

# Quantum Computation - Lecture 09 - Quantum Simulation

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A tree decomposition of a graph  $G$ :

- A tree  $\mathcal{T}$
- A function that maps each vertex  $w \in V(\mathcal{T})$  to a subset  $B_w \subseteq V(G)$ .
  - ▶  $\bigcup_{v \in V(\mathcal{T})} B_v = V(G)$
  - ▶  $\forall \{u, v\} \in E(G), \exists w \in V(\mathcal{T}), \{u, v\} \subseteq B_w$
  - ▶  $\forall u \in V(G)$  the set of vertices  $w \in V(\mathcal{T})$  with  $u \in B_w$  form a connected subtree.
- Width of a tree:  $\max_{w \in V(\mathcal{T})} |B_w| - 1$

- Equivalent definition: Elimination Width:
- Let  $\pi$  be an ordering of the vertices of  $G$ .
- Start with  $\pi(1)$ .
- Add an edge connecting any two pair of neighbors of  $\pi(1)$  that were not previously adjacent.
- remove  $\pi(1)$ .
- Restart the process with  $\pi(2)$  and so on...
- The induced width of a vertex is the number of neighbors of a vertex at the time it is being eliminated.
- The elimination width is equal to the tree-width.

- State Space of a Qubit:  $\mathcal{H} = \mathbb{C}^2$
- Basis for  $\mathcal{H}$ :  $|0\rangle, |1\rangle$
- Space of operators on a vector space  $V$ :  $L(V)$
- Density Operator on  $n$  qubits:  $\rho \in L(\mathcal{H}^{\otimes n})$ , with  $Tr(\rho) = 1$ .
- If  $x = x_1x_2\dots x_n \in \{0, 1\}^n$  then  $\rho_x = \otimes_{i=1}^n |x_i\rangle\langle x_i|$  is a density operator of the state  $|x\rangle = \otimes_{i=1}^n |x_i\rangle$ .

- Graph of a quantum circuit  $C$ :  $G_C$ 
  - ▶ A vertex  $v_U$  for each gate  $U$ .
  - ▶ A vertex  $v_i$  for each input  $i$
  - ▶ A vertex  $v_o$  for each output  $o$
  - ▶ An edge  $(v_U, v_{U'})$  if an output of  $U$  is an input of  $U'$ .

- Rank- $k$  tensor in an  $m$ -dimensional space  $g = [g_{i_1, i_2, \dots, i_k}]$  is a  $m^k$ -dimensional array
- rank-0 tensor: Complex number
- rank-1 tensor: vector
- rank-2 tensor: Usual Matrix

- Here we will be interested in dimension-4 tensors
- Each index of the tensor will run through the set

$$II = \{|0\rangle\langle 0|, |0\rangle\langle 1|, |1\rangle\langle 0|, |1\rangle\langle 1|\} \quad (1)$$

- Tensor associated to a density operator  $\rho$ :

$$\rho_{\sigma_1, \sigma_2, \dots, \sigma_a} = \text{tr}(\rho \cdot (\otimes_{i=1}^a \sigma_i)^\dagger) \quad (2)$$

- Tensor associated to a superoperator  $Q$  acting on  $a$  input qubits and  $b$  output qubits.

$$Q_{\sigma_1, \dots, \sigma_a, \tau_1, \dots, \tau_b} = \text{tr}(Q(\otimes_{i=1}^a \sigma_i) \cdot (\otimes_{j=1}^b \tau_j)^\dagger) \quad (3)$$

- $g = [g_{i_1, \dots, i_l, j_1, \dots, j_k}]$
- $h = [h_{i_1, \dots, i_l, j'_1, \dots, j'_{k'}}]$
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$$f_{j_1, \dots, j_k, j'_1, \dots, j'_{k'}} = \sum_{i_1, \dots, i_l} g_{i_1, \dots, i_l, j_1, \dots, j_k} \cdot h_{i_1, \dots, i_l, j'_1, \dots, j'_{k'}} \quad (4)$$

- If all outputs of a density matrix  $\rho$  are connected to the inputs of  $Q$  then the contraction of  $\rho$  and  $Q$  gives the tensor corresponding to the density matrix  $Q\rho Q^\dagger$ .



- Measurement scenario on  $m$  qubits:  $\tau : [m] \rightarrow L(\mathbb{C}^2)$  such that  $\tau(i)$  is a single-qubit POVM measurement element.
- If a qubit is not to be measured we can set  $\tau(i) = I$
- Contracting all the gates to the single output measurement gives the output probability.

- Contraction of an edge  $e$ : removes  $e$  and replaces its end vertices with a single vertex.
- Contraction ordering: Ordering of the edges of  $G$

$$\pi : \pi(1), \pi(2), \dots, \pi(|E(G)|)$$

- Complexity of  $\pi$  is the maximum degree of a merged vertex during the contraction process.
- Contraction complexity of  $G$ :  $cc(G)$  is the minimum complexity of a contraction ordering.
- Obs: Only the degree of the merged vertex count: For instance, if  $G$  is a path  $cc(G) = 1$  and  $\Delta(G) = 2$

- Line Graph of  $G$ :  $G^*$  whose vertices are the edges of  $G$  and two vertices  $e_1, e_2$  of  $G^*$  are connected if  $e_1 \cap e_2 \neq \emptyset$ .
- For any graph  $G$ ,  $cc(G) = tw(G^*)$
- Given a tree decomposition of  $G^*$  of width  $d$ , one can determine efficiently a contraction ordering  $cc(\pi) \leq d$ .
- Robertson-Seymour: There is a deterministic algorithm that given a graph  $G$  outputs a tree decomposition of  $G$  of width  $O(tw(G))$  in time  $|V(G)|^{O(1)} \exp[O(tw(G))]$ .
- $(\frac{tw(G)-1}{2}) \leq tw(G^*) \leq \Delta(G)(tw(G) + 1) - 1$
- Corollary: If the gates of a quantum circuit have at most  $d$  outputs, we have that

$$(tw(G) - 1)/2 \leq cc(G) = tw(G^*) \leq d(tw(G) + 1) - 1$$