CS621/CSL611
Quantum Computing For Computer Scientists

The Leap from Classical to Quantum

Dhiman Saha

Winter 2024

IIT Bhilai

The Leap from Classical to Quantum

- Graphs without weights will model classical deterministic systems.
- Graphs weighted with real numbers will model classical probabilistic systems.
- Graphs weighted with complex numbers and will model quantum systems.

The double-slit experiment

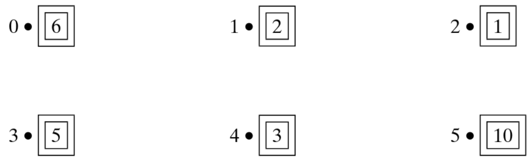
Computer science/graph-theoretic version of the double-slit experiment, perhaps the most important experiment in quantum mechanics.

Classical Deterministic Systems

Graph Modeling of the “State” of a Deterministic System

Example

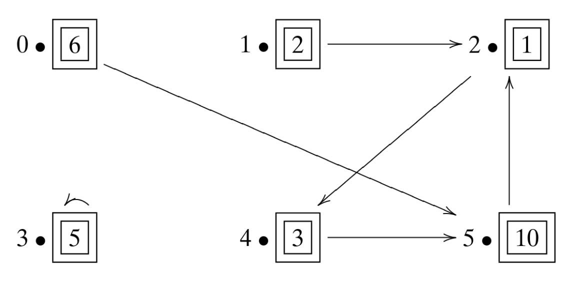
Let there be 6 vertices in a graph and a total of 27 marbles. We might place 6 marbles on vertex 0, 2 marbles on vertex 1, and the rest as described by this picture



- We shall denote this state as $X = [6, 2, 1, 5, 3, 10]^T$

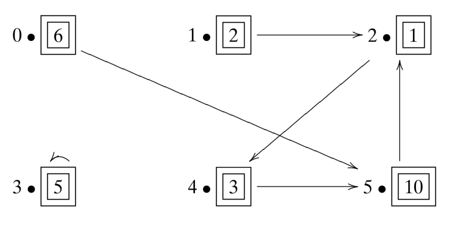
Capturing the "Dynamics" of the System

- Dynamics of the system can be represented by a graph with directed edges



- The idea is that if an arrow exists from vertex i to vertex j, then in one time click, all the marbles on vertex i will shift to vertex j.

$$M = \begin{array}{cc} & \begin{array}{cccccc} \mathbf{0} & \mathbf{1} & \mathbf{2} & \mathbf{3} & \mathbf{4} & \mathbf{5} \end{array} \\ \begin{array}{c} \mathbf{0} \\ \mathbf{1} \\ \mathbf{2} \\ \mathbf{3} \\ \mathbf{4} \\ \mathbf{5} \end{array} & \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 \end{bmatrix} \end{array},$$



- Here $M[i, j] = 1$ if and only if there is an arrow from vertex j to vertex i[1].
- The requirement that every vertex has exactly one outgoing edge corresponds to the fact that every column of the Boolean adjacency matrix contains exactly one 1.

[1] Note that the direction is reversed for reasons to be described later.

- Lets say that we multiply M by a state of the system $X = [6, 2, 1, 5, 3, 10]^T$. Then we have

$$MX = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 6 \\ 2 \\ 1 \\ 5 \\ 3 \\ 10 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 12 \\ 5 \\ 1 \\ 9 \end{bmatrix} = Y.$$

Interpretation

If X describes the state of the system at time t, then Y is the state of the system at time $t+1$, i.e., after one time click.

Exercise

- Using the dynamics given below, determine what the state of the system would be if you start with the state

$$[5, 5, 0, 2, 0, 15]^T$$

$$M = \begin{array}{c c} & \begin{array}{cccccc} \mathbf{0} & \mathbf{1} & \mathbf{2} & \mathbf{3} & \mathbf{4} & \mathbf{5} \end{array} \\ \begin{array}{c} \mathbf{0} \\ \mathbf{1} \\ \mathbf{2} \\ \mathbf{3} \\ \mathbf{4} \\ \mathbf{5} \end{array} & \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 \end{bmatrix} \end{array},$$

- In general, any simple directed graph with n vertices can be represented by an $n-by-n$ matrix M having entries as

$$
\begin{aligned}
M[i,j] &= 1 \text{ if and only if there is an edge from vertex } j \text{ to vertex } i. \\
&= 1 \text{ if and only if there is a path of length 1 from vertex } j \text{ to vertex}
\end{aligned}
$$

- If $X = [x_0, x_1, \cdots, x_{n-1}]^T$ is a column vector that corresponds to placing x_i marbles on vertex i, and
- If $MX = Y$ where $Y = [y_0, y_1, ..., y_{n-1}]^T$, then there are y_j marbles on vertex j after one time click.
- M is thus a way of describing how the state of the marbles can change from time t to time $t+1$.

Relation with Interpreting Quantum Systems

- (finite-dimensional) quantum mechanics works the same way.
- States of a system are represented by column vectors, and the way in which the system changes in one time click is represented by matrices.
- Multiplying a matrix with a column vector yields a subsequent state of the system.

Generalizing multiple iteration

- In general, multiplying an $n - by - n$ matrix by itself several times will produce another matrix whose i, jth entry will indicate whether there is a path after several time clicks.
- Consider $X = [x_0, x_1, \cdots, x_{n-1}]^T$ to be the state where one places x_0 marbles on vertex 0, x_1 marbles on vertex $1, \cdots, x_{n-1}$ marbles on vertex $n - 1$.
- Then, after k steps, the state of the marbles is Y, where $Y = [y_0, y_1, \cdots, y_{n-1}]^T = M^k X$.
- In other words, y_j is the number of marbles on vertex j after k steps.

Relation with Interpreting Quantum Systems

- In quantum mechanics, if there are two or more matrices that manipulate states, the action of one followed by another is described by their **product**.
- We shall take different states of systems and multiply the states by various matrices (of the appropriate type) to obtain other ones.
- These new states will again be multiplied by other matrices until we attain the desired end state.

The Quantum Flow

- In quantum computing, we shall start with an initial state, described by a vector of numbers.
- The initial state will essentially be the input to the system.
- Operations in a quantum computer will correspond to multiplying the vector with matrices.
- The output will be the state of the system when we are finished carrying out all the operations.

- The states of a system correspond to column vectors (state vectors).
- The dynamics of a system correspond to matrices.
- To progress from one state to another in one time step, one must multiply the state vector by a matrix.
- Multiple step dynamics are obtained via matrix multiplication.

Write a program that performs our little marble experiment.

- The program should allow the user to enter a Boolean matrix that describes the ways that marbles move.
- Make sure that the matrix follows our requirement.
- The user should also be permitted to enter a starting state of how many marbles are on each vertex.
- Then the user enters how many time clicks she wants to proceed.
- The computer should then calculate and output the state of the system after those time clicks.