Classical Simulation of Quantum Computation

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Definition

- ***Classical simulation of a quantum system***
- the techniques for efficiently simulating quantum circuits on a classical computer

- ***Quantum simulation***
- a branch of quantum technology that studies the structures and properties of electronic or molecular systems

Strong vs Weak Simulation

Definition 9.1 *Strong simulation* aims to *calculate the probabilities* of the output measurement outcomes efficiently with high accuracy using a classical computer.

$$P(\alpha), \forall \alpha$$

Definition 9.2 *Weak simulation* aims to *sample once* from the output distribution efficiently using a classical computer.

$$P(0 \dots 0)$$

- They are different
- Strong simulation $\longrightarrow$ weak simulation

Distance Measures

Definition 9.3 The *total variation distance* between p and q is defined as

$$\mathrm{d_{TV}}(p,q) = \frac{1}{2}\sum_{i=1}^{d}|p_i - q_i| = \frac{1}{2}||p - q||_1.$$

The total variation distance, which takes value between 0 and 1, measures the worst probability discrepancy between a sample from p and a sample from q, i.e., $\mathrm{d_{TV}}(p,q) = \max_{x\in\Omega} |\mathbf{Pr}_p[x] - \mathbf{Pr}_q[x]|$.

Distance Measures

Definition 9.4 The ℓ_2 *distance* between p and q is defined as

$$\mathrm{d}_{\ell_2}(p,q) = \left(\sum_{i=1}^{d}(p_i - q_i)^2\right)^{1/2} = ||p-q||_2.$$

The ℓ_2 distance, which takes value between 0 and $\sqrt{2}$, is related to the total variation distance by $\mathrm{d}_{\ell_2}(p,q) \leq 2\mathrm{d}_{\mathrm{TV}}(p,q) \leq \sqrt{d}\,\mathrm{d}_{\ell_2}(p,q)$.

Distance Measures

Definition 9.5 The *Hellinger distance* between p and q is defined as

$$\mathrm{d_H}(p, q) = \left(\sum_{i=1}^{d} (\sqrt{p_i} - \sqrt{q_i})^2 \right)^{1/2}.$$

The Hellinger distance, which take value between 0 and $\sqrt{2}$, is related to the total variation distance by $\mathrm{d}_\mathrm{H}^2(p, q) \leq 2\mathrm{d}_\mathrm{TV}(p, q) \leq 2\mathrm{d}_\mathrm{H}(p, q)$.

Distance Measures

Definition 9.6 The *trace distance* between two mixed states ρ and σ is defined as

$$D_{tr}(\rho, \sigma) = \frac{1}{2}||\rho - \sigma||_1 = \frac{1}{2}\text{tr}\left(\sqrt{(\rho - \sigma)^\dagger(\rho - \sigma)}\right).$$

The trace distance, which takes value between 0 and 1, can be viewed as the quantum analogue of the total variation distance, in that D_{tr} calculates the maximum probability that two states ρ and σ can be discriminated by measurements.

Distance Measures

Definition 9.7 The *Hilbert–Schmidt distance* between ρ and σ is defined as

$$D_{HS}(\rho, \sigma) = ||\rho - \sigma||_F = \operatorname{tr}\left((\rho - \sigma)^2\right)^{1/2},$$

where $||\cdot||_F$ is also called the Frobenius norm. The Hilbert–Schmidt distance is the quantum analogue of the ℓ_2 distance. It relates to the trace distance by $D_{HS}(\rho, \sigma) \leq 2\, D_{tr}(\rho, \sigma) \leq \sqrt{d}\, D_{HS}(\rho, \sigma)$.

Distance Measures

Definition 9.8 The *Bures distance* between ρ and σ is defined as

$$\mathrm{D_B}(\rho, \sigma) = (2(1 - F(\rho, \sigma)))^{1/2},$$

where $F(\rho, \sigma) = ||\sqrt{\rho}\sqrt{\sigma}||_1$ is the fidelity between the two mixed states ρ and σ. The Bures distance is the quantum analogue of the Hellinger distance. It relates to the trace distance by $\mathrm{D_B^2}(\rho, \sigma) \leq 2\mathrm{D_{tr}}(\rho, \sigma) \leq 2\mathrm{D_B}(\rho, \sigma)$.

Simulation Techniques covered

- Density Matrices: the Schrodinger picture
- Stabilizer Formalism: the Heisenberg picture
- Tensor Network
- Graphical Models

Density Matrices: the Schrodinger picture

Through time, a quantum state is evolved to another by some unitary transformation U:

$$|\psi(0)\rangle \xrightarrow{time} |\psi(t)\rangle = U\,|\psi(0)\rangle\,.$$

Probability of an outcome x *(*$U=U_m \ldots U_2\, U_1$*)*

$$p(x) = |\,\langle x|U|0\ldots 0\rangle\,|^2.$$

- weak simulation vs strong simulation

- *# of qubits* 2^n
- *# of multiplications* $O(2^{2n})$ *and then summing them*
- *time cost =* $O\,(m2^{2n})$

Stabilizer Formalism: the Heisenberg picture

$$A(0) \xrightarrow{time} A(t) = U^\dagger A(0) U$$

Definition 9.9 A quantum gate is a *stabilizer gate* if it is generated from the Clifford group $S = \langle \text{CNOT, H, S} \rangle$. In other words, it is a product of $g \in S$.

For example, all Pauli gates belong to this set: $X = HZH$, $Y = iXZ$, $Z = SS$. Notice that a stabilizer gate S conjugates a gate from the Pauli group back to the Pauli group: $SP_i S^\dagger = P_j$ up to a phase factor, where $P_i, P_j \in \mathcal{P}$.

Definition 9.10 A state is a *stabilizer state* if it can be prepared from $|00\ldots0\rangle$ using stabilizer gates.

Definition 9.11 A quantum circuit is called a *stabilizer circuit* if it is made of stabilizer gates applied on input state $|00\ldots0\rangle$, and measurements in the computational basis.

Stabilizer Formalism: the Heisenberg picture

Definition 9.12 $|\psi\rangle$ is stabilized by a quantum circuit U, if $U|\psi\rangle = |\psi\rangle$.

Theorem 9.13 Gottesman–Knill theorem [362] *states that there exists classical algorithm that simulates any stabilizer circuit in polynomial time.*

In simulation, we do not need to keep track of the amplitudes of state vector anymore; rather we can keep track of the stabilizer operators. Let us now examine how to update the stabilizer group when applying a quantum gate:

$$|+\rangle \otimes |0\rangle \xrightarrow{I \otimes H} |+\rangle \otimes |+\rangle .$$

Tensor Network

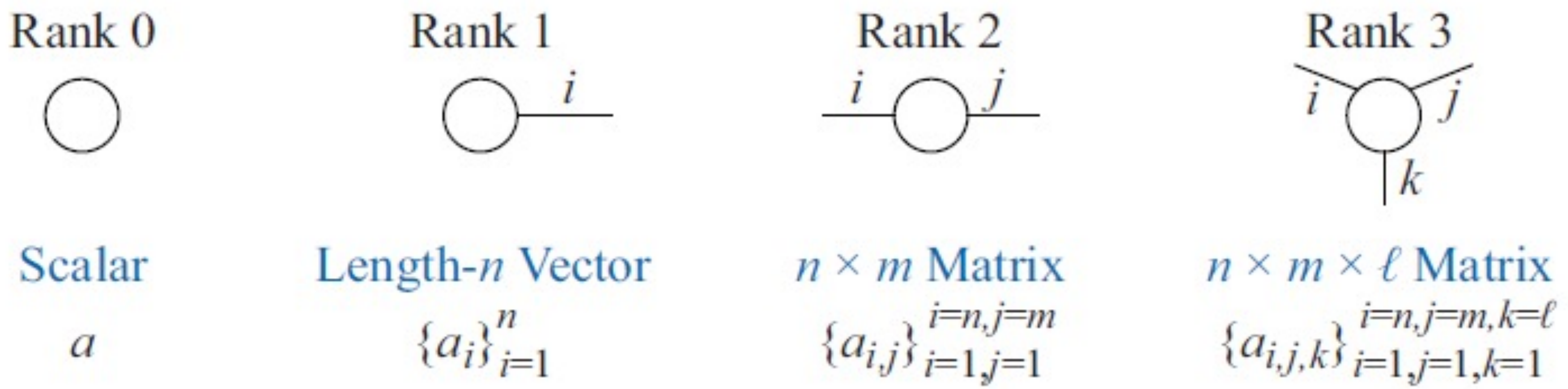

Figure 9.1: Graphical representation of tensors and their mathematical definitions.

Tensor Network

- Qubit state: vector $\rightarrow$ 1-d tensor.
- Single-qubit gate: 2×2 matrix (i.e., qubit input index (column) and qubit output index (row)) $\rightarrow$ 2-d tensor.
- Two-qubit gate: instead of a 4×4 matrix, we can index an entry by 4 indices, namely the qubit 1 input, the qubit 1 output, the qubit 2 input, and the qubit 2 output $\rightarrow$ 4-d tensor.

Tensor Network

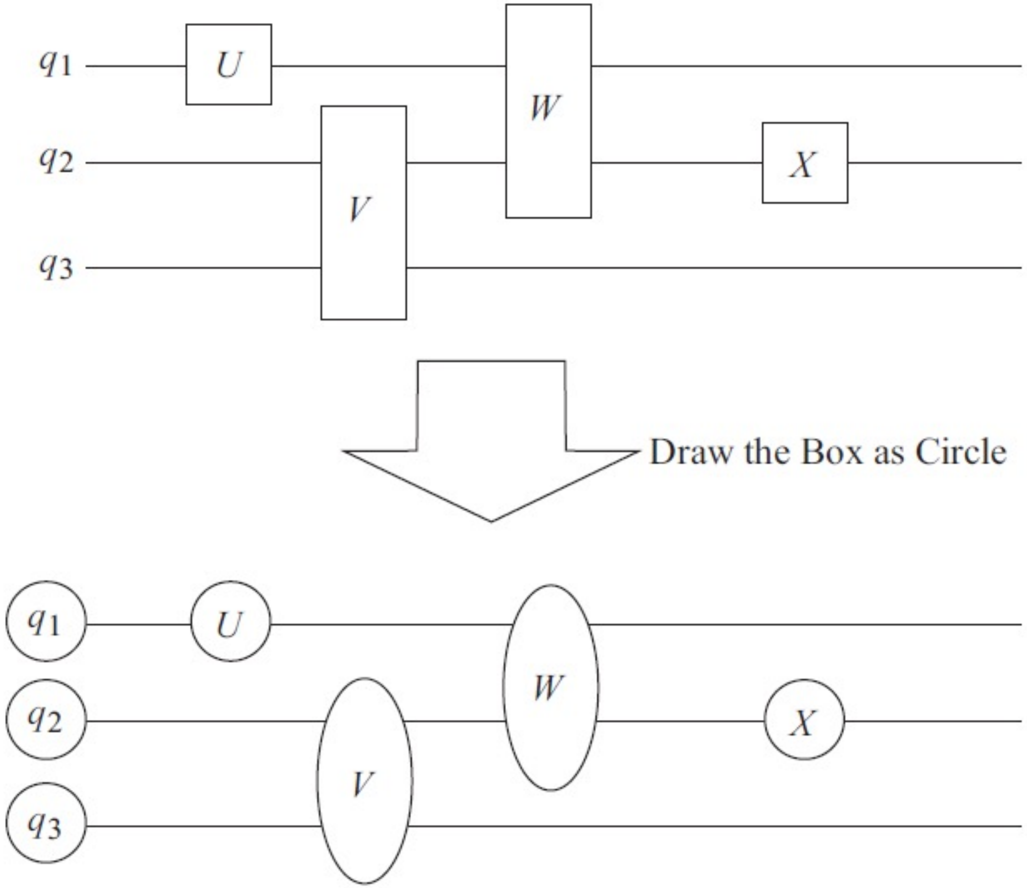

Figure 9.2: Converting from a quantum circuit to a tensor network.

Tensor Network Contraction

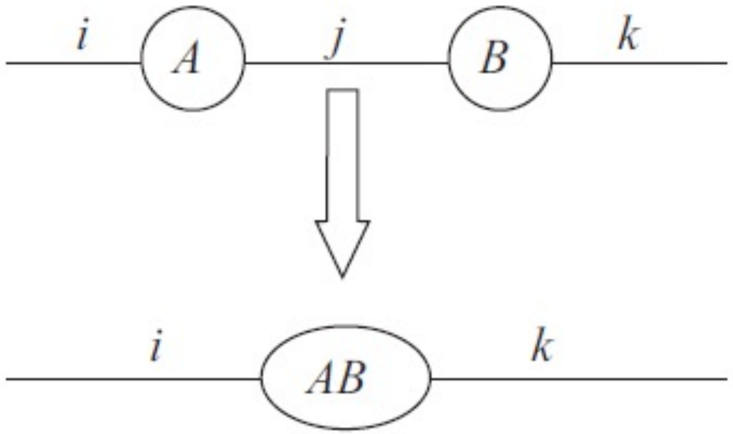

Figure 9.3: Contracting two rank-2 tensors, A and B, is equivalent to the matrix multiplication $C = AB$.

Tensor Network Contraction

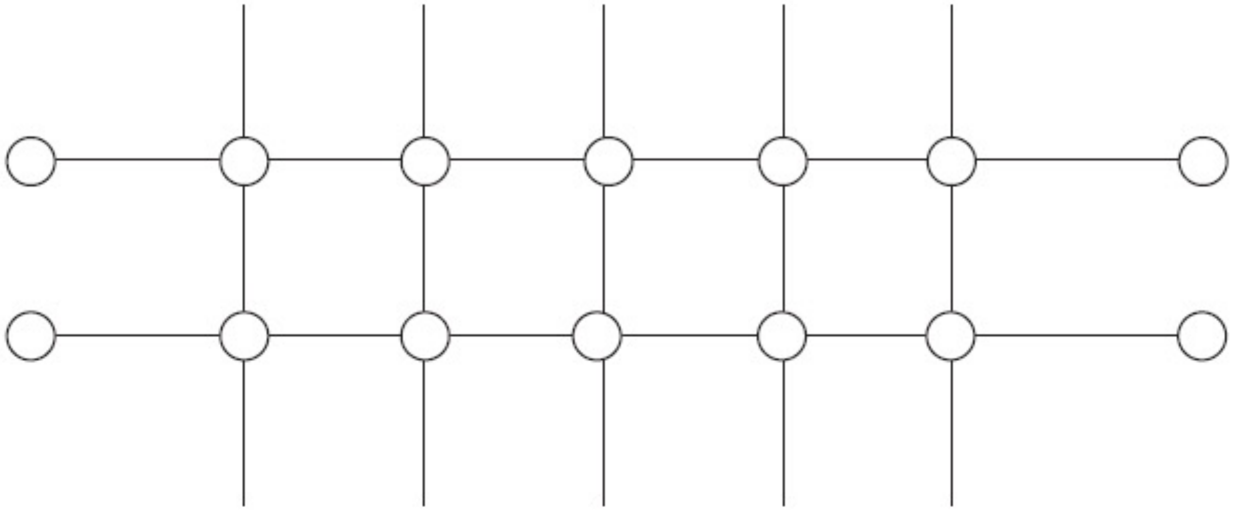

Figure 9.4: Part of a generic tensor network, consisting of ten rank-4 tensors and four rank-1 tensors.

$$\sum_j A_i^j B_j^k = C_i^k .$$

Tensor Network Contraction

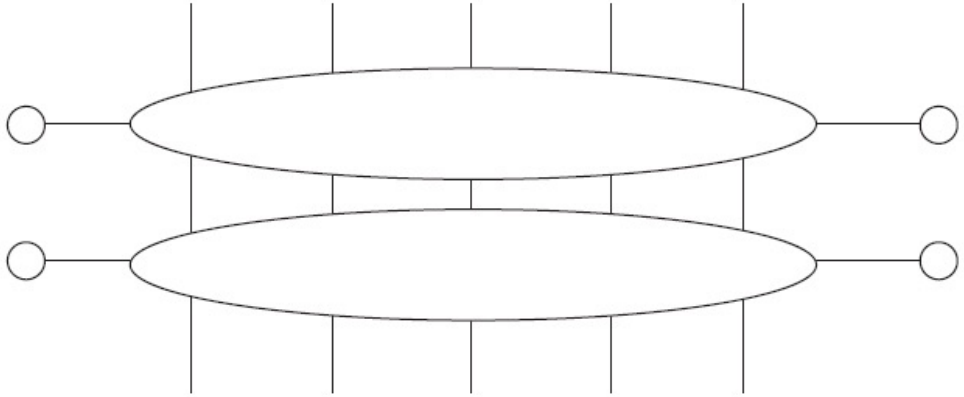

Figure 9.5: First strategy of contraction that results in two rank-12 tensors and four rank-1 tensors. Then contracting the two rank-12 tensors involves contracting 5 edges at once, by summing over 2^5 terms.

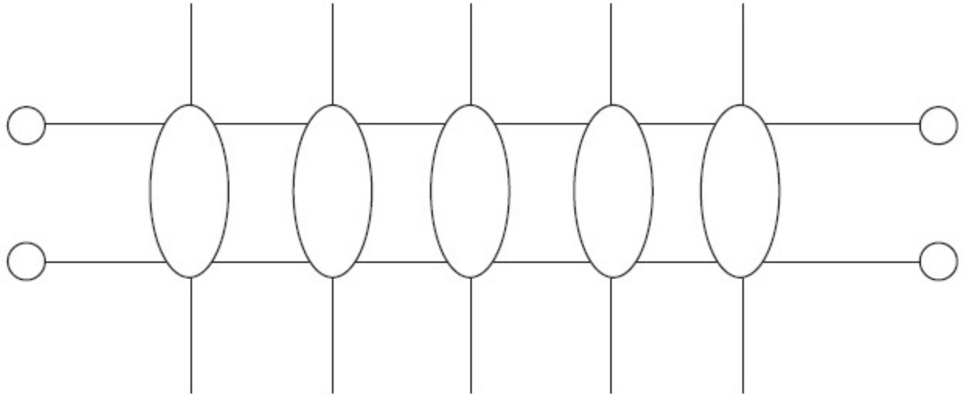

Figure 9.6: Second strategy of contraction that results in five rank-6 tensors and four rank-1 tensors. Then contracting the five rank-6 tensors involves contracting from left to right 2 edges at a time, by summing over 2^2 terms four times.

Tensor Network -> Undirected Graphical Models

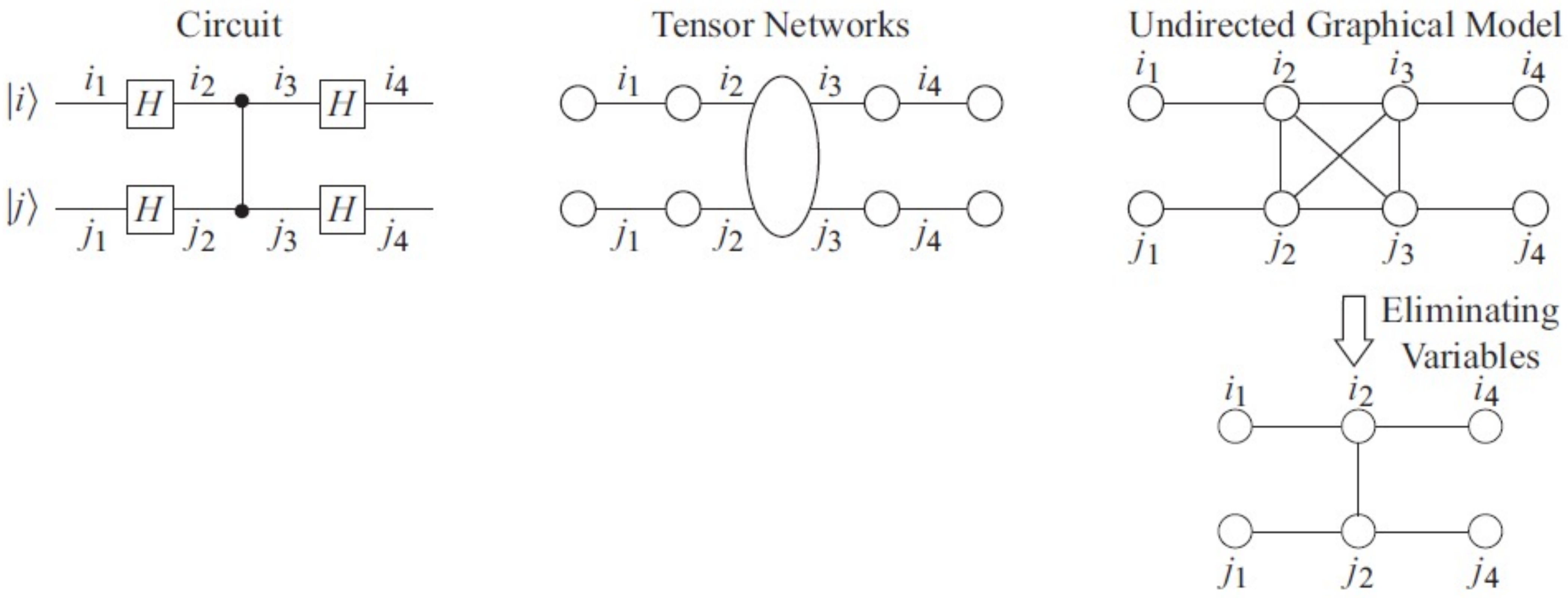

Figure 9.7: Converting from a quantum circuit, to a tensor network, then to an undirected graphical model. Note on bottom-right panel is the reduced graph using a technique called variable elimination.

Undirected Graphical Models

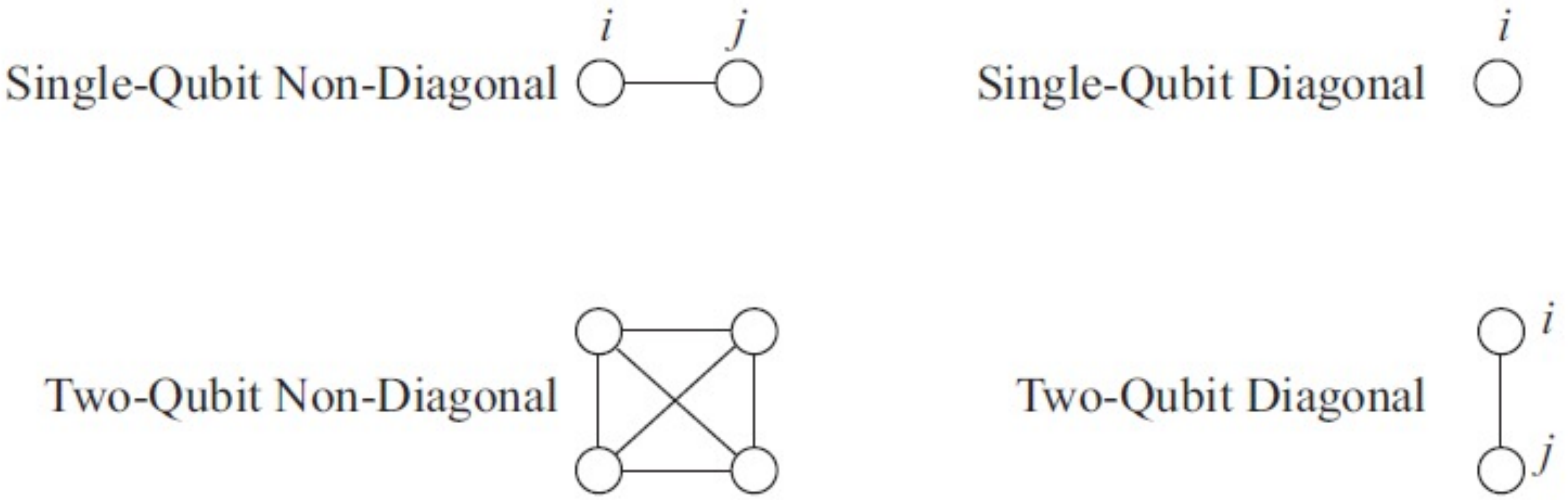

Figure 9.8: In the undirected graphical model, diagonal gates have simplified graph components with fewer indices to sum over.

QUESTIONS & COMMENTS?