QUANTUM CIRCUITS AS CONTRACTION PROVIDERS FOR tnreason

RESEARCH NOTES IN THE ENEXA PROJECT

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By its central axioms, quantum mechanics of multiple qubits is formulated by tensors capturing states and discrete time evolutions. Quantum circuits are contractions of multiple tensors and therefore tensor networks, and measurement probabilities are given by contractions. Here we investigate how we can exploit these as contraction provider for tnreason .

1 Comparing tensor networks and quantum circuits

First of all, we need to extend to complex tensors, which are maps

$$\tau : \bigtimes_{k\in[d]} [2] \to \mathbb{C}$$

with image in $\mathbb{C}$ instead of $\mathbb{R}$ as in the report.

A coarse comparison of the nomenclature used for quantum circuits and tensor networks:

Quantum Circuit	**Tensor Network**
Qubit	Boolean Variable
Quantum Gate	Unitary Tensor
Quantum Circuit	Tensor Network on a graph

Some constraints appear for a tensor network to be a quantum circuit

- **Unitarity of each gate:** That is the variables of each tensor are bipartite into sets A^{in} and A^{out} of same cardinality and the basis encoding with respect to this bipartition, that is
$$T_{\mathrm{in}\to\mathrm{out}}[X_{\mathrm{in}}, X_{\mathrm{out}}] : \bigotimes_{k\in A^{\mathrm{in}}} \mathbb{C}^2 \to \bigotimes_{k\in A^{\mathrm{out}}} \mathbb{C}^2 \,,$$
is a unitary map, that is
$$(T_{\mathrm{in}\to\mathrm{out}})^H \circ (T_{\mathrm{in}\to\mathrm{out}}) = \left\langle T_{\mathrm{in}\to\mathrm{out}}[X_{\mathrm{in}}, Y], \overline{T}_{\mathrm{in}\to\mathrm{out}}[Y, X_{\mathrm{out}}]\right\rangle [X_{\mathrm{out}}, X_{\mathrm{in}}] = \delta\left[X_{\mathrm{out}}, X_{\mathrm{in}}\right].$$
- **Acylicity:** Incoming and outgoing variables of each tensor core provide a direction of each edge tensor. With respect to this directionality the graph underlying the tensor network has to be acyclic.
- **Incoming-Outgoing structure:** Variable appear at most once as incoming and at most once as outgoing variables. Those appearing either as incoming or as outgoing are the input and the output variables of the whole circuit.

The unitary tensors can be aligned layerwise, if and only if the last two assumption hold, i.e. the directed graph is acylic and each variable appears at most once as an incoming and at most once as an outgoing variable.

2 Encoding Schemes

We investigate here quantum pendants to the function encoding schemes used in tnreason .

2.1 Coordinate encoding

Definition 1. *Given a function $\mathbb{P} : \bigtimes_{k\in[d]}[2] \to \mathbb{R}^+$ with $\langle\mathbb{P}\rangle[\varnothing] = 1$ the coordinate encoding quantum state is*

$$\psi^{\mathbb{P}}[X_{[d]}] = \sum_{x_{[d]}\in\bigtimes_{k\in[d]}[m_k]} \sqrt{\mathbb{P}\left[X_{[d]} = x_{[d]}\right]} \cdot \epsilon_{x_{[d]}}\left[X_{[d]}\right] .$$

This coincides with the q-sample scheme of encoding in [Low et al. - Quantum Inference on Bayesian Networks].

2.2 Basis encoding

Definition 2. *Given a function $q : \bigtimes_{k\in[d]}[2] \to \bigtimes_{l\in[p]}[2]$ the basis encoding circuit is the unitary tensor*

$$\begin{aligned} &U^q[X_{\text{in},[d]} = x_{\text{in},[d]}, X_{\text{out},[d]} = x_{\text{out},[d]}, Y_{\text{in},q}, Y_{\text{out},q}] \\ &= \begin{cases} 0[Y_{\text{in}}, Y_{\text{out}}] & \textit{if} \quad X_{\text{in},[d]} \neq X_{\text{out},[d]} \\ \epsilon_0\left[Y_{\text{in}}\right] \otimes \epsilon_{q(X_{\text{in},[d]}=x_{\text{in},[d]})}\left[Y_{\text{out},q}\right] + \left(\mathbb{I}\left[Y_{\text{in}}\right] - \epsilon_0\left[Y_{\text{in}}\right]\right) \otimes \epsilon_{\neg q(X_{\text{in},[d]}=x_{\text{in},[d]})}\left[Y_{\text{out},q}\right] & \textit{else} \end{cases} \end{aligned}$$

Here by $\neg q$ we denote an arbitrary function which never coincides with q.

The decomposition by contraction property of basis encodings is now a composition of circuits property, as stated in the next lemma.

Lemma 1. *We have for functions $q : \bigtimes_{k\in[d]}[2] \to \bigtimes_{l\in[p]}[2]$, $g : \bigtimes_{l\in[p]}[2] \to \bigtimes_{s\in[r]}[2]$*

$$\begin{aligned} U^{g\circ q}[X_{\text{in},[d]}, X_{\text{out},[d]}, Y_{\text{in},g\circ q}, Y_{\text{out},g\circ q}] = \big\langle &\epsilon_0\left[Y_{\text{in},q}\right], \\ &U^q[X_{\text{in},[d]}, X_{\text{out},[d]}, Y_{\text{in},q}, Y_{\text{out},q}], \\ &U^g[Y_{\text{out},q}, Y_{\text{out},}, Y_{\text{in},g\circ q}, Y_{\text{out},g\circ q}]\big\rangle\left[X_{\text{in},[d]}, X_{\text{out},[d]}, Y_{\text{in},g\circ q}, Y_{\text{out},g\circ q}\right] . \end{aligned}$$

Concatenating two basis encoding circuits is the basis encoding circuit of their modulus 2 sum.

A basis+ elementary function can be encoded by a single controlled NOT operation with auxiliary X qubits.

This motivates the mod2-basis+ CP decomposition of tensors.

Definition 3. *Given a boolean tensor τ, a mod2-basis+ CP decomposition is a collection $\mathcal{M}$ of tuples (A, x_A) with such that for any $x_{[d]} \in \bigtimes_{k\in[d]}[m_k]$*

$$\tau\left[X_{[d]} = x_{[d]}\right] = \bigoplus_{(A,x_A)\in\mathcal{M}} \langle\epsilon_{x_A}\left[X_A\right]\rangle\left[X_{[d]} = x_{[d]}\right] .$$

Having a mod2-basis+ CP decomposition of rank r to a connective, we need r controlled NOT gates to prepare the basis encoding. Given a syntactical decomposition of a boolean statistics, we prepare the basis encoding as a circuit with:

- **Fine Structure:** Represent each logical connective based on its mod2-basis+ CP decomposition, as a concatenation of basis encoding circuits with the same variables.
- **Coarse Structure:** Arrange the logical connective representing circuits according to the syntactical hypergraph, where parent head variables appear as distributed variables at their children.

3 Representing Computation Activation Networks as Quantum Circuits

$\mathrm{tnreason}$ provides tensor network representations of knowledge bases and exponential families following a Computation Activation architecture. Here are some ideas to utilize quantum circuits for sampling Computation Activation Networks.

3.1 Value Qubits

We introduce a value qubit, which stores in its coefficient to the first state the probability of the configuration. When we have a probability tensor, this can be prepared, since all values are in $[0, 1]$. The value qubit is intialized by the zeroth one hot encoding ($|0\rangle$) and rotated by a controlled rotation gate, which is controlled by the variable qubits.

3.2 Polynomial Sparsity

Each monomial can be prepared by a multiple-controlled NOT gate, where the control qubits are the affected variables and the target qubit is the value qubit. When we sum monomials wrt modulus 2 calculus, then the preparation is a sequence of such circuits. In such way, we can prepare any propositional formula.

3.3 Decomposition Sparsity

We can decompose any propositional formula into logical connectives and prepare to each a modulus 2 circuit implementation. This works, when the target qubit of one connective is used as a value qubit of another.

3.4 Quantum Rejection Sampling

Note, that the variable qubits are uniformly distributed when only the computation circuit is applied. When sampling the probability distribution, we need the value qubit to be in state 1 in order for the sample to be valid. Any other states will have to be rejected.

Classically, this can be simulated in the same way: Just draw the variables from uniform, calculate the value qubit by a logical circuit inference and accept with probability by the computed value.

For this procedure to be more effective (and in particular not having an efficient classical pendant), we need amplitude amplification on the value qubit. This can provide a square root speedup in the complexity compared with classical rejection sampling.

4 POVM measurements as contractions

The main difficulty of using quantum circuits as contraction providers is that we can only extract information through measurments. Therefore measurement is the only way to execute contractions of the circuit, which come with restrictions when interested in contraction with open variables.

The most general measurement formalism is through a POVM, a set $\{E_y \,:\, y \in [r]\}$ of positive operators with

$$\sum_{y\in[r]} E_y = I$$

Measuring a pure state $|\psi\rangle$ We then get outcome m with probability

$$\langle\psi|E_y|\psi\rangle$$

We define a measurement variable Y taking indices $y \in [r]$ and a measurement tensor

$$E[Y, X_{\mathrm{in}}, X_{\mathrm{out}}]$$

with slices

$$E[Y = y, X_{\mathrm{in}}, X_{\mathrm{out}}] = E_y \,.$$

Repeating the measurement asymptotically on a state $|\psi\rangle$ prepared by a quantum circuit $\tau^{\mathcal{G}}$ acting on the trivial start state $\mathbb{I}$, we denote the measurement outcome by y^j. In the limit $m \to \infty$ we get almost surely

$$\frac{1}{m}\sum_{j\in[m]} \epsilon_{y^j}\left[Y\right] \to \left\langle \tau^{\mathcal{G}}[X_{\mathrm{in}}], E[Y, X_{\mathrm{in}}, X_{\mathrm{out}}], \tau^{\tilde{\mathcal{G}}}[X_{\mathrm{out}}]\right\rangle [Y] \,.$$