Quantum Gates, Circuits, and Entanglement

EVA: Quantum Machine Learning – Lecture 2

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Roadmap

1. Single-qubit gates and matrix action
2. Multi-qubit systems and tensor products
3. Entanglement: Bell and GHZ states
4. Quantum circuits as computational graphs

Practice session follows this lecture: math tasks M2.1–M2.4 and programming tasks P2.1–P2.4.

Single-qubit gates

Convention reminder

In circuit notation, each qubit starts in

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

unless a different preparation step is shown.

To start from another state:

- apply X to prepare $|1\rangle$
- apply H to prepare $|+\rangle$
- apply explicit initialization (software level)

Quantum gates as unitary operators

A valid gate U is unitary:

$$U^\dagger U = I$$

For a state $|\psi\rangle$, gate action is linear:

$$\left|\psi'\right\rangle = U\,|\psi\rangle$$

Why unitarity matters:

- preserves normalization $\|\psi\| = 1$
- gives reversible evolution before measurement

Pauli gates X, Y, Z

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Gate	Action on $\|0\rangle$	Action on $\|1\rangle$
X	$\|1\rangle$	$\|0\rangle$
Y	$i\,\|1\rangle$	$-i\,\|0\rangle$
Z	$\|0\rangle$	$-\,\|1\rangle$

`lecture_02_demo.ipynb`, Demo 1: single-qubit gate action.

Hadamard, phase, and $\pi/8$ gates

$$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}, \quad T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix}$$

- $H\left|0\right\rangle = \left|+\right\rangle$, $H\left|1\right\rangle = \left|-\right\rangle$
- S and T change phase of $\left|1\right\rangle$ relative to $\left|0\right\rangle$
- $T^2 = S$, $S^2 = Z$

Rotation gates and trainable parameters

$$R_x(\theta) = e^{-i\theta X/2}, \quad R_y(\theta) = e^{-i\theta Y/2}, \quad R_z(\theta) = e^{-i\theta Z/2}$$

Explicitly:

$$R_y(\theta) = \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}$$

At $\theta = \pi$, each rotation equals $-i$ times a Pauli gate (global phase included).

`lecture_02_demo.ipynb`, Demo 5: parameterized $R_y(\theta)$.

Conjugation identity: $HXH = Z$

Matrix multiplication gives:

$$HXH = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix} = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} = Z$$

So H changes basis between X- and Z-eigenstates.

`lecture_02_demo.ipynb`, Demo 1: matrix action and identities.

A first universality statement

Any single-qubit unitary can be decomposed as

$$U = e^{i\alpha} R_z(\beta) R_y(\gamma) R_z(\delta)$$

for real angles $\alpha, \beta, \gamma, \delta$.

Interpretation:

- rotations already span all single-qubit transformations
- parameterized gates are natural trainable blocks for QML

Multi-qubit systems

Tensor product state space

For two qubits:

$$|\psi\rangle_{AB} = |\psi\rangle_A \otimes |\psi\rangle_B$$

Computational basis:

$$|00\rangle, |01\rangle, |10\rangle, |11\rangle$$

where, for example,

$$|10\rangle = |1\rangle \otimes |0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

Why Hilbert space grows as 2^n

n qubits span a complex vector space of dimension 2^n.

Qubits n	Basis states	Dimension
1	$\|0\rangle, \|1\rangle$	2
2	$\|00\rangle, \ldots, \|11\rangle$	4
5	32 basis strings	32
20	$1,048,576$ basis strings	2^{20}

This scaling motivates quantum feature spaces in QML.

Example: $(H \otimes I)\,|00\rangle$

Start from

$$|00\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

Apply

$$H \otimes I = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix}$$

Then

$$(H \otimes I)\,|00\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |10\rangle)$$

CNOT gate

CNOT on control qubit 0 and target qubit 1:

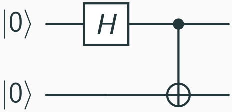
$$\text{CNOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

Input	Output
$\lvert 00\rangle$	$\lvert 00\rangle$
$\lvert 01\rangle$	$\lvert 01\rangle$
$\lvert 10\rangle$	$\lvert 11\rangle$
$\lvert 11\rangle$	$\lvert 10\rangle$

Entanglement

Creating a Bell state

Circuit:



State evolution:

$$|00\rangle \xrightarrow{H\otimes I} \frac{1}{\sqrt{2}}(|00\rangle + |10\rangle) \xrightarrow{\text{CNOT}} \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) = \left|\Phi^+\right\rangle$$

`lecture_02_demo.ipynb`, Demo 2: Bell state step-by-step.

Why $|\Phi^+\rangle$ is entangled

Assume separability:

$$\left|\Phi^+\right\rangle = (a\,|0\rangle + b\,|1\rangle) \otimes (c\,|0\rangle + d\,|1\rangle)$$

Then coefficients must satisfy

$$ac = \frac{1}{\sqrt{2}}, \quad ad = 0, \quad bc = 0, \quad bd = \frac{1}{\sqrt{2}}$$

From $ad = 0$: either $a = 0$ or $d = 0$.

- $a = 0 \Rightarrow ac = 0$ contradicts $ac = \frac{1}{\sqrt{2}}$
- $d = 0 \Rightarrow bd = 0$ contradicts $bd = \frac{1}{\sqrt{2}}$

Contradiction: $|\Phi^+\rangle$ is not separable.

`lecture_02_demo.ipynb`, Demo 2: Bell-state construction context.

All four Bell states

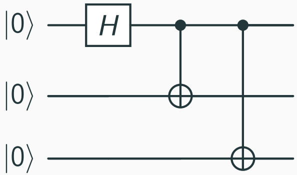
$$\left|\Phi^{\pm}\right\rangle = \frac{|00\rangle \pm |11\rangle}{\sqrt{2}}, \qquad \left|\Psi^{\pm}\right\rangle = \frac{|01\rangle \pm |10\rangle}{\sqrt{2}}$$

State	Construction from $|00\rangle$	Nonzero outcomes
$\left|\Phi^{+}\right\rangle$	$H(0)$, $\mathrm{CX}(0,1)$	00, 11
$\left|\Phi^{-}\right\rangle$	$H(0)$, $Z(0)$, $\mathrm{CX}(0,1)$	00, 11
$\left|\Psi^{+}\right\rangle$	$H(0)$, $\mathrm{CX}(0,1)$, $X(1)$	01, 10
$\left|\Psi^{-}\right\rangle$	$H(0)$, $Z(0)$, $\mathrm{CX}(0,1)$, $X(1)$	01, 10

GHZ state as Bell generalization

Three-qubit Greenberger-Horne-Zeilinger (GHZ) state:

$$|\mathrm{GHZ}\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$$



`lecture_02_demo.ipynb`, Demo 4: GHZ state.

No-cloning theorem (statement)

There is no unitary U such that

$$U\left(|\psi\rangle\,|0\rangle\right) = |\psi\rangle\,|\psi\rangle$$

for every unknown $|\psi\rangle$.

Proof sketch by linearity:

- Suppose cloning works for $|0\rangle$ and $|1\rangle$
- For $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$, linearity gives

$$U(|+\rangle\,|0\rangle) = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

- But exact cloning requires

$$|+\rangle\,|+\rangle = \frac{1}{2}(|00\rangle + |01\rangle + |10\rangle + |11\rangle)$$

Not equal: universal cloning is impossible.

Circuits as computational graphs

Depth, width, and parameter count

For a gate-based quantum model:

- **width**: number of qubits
- **depth**: number of sequential gate layers
- **parameters**: rotation angles in trainable gates

These quantities are direct analogs of model size in classical ML, but hardware noise makes depth especially expensive on NISQ devices.

Neural-network analogy

Classical ML object	Quantum analog	Role
layer weights	rotation angles θ	trainable parameters
forward pass	gate sequence $U(\theta)$	state transformation
activation/readout	measurement	output nonlinearity
network depth	circuit depth	expressivity vs trainability

This analogy becomes concrete in variational quantum circuits starting in Classes 6–7.

State evolution through a circuit

Bell-state circuit snapshots:

$$|00\rangle \xrightarrow{H(q_0)} \frac{1}{\sqrt{2}}(|00\rangle + |10\rangle) \xrightarrow{\mathrm{CX}(q_0, q_1)} \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

Corresponding probabilities:

$$P_{\text{init}} = (1, 0, 0, 0)$$

$$P_{\text{after } H} = \left(\frac{1}{2}, 0, \frac{1}{2}, 0\right)$$

$$P_{\text{after CX}} = \left(\frac{1}{2}, 0, 0, \frac{1}{2}\right)$$

`lecture_02_demo.ipynb`, Demo 2: state evolution snapshots.

Measurement and shot statistics

For a circuit output state $|\psi\rangle$, a single measurement gives one bitstring sample. To estimate probabilities, we repeat the circuit.

If the true probability of outcome x is p_x, then after N shots:

$$\hat{p}_x = \frac{\text{counts}(x)}{N}$$

has statistical uncertainty roughly

$$\sigma(\hat{p}_x) \approx \sqrt{\frac{p_x(1 - p_x)}{N}}$$

More shots reduce noise, but increase runtime.

Live demo snippet: Bell states in Qiskit

```
from qiskit import QuantumCircuit
from qiskit.primitives import StatevectorSampler

qc = QuantumCircuit(2)
qc.h(0)
qc.cx(0, 1)
qc.measure_all()

counts = StatevectorSampler().run([qc], shots=1024).result()
```

`lecture_02_demo.ipynb`, Demo 3: Bell-state counts.

Live demo snippet: $R_y(\theta)$ in PennyLane

```
import pennylane as qml

dev = qml.device("default.qubit", wires=1)
@qml.qnode(dev)
def ry_expval(theta):
    qml.RY(theta, wires=0)
    return qml.expval(qml.PauliZ(0))
```

Analytical target for this circuit:

$$\langle Z \rangle = \cos\theta$$

`lecture_02_demo.ipynb`, Demo 5: $R_y(\theta)$ expectation.

Summary

- Gates are unitary matrices acting on state vectors
- Tensor products build multi-qubit state spaces of size 2^n
- CNOT plus single-qubit gates generates entanglement
- Bell and GHZ states are canonical entangled resources
- Circuits can be read as trainable computational graphs

Next class: measurement, observables, expectation values, and the sampler/estimator workflow.

References i

1. Nielsen and Chuang, *Quantum Computation and Quantum Information*, Cambridge University Press (2010).
2. Schuld and Petruccione, *Supervised Learning with Quantum Computers*, Springer (2018).
3. IBM Quantum documentation: `https://docs.quantum.ibm.com/`
4. PennyLane documentation: `https://docs.pennylane.ai/`