, even on unstructured graphs and even when the underlying computation is a \#P-hard problem \cite{44}.

In this work, we exploit the connection with statistical mechanics and the efficiency of tensor network methods to evaluate the Jones polynomial in the general \#P-hard case. Specifically, we introduce tensor network contraction algorithms that evaluate \(V_K(t)\) at values of \(t\) away from the “easy” ones, yet achieve demonstrably advantageous computation times that indicate subexponential scaling as a function of the number of crossings in \(K\) for the \textit{typical} case. Our work thus furnishes a useful numerical tool for the evaluation of an essential knot invariant.

We begin with a preliminary review of the relation between the Potts model partition function and the Jones polynomial, starting with the relevant knot theory terminology. A knot \(K\) consists of an embedding of the circle \(S^1\) in \(\mathbb{R}^3\). A knot diagram is the projection of the knot to \(\mathbb{R}^2\), where the information about which strand is over which at every crossing is preserved. Intuitively, a knot diagram is what one produces when one attempts to draw a knot in two dimensions. Discarding the infor-
A knot can be oriented by choosing a direction along the strand. There are two ways to do this but they are equivalent. Each crossing obtains a twist sign \( \epsilon_c \), according to the direction of the strands exiting the crossing; if the strands cross in a clockwise (counterclockwise) fashion then the crossing obtains a positive (negative) twist sign. The sum of all the twist signs is called writhe, \( w_K = \sum_c \epsilon_c \), and characterizes the knot chirality. The Jones polynomial is sensitive to the knot chirality as it can distinguish mirrored knots.

For any knot diagram, a planar graph \( G \) called the Tait graph is defined as follows. The two-dimensional regions defined by the knot diagram can be bicoloured with, say, black and white, so that no two adjacent regions share a colour. There are two ways to do this, and so we choose the convention that the unique unbounded region is white. Then, vertices \( v \in V \), where \( V \) is the vertex set of \( G \), correspond to the black regions. Edges \( e = (v, v') \in E \), where \( (v, v') \in V \times V \) and \( E \) is the edge set of \( G \), are such that they connect black regions through the knot diagram crossings. The vertex degree is denoted \( d_v \) and counts the number of incident edges to that vertex. We have used the same symbol for crossings and the corresponding edges. The edges are decorated by Tait signs \( \varepsilon_c \) which are determined by the following rule. If the region to the left (right) is black when exiting a crossing on the over strand, then the crossing obtains a positive (negative) Tait sign. The sum of all tait signs is called Tait number, \( \tau_K = \sum_c \varepsilon_c \).

We now restate the relation between the \( q \)-state Potts model partition function \( Z(q) \) and the Jones polynomial \( V_K(t) \) of a knot \( K \) [45, 46]. A Potts model is placed on \( G \) by defining spins with \( q \) available states \( \sigma_v = 0, \ldots, q - 1 \) to reside on the vertices \( v = 1, \ldots, n_G \). The Tait-signs \( \varepsilon_c = \pm \) that decorate the Tait graph’s edges determine the interaction strength between spins, which take two corresponding values \( J_{\pm} \). Their relation with the Jones variable is \( e^{J_\pm} = -t^{\pm} \) and the Jones variable is determined by fixing \( q \in \mathbb{N} \) via Eq. (1). The Potts partition function over all spin-states \( \{ \sigma \} \) is

\[
Z(q) = \sum_{\{ \sigma \}} \prod_{\{ v, v' \}} T_{\sigma_v, \sigma_{v'}}^{\epsilon_{v, v'}}, \quad (2)
\]

\[
T_{\sigma_v, \sigma_{v'}} = 1 - (1 + t^{-\varepsilon_c})\delta_{\sigma_v, \sigma_{v'}}. \quad (3)
\]

Multiplying the partition function with the appropriate prefactor, which accounts for twists and ensures that the unknot returns \( V_\bigcirc = 1, \forall t \in \mathbb{C} \), we write

\[
V_K(t(q)) = A(q)Z(q), \quad (4)
\]

with \( A(q) = (1 - q^{\pm} - q^{-1})^{n_G} w_K(q) t^{\frac{1}{2} \tau_K} \).

Evaluation of \( Z(q) \) on arbitrary graphs is a \#P-hard problem [47]. Regardless of this complexity, in this work we will use tensor network methods [44] to obtain \( Z(q) \) for Tait graphs \( G \) exactly. From a graph \( G \) we construct a tensor network \( G_T \) encoding the Potts model as follows. Each vertex \( v \) is endowed with a spin tensor (also known as a COPY tensor) of the form

\[
\tilde{T}_{\{ \sigma_e \}_{i=1}^{d_v}}^{d_v} = \delta_{\sigma_{v_1}, \sigma_{v_2}, \ldots, \sigma_{v_d_v}}, \quad (5)
\]

which is a generalized \( q^{d_v} \)-dimensional Kronecker tensor. Each edge obtains a vertex on which we place the interaction tensor \( T \) of Eq. (3), which is always a \( q \times q \) matrix. Full contraction of \( G_T \) yields \( Z(q) \). This amounts to performing a sequence of tensor contractions, each being a dot product over the common index of two adjacent tensors in \( G_T \). The partition function is then equivalently expressed as

\[
Z(q) = \sum_{\{ \sigma \}} \prod_{\{ v, v' \}} T_{\sigma_v, \sigma_{v'}} \prod_v \tilde{T}_{\{ \sigma_e \}_{i=1}^{d_v}}^{d_v}. \quad (6)
\]

Every contraction step yields a graph minor \( H \) of the initial graph. Thus, when contracting a tensor network \( G_T \), there occurs at least one tensor of dimension equal to the maximal vertex degree over all minors \( \Delta_H = \max_H \max_v d_v \).

In general, finding the optimal contraction sequence so that \( \Delta_H \) grows favourably slowly, is an NP-complete
Figure 2. (Top) Scaling of average number of vertices $\langle n_v \rangle$ (triangles) and edges $\langle n_e \rangle$ (dots) (logscale) of simplified Tait graphs with the grid size $L$ (logscale) of the random grid walk. Dashed and solid red lines are linear fits on the last 15 data points with slopes 2.0132 and 2.0742, respectively. (Bottom) Ratio $\langle n_v \rangle / \langle n_e \rangle$ versus $L$ converging to $\sim 2$, compatible with the lower bound $1$ (dashed line) for random planar graphs. (Inset) Ratio versus $L$ (logscale) of average maximal degree $\langle \Delta G \rangle$ (dashed line) for random planar graphs for each $L$. We sampled 200 knots and error bars are standard mean error.

Figure 3. Scaling with grid walk size $L$ (top) and with crossing number $\sqrt{\langle n_c \rangle}$ (bottom) of average maximal degree $\langle \Delta H \rangle$ encountered under greedy (red squares) and METIS (green triangles) contraction of $G$. Solid lines are linear fits (on the last 10 data points) showing the asymptotic behaviour. Black dots represent average maximal degrees $\langle \Delta G \rangle$ of $G$. (Inset) Instance-by-instance comparison of $\Delta H$ for the two contraction methods. The same data is used as for Fig. 2. Data points $\langle n_c \rangle$ are obtained by binning the interval between max $n_c$ for min $L$ and min $n_c$ for max $L$ and placing symbols at the mean of each bin. This is due to the fact that by sampling graphs for each $L$ we obtain a finite-variance distribution over $n_c$. Error bars are standard mean error.

graph-theoretic problem [48–51]. Practical contraction schemes for tensor networks is an active field of research [52]. We employ contraction methods introduced in Ref. [44], here dubbed greedy and METIS, which were developed for fast evaluation of partition functions similar to $Z(q)$. In the greedy method, the “cheapest” edge contraction in terms of the resulting $\Delta H$ is performed. On the other hand, METIS heuristically constructs a separator hierarchy using the METIS algorithm [53], attempting to minimize the cut length while splitting the graph into comparably large components. The contraction is performed following the separator hierarchy in a coarse graining fashion. For details we point to Ref. [44]. We provide an example script demonstrating the evaluation of $V_K(t)$ in an online repository [54].

To investigate the performance of our numerical scheme, we require a procedure for generating random knots, whose Tait graphs we can use to evaluate the Jones polynomial. Since Tait graphs are planar and connected by construction, one may be tempted to just generate random connected planar graphs. However, not any planar connected graph corresponds to a knot shadow.

A generic planar connected graph corresponds to a link shadow, where a link is viewed as the embedding of multiple nonintersecting $S^1$ components. Instead, we employ the random grid walk method [55, 56] to sample random knot diagrams, ensuring by construction that the number of components is always one. A grid walk consists of horizontal segments and vertical segments, where vertical segments always pass over horizontal ones. The walk is encoded by a random permutation of coordinates $x, y \in S_L$, where $L$ is the linear grid size, and steps of the form $(x_i, y_i) \rightarrow (x_i, y_{i+1}) \rightarrow (x_{i+1}, y_{i+1})$. Since all knots have a grid walk representation, any knot is accessible via this procedure. An example grid walk is shown in Fig. 1 (bottom-left).

For a given orientation of the grid diagram, each crossing has a twist sign. All possible configurations are shown in Fig. 1 (top-left), and summing over them we obtain the writhe. The bicoloured knot along with its $G$ are shown Fig. 1 (bottom-right). Keeping in mind that vertical segments pass over horizontal ones, the colour pat-
tern around a crossing determines the Tait signs $\varepsilon_v$, as shown in Fig. 1 (top-right), and so the Tait number is readily available.

With a construction that allows us to randomly sample knots at hand, we now investigate properties of the corresponding Tait graphs $G$. First, we perform Reidemeister moves that leave the knot topology invariant but simplify the graph. In particular, a Reidemeister I introduces or removes a twist in the knot. We employ it to remove loops, i.e., edges of the form $(v, v)$, as well as spikes, i.e., degree-1 vertices, from the Tait graph. Note that a Reidemeister I move changes the writhe by 1. A Reidemeister II move amounts to overlaying a strand over or under another, or inversely combing the strands so they do not cross. These moves are usually referred to as poke and unpoke, respectively. In terms of $G$, we perform unpokes in order to remove double edges $c, c' = (v, v')$ with $\varepsilon_v = -\varepsilon_{v'}$. We then study the scaling of graph invariants of the resulting simplified graphs.

In Fig. 2 (top) we provide evidence for quadratic scaling of average number of vertices, $\langle n_v \rangle \sim L^2$, and average number of edges, $\langle n_e \rangle \sim L^2$, for simplified Tait graphs $G$ obtained by the random grid walk. In Fig. 2 (bottom) it is shown that the ratio of the average number of edges over the average number of vertices converges to $\sim 2$ as the size of the Tait graphs increases. This convergent behavior is compatible with the lower bound $\frac{\Delta_G}{c}$ of this ratio for random planar graphs [57]. Furthermore, for random planar graphs the average maximal degree $\langle \Delta_G \rangle$, defined as $\Delta_G = \max_v d_v$, scales logarithmically with the graph size [58]. This is also confirmed for the simplified Tait graphs sampled by the random grid walk, as shown in Fig. 2 (inset).

The central quantity of interest for the purposes of tensor network contraction is the maximal degree $\Delta_H$ encountered in the sequence of minors $H$ occurring during contracting $G$. This quantity characterizes the complexity of the algorithm, in the sense that runtime and memory requirements scale as $O(q^{\Delta_H})$.

In Fig. 3 we show the scaling of the average $\Delta_H$ with the grid-walk size $L$. We find an asymptotically linear scaling with $L$, which implies runtime scaling $O(q\sqrt{n_c})$. Both contraction methods perform similarly, with METIS exhibiting marginally better scaling, yet only outperforming greedy for larger graphs ($n_c \gtrsim 900$). We therefore use greedy to explicitly compute the time of the Jones polynomial for realistically accessible graph sizes. Results for the case of $q = 5$ are shown in Fig. 4. The favorable typical-case scaling allows us to comfortably evaluate the Jones polynomial at $q = 5$ for knots with $n_c > 40$. For comparison, the largest calculations of the full expression for the Jones polynomial reported in the literature are for $n_c = 22$ [29–33].

The main bottleneck in these benchmarks is memory usage. For each $n_c$, there are exceptional knots that yield atypically large $\Delta_H$ and thus evaluation of $V_K(t)$ requires contraction of large tensors. With larger $q$, these exceptional cases may overflow the available memory, even though typical cases with the same $n_c$ are easily amenable. For the $q = 5$ example in Fig. 4, such exceptional knots occur at $n_c = 48$. On the other hand, for any particular knot of interest, one can test various graph contraction schemes to find the most favorable $\Delta_H$ and thus gauge the resources required a priori.

In conclusion, we have developed a concrete methodology, based on tensor networks, for the evaluation of the Jones polynomial of arbitrary knots and demonstrated favorable performance of actual implementations. Due to the broad relevance of knot invariants, our methods have wide applicability: classification of knotted polymers [3], quantification of turbulence in classical and quantum fluids [5], and study of the Jones conjecture [59] are just a few examples of problems that require computation of knot polynomials. We therefore believe that the techniques introduced here can have multifaceted impact. They also admit several extensions. For example, it is possible to obtain the coefficients of $V_K(t)$ via polynomial interpolation between evaluations at a number of values of $t$ equal to the degree of $V_K(t)$, for which easily obtainable bounds exist [1]. Moreover, in analogy with condensed matter applications of tensor networks, where truncation of singular values along edges of the network lead to accurate approximations of a desired physical quantity, appropriate truncation procedures may allow one to obtain controlled approximations of the Jones polynomial, and potentially other knot invariants. It is also interesting to consider whether our algorithms can be extended to cases of $q \in \mathbb{R}$ [60, 61].

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Figure 4. Scaling of average runtime $\langle r_{Z(q)} \rangle$ of calculating $Z(q)$ for $q = 5$ via contracting $G_T$ with greedy as a function of $L$ (green triangles) and $n_c$ (red squares, error bars smaller than markers), as shown by the linear fits (solid lines). For each data point we sampled 1000 knots. The data for each $n_c$ was gathered by inverting the quadratic fit $\langle n_c \rangle(L)$ of Fig. 2 (Top) to obtain $L(\langle n_c \rangle)$ and sampling knots for the appropriate $L$ until we gather 1000 knots for each $n_c$ up to $n_c = 46$. Error bars are standard mean error. Calculations were performed on a single core of an Intel Core i7-5820K 3.30 GHz processor with 47 GiB RAM.
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