Quantum walks

Ashley Montanaro

Centre for Quantum Information and Foundations, Department of Applied Mathematics and Theoretical Physics, University of Cambridge

November 29, 2011

Quantum walks

• This lecture is about a generalisation of the fundamental concept of random walks (aka Markov chains) to quantum computation.

• We start with the most basic random walk possible: a walk on the line.

• Take the real line

and put a particle on the line, initially at position 0.

• Take the real line

and put a particle on the line, initially at position 0.

• Take the real line

and put a particle on the line, initially at position 0.

• Take the real line

and put a particle on the line, initially at position 0.

• Take the real line

and put a particle on the line, initially at position 0.

• Take the real line

and put a particle on the line, initially at position 0.

• Take the real line

and put a particle on the line, initially at position 0.

• Take the real line

and put a particle on the line, initially at position 0.

- At each step, toss a fair coin and move distance 1 either to the right or to the left.
- It is easy to calculate that the probability of being found at position *x* after *t* steps is exactly

$$\frac{1}{2^t} \begin{pmatrix} t \\ \frac{t+x}{2} \end{pmatrix}$$
,

where we define $\binom{t}{r} = 0$ for non-integer *r*.

Random walk on the line (even times)

Random walk on the line (100 steps)



Consider a quantum system with two registers |x⟩|c⟩, where the first holds an integer position x and the second holds a coin state c ∈ {L, R}.

- Consider a quantum system with two registers |x⟩|c⟩, where the first holds an integer position x and the second holds a coin state c ∈ {L, R}.
- Just like the classical walk, at each step our quantum walk will flip a coin and then decide which way to go.

- Consider a quantum system with two registers |x⟩|c⟩, where the first holds an integer position x and the second holds a coin state c ∈ {L, R}.
- Just like the classical walk, at each step our quantum walk will flip a coin and then decide which way to go.
- These two operations will be unitary: a coin operator *C*, and a shift operator *S*.

- Consider a quantum system with two registers |x⟩|c⟩, where the first holds an integer position x and the second holds a coin state c ∈ {L, R}.
- Just like the classical walk, at each step our quantum walk will flip a coin and then decide which way to go.
- These two operations will be unitary: a coin operator *C*, and a shift operator *S*.
- The coin operator acts solely on the coin register, and consists of a Hadamard operation:

$$C|L\rangle = rac{1}{\sqrt{2}} \left(|L\rangle + |R\rangle\right), \ \ C|R\rangle = rac{1}{\sqrt{2}} \left(|L\rangle - |R\rangle\right).$$

- Consider a quantum system with two registers |x⟩|c⟩, where the first holds an integer position x and the second holds a coin state c ∈ {L, R}.
- Just like the classical walk, at each step our quantum walk will flip a coin and then decide which way to go.
- These two operations will be unitary: a coin operator *C*, and a shift operator *S*.
- The coin operator acts solely on the coin register, and consists of a Hadamard operation:

$$C|L\rangle = rac{1}{\sqrt{2}}\left(|L\rangle + |R\rangle\right), \ \ C|R\rangle = rac{1}{\sqrt{2}}\left(|L\rangle - |R\rangle\right).$$

• The shift operator acts on both registers, and simply moves the walker in the direction indicated by the coin state:

$$S|x\rangle|L\rangle = |x-1\rangle|L\rangle, \ S|x\rangle|R\rangle = |x+1\rangle|R\rangle.$$

• So a quantum walk on the line for *t* steps consists of applying the unitary operator $(S(I \otimes C))^t$ to some initial state, then measuring the position register.

- So a quantum walk on the line for *t* steps consists of applying the unitary operator $(S(I \otimes C))^t$ to some initial state, then measuring the position register.
- Note: we only measure the position at the end, not after each step.

- So a quantum walk on the line for *t* steps consists of applying the unitary operator $(S(I \otimes C))^t$ to some initial state, then measuring the position register.
- Note: we only measure the position at the end, not after each step.
- This simple process can lead to some fairly complicated results!
- Consider the first few steps of a quantum walk with initial state |0⟩|L⟩ (position 0, facing left).

$$|0\rangle|L\rangle \quad \mapsto \quad \frac{1}{\sqrt{2}}\left(|-1\rangle|L\rangle + |1\rangle|R\rangle\right)$$

$$\begin{aligned} |0\rangle|L\rangle &\mapsto \frac{1}{\sqrt{2}}\left(|-1\rangle|L\rangle + |1\rangle|R\rangle\right) \\ &\mapsto \frac{1}{2}\left(|-2\rangle|L\rangle + |0\rangle|R\rangle + |0\rangle|L\rangle - |2\rangle|R\rangle\right) \end{aligned}$$

$$\begin{split} |0\rangle|L\rangle &\mapsto \frac{1}{\sqrt{2}}\left(|-1\rangle|L\rangle + |1\rangle|R\rangle\right) \\ &\mapsto \frac{1}{2}\left(|-2\rangle|L\rangle + |0\rangle|R\rangle + |0\rangle|L\rangle - |2\rangle|R\rangle\right) \\ &\mapsto \frac{1}{2\sqrt{2}}\left(|-3\rangle|L\rangle + |-1\rangle|R\rangle + 2|-1\rangle|L\rangle - |1\rangle|L\rangle + |3\rangle|R\rangle) \end{split}$$

$$\begin{aligned} |0\rangle|L\rangle &\mapsto \frac{1}{\sqrt{2}}\left(|-1\rangle|L\rangle + |1\rangle|R\rangle\right) \\ &\mapsto \frac{1}{2}\left(|-2\rangle|L\rangle + |0\rangle|R\rangle + |0\rangle|L\rangle - |2\rangle|R\rangle\right) \\ &\mapsto \frac{1}{2\sqrt{2}}\left(|-3\rangle|L\rangle + |-1\rangle|R\rangle + 2|-1\rangle|L\rangle - |1\rangle|L\rangle + |3\rangle|R\rangle\right) \\ &\mapsto \dots \end{aligned}$$

$$\begin{split} |0\rangle|L\rangle &\mapsto \frac{1}{\sqrt{2}}\left(|-1\rangle|L\rangle + |1\rangle|R\rangle\right) \\ &\mapsto \frac{1}{2}\left(|-2\rangle|L\rangle + |0\rangle|R\rangle + |0\rangle|L\rangle - |2\rangle|R\rangle\right) \\ &\mapsto \frac{1}{2\sqrt{2}}\left(|-3\rangle|L\rangle + |-1\rangle|R\rangle + 2|-1\rangle|L\rangle - |1\rangle|L\rangle + |3\rangle|R\rangle\right) \\ &\mapsto \dots \end{split}$$

• Measuring after the third step yields position -3, 1 and 3 with probability 1/8 each, and position -1 with probability 5/8.

$$\begin{split} |0\rangle|L\rangle &\mapsto \frac{1}{\sqrt{2}}\left(|-1\rangle|L\rangle + |1\rangle|R\rangle\right) \\ &\mapsto \frac{1}{2}\left(|-2\rangle|L\rangle + |0\rangle|R\rangle + |0\rangle|L\rangle - |2\rangle|R\rangle\right) \\ &\mapsto \frac{1}{2\sqrt{2}}\left(|-3\rangle|L\rangle + |-1\rangle|R\rangle + 2|-1\rangle|L\rangle - |1\rangle|L\rangle + |3\rangle|R\rangle\right) \\ &\mapsto \dots \end{split}$$

- Measuring after the third step yields position -3, 1 and 3 with probability 1/8 each, and position -1 with probability 5/8.
- By contrast, the classical walk is found in position -3 or 3 with probability 1/8 each, and -1 and 1 with probability 3/8 each.

$$\begin{split} |0\rangle|L\rangle &\mapsto \frac{1}{\sqrt{2}}\left(|-1\rangle|L\rangle + |1\rangle|R\rangle\right) \\ &\mapsto \frac{1}{2}\left(|-2\rangle|L\rangle + |0\rangle|R\rangle + |0\rangle|L\rangle - |2\rangle|R\rangle\right) \\ &\mapsto \frac{1}{2\sqrt{2}}\left(|-3\rangle|L\rangle + |-1\rangle|R\rangle + 2|-1\rangle|L\rangle - |1\rangle|L\rangle + |3\rangle|R\rangle\right) \\ &\mapsto \dots \end{split}$$

- Measuring after the third step yields position -3, 1 and 3 with probability 1/8 each, and position -1 with probability 5/8.
- By contrast, the classical walk is found in position -3 or 3 with probability 1/8 each, and -1 and 1 with probability 3/8 each.
- The bias of the quantum walk is an effect of interference.

Hadamard walk on the line (even times 0-10)

Hadamard walk on the line (even times 12-100)

• Unlike the classical walk, the quantum walk is not symmetric about 0. This can be "fixed" by changing the initial coin state to $\frac{1}{\sqrt{2}}|0\rangle(|L\rangle + i|R\rangle)$, or using a different coin operator.

- Unlike the classical walk, the quantum walk is not symmetric about 0. This can be "fixed" by changing the initial coin state to $\frac{1}{\sqrt{2}}|0\rangle(|L\rangle + i|R\rangle)$, or using a different coin operator.
- Unlike the classical random walk, at time *t* > 0 the walker is not most likely to be found at the origin.

- Unlike the classical walk, the quantum walk is not symmetric about 0. This can be "fixed" by changing the initial coin state to $\frac{1}{\sqrt{2}}|0\rangle(|L\rangle + i|R\rangle)$, or using a different coin operator.
- Unlike the classical random walk, at time *t* > 0 the walker is not most likely to be found at the origin.
- The quantum walk seems to spread out more quickly from the origin. Classically, the variance in position after *t* steps is *O*(*t*), but in the quantum case it turns out to be of order *t*².

- Unlike the classical walk, the quantum walk is not symmetric about 0. This can be "fixed" by changing the initial coin state to $\frac{1}{\sqrt{2}}|0\rangle(|L\rangle + i|R\rangle)$, or using a different coin operator.
- Unlike the classical random walk, at time *t* > 0 the walker is not most likely to be found at the origin.
- The quantum walk seems to spread out more quickly from the origin. Classically, the variance in position after *t* steps is *O*(*t*), but in the quantum case it turns out to be of order *t*².
- This is noticeably more difficult to prove than the classical proof.

Quantum vs. classical walk on the line (even times 12-100)

Random walks on general graphs

There is a natural generalisation of the classical random walk on the line to a random walk on an arbitrary graph G with mvertices.

Random walks on general graphs

There is a natural generalisation of the classical random walk on the line to a random walk on an arbitrary graph G with mvertices.

- The walker is positioned at a vertex of *G*, and at each time step, it chooses an adjacent vertex to move to, uniformly at random.
- Here we will consider only <u>undirected</u> and <u>regular</u> graphs where:
 - the ability to move from A to B implies the ability to move from B to A;
 - every vertex has degree *d*.
Random walks on general graphs

 The probability of being at vertex *j* after *t* steps, given that the walk started at vertex *i*, is just (*j*|*M*^t|*i*) for some matrix *M*, where

$$M_{ij} = \begin{cases} \frac{1}{d} & \text{if } i \text{ is connected to } j \\ 0 & \text{otherwise.} \end{cases}$$

• To quantise this, we still have position and coin registers, but now the position register is *m*-dimensional and the coin register is *d*-dimensional.

• Label each vertex with a distinct integer between 1 and *m*. For each vertex, label its outgoing edges with distinct integers between 1 and *d* such that, for each *i*, edges labelled with *i* form a cycle.

- Label each vertex with a distinct integer between 1 and *m*. For each vertex, label its outgoing edges with distinct integers between 1 and *d* such that, for each *i*, edges labelled with *i* form a cycle.
- For each vertex v ∈ {1,..., m}, let N(v, i) denote the i'th neighbour of v (i.e. the vertex at the other end of the i'th edge).

- Label each vertex with a distinct integer between 1 and *m*. For each vertex, label its outgoing edges with distinct integers between 1 and *d* such that, for each *i*, edges labelled with *i* form a cycle.
- For each vertex v ∈ {1,..., m}, let N(v, i) denote the i'th neighbour of v (i.e. the vertex at the other end of the i'th edge).
- Our quantum walk will once again consist of alternating shift and coin operators *S* and *C*, i.e. each step is of the form (*S*(*I* ⊗ *C*)). The shift operator simply performs the map

 $S|v\rangle|i\rangle = |N(v,i)\rangle|i\rangle.$

- Label each vertex with a distinct integer between 1 and *m*. For each vertex, label its outgoing edges with distinct integers between 1 and *d* such that, for each *i*, edges labelled with *i* form a cycle.
- For each vertex v ∈ {1,..., m}, let N(v, i) denote the i'th neighbour of v (i.e. the vertex at the other end of the i'th edge).
- Our quantum walk will once again consist of alternating shift and coin operators *S* and *C*, i.e. each step is of the form (*S*(*I* ⊗ *C*)). The shift operator simply performs the map

 $S|v\rangle|i\rangle = |N(v,i)\rangle|i\rangle.$

• As the coin register is now *d*-dimensional, we have many possible choices for *C*.

• One reasonable choice for *C* is the so-called *Grover* coin,

$$C = \begin{pmatrix} \frac{2}{d} - 1 & \frac{2}{d} & \dots & \frac{2}{d} \\ \frac{2}{d} & \frac{2}{d} - 1 & \dots & \frac{2}{d} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{2}{d} & \frac{2}{d} & \dots & \frac{2}{d} - 1 \end{pmatrix}$$

.

This is just the iteration used in Grover's algorithm.

• One reasonable choice for C is the so-called Grover coin,

$$C = \begin{pmatrix} \frac{2}{d} - 1 & \frac{2}{d} & \dots & \frac{2}{d} \\ \frac{2}{d} & \frac{2}{d} - 1 & \dots & \frac{2}{d} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{2}{d} & \frac{2}{d} & \dots & \frac{2}{d} - 1 \end{pmatrix}$$

This is just the iteration used in Grover's algorithm.

• This operator is an appealing choice because it is permutation-symmetric (i.e. treats all edges equally), and it is far away from the identity matrix (i.e. has a large mixing effect).

• One reasonable choice for C is the so-called Grover coin,

$$C = \begin{pmatrix} \frac{2}{d} - 1 & \frac{2}{d} & \dots & \frac{2}{d} \\ \frac{2}{d} & \frac{2}{d} - 1 & \dots & \frac{2}{d} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{2}{d} & \frac{2}{d} & \dots & \frac{2}{d} - 1 \end{pmatrix}$$

This is just the iteration used in Grover's algorithm.

- This operator is an appealing choice because it is permutation-symmetric (i.e. treats all edges equally), and it is far away from the identity matrix (i.e. has a large mixing effect).
- If d = 2, we would get $C = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, so in this case the coins used earlier for the walk on the line lead to more interesting behaviour.

• Note that, as the quantum walk consists only of unitary operations, the position of the walker does not tend to a limiting distribution over the vertices of *G*, by contrast with the classical random walk.

The hypercube

We now focus on one particularly interesting graph: the *n*-dimensional hypercube (aka the Cayley graph of the group Zⁿ₂).

The hypercube

- We now focus on one particularly interesting graph: the *n*-dimensional hypercube (aka the Cayley graph of the group Zⁿ₂).
- This is the graph whose vertices are *n*-bit strings which are adjacent if they differ in exactly one bit.

The hypercube

- We now focus on one particularly interesting graph: the *n*-dimensional hypercube (aka the Cayley graph of the group Zⁿ₂).
- This is the graph whose vertices are *n*-bit strings which are adjacent if they differ in exactly one bit.
- We will be interested in the expected time it takes for a random walk on this graph to travel from the "all zeroes" string 0^{*n*} to the "all ones" string 1^{*n*}, i.e. to traverse the graph from one extremity to the other, which is known as the hitting time from 0^{*n*} to 1^{*n*}.

Classically, this time can be analysed by mapping the walk to a (biased) random walk on the line.

Classically, this time can be analysed by mapping the walk to a (biased) random walk on the line.

• Imagine the walker is currently at a vertex with Hamming weight *k*.

Classically, this time can be analysed by mapping the walk to a (biased) random walk on the line.

- Imagine the walker is currently at a vertex with Hamming weight *k*.
- The probability of moving to a vertex with Hamming weight (k-1) is k/n, and the probability of moving to a vertex with Hamming weight (k + 1) is 1 k/n.

Classically, this time can be analysed by mapping the walk to a (biased) random walk on the line.

- Imagine the walker is currently at a vertex with Hamming weight *k*.
- The probability of moving to a vertex with Hamming weight (k 1) is k/n, and the probability of moving to a vertex with Hamming weight (k + 1) is 1 k/n.
- As *k* increases, the probability of a step leading to the Hamming weight increasing decreases, so intuitively the walker becomes "stuck" in the "middle" of the graph (i.e. near Hamming weight *n*/2).

Classically, this time can be analysed by mapping the walk to a (biased) random walk on the line.

- Imagine the walker is currently at a vertex with Hamming weight *k*.
- The probability of moving to a vertex with Hamming weight (k-1) is k/n, and the probability of moving to a vertex with Hamming weight (k + 1) is 1 k/n.
- As *k* increases, the probability of a step leading to the Hamming weight increasing decreases, so intuitively the walker becomes "stuck" in the "middle" of the graph (i.e. near Hamming weight *n*/2).

Proposition

The hitting time from 0^n to 1^n is at least $2^n - 1$.

Theorem

If a quantum walk on the hypercube is performed for $T \approx \frac{\pi}{2}n$ steps starting in position 0^n , and the position register is measured, the outcome 1^n is obtained with probability 1 - O(polylog(n)/n).

Theorem

If a quantum walk on the hypercube is performed for $T \approx \frac{\pi}{2}n$ steps starting in position 0^n , and the position register is measured, the outcome 1^n is obtained with probability 1 - O(polylog(n)/n).

Similarly to the classical case, we can simplify this to a walk on the line. Define a set of 2n states $\{|v_k, L\rangle, |v_k, R\rangle\}$ indexed by k = 0, ..., n as follows:

$$\begin{aligned} |\upsilon_k, L\rangle &:= \frac{1}{\sqrt{k\binom{n}{k}}} \sum_{x, |x|=k} \sum_{i, x_i=1} |x\rangle |i\rangle, \\ |\upsilon_k, R\rangle &:= \frac{1}{\sqrt{(n-k)\binom{n}{k}}} \sum_{x, |x|=k} \sum_{i, x_i=0} |x\rangle |i\rangle. \end{aligned}$$

(The special cases $|v_0, L\rangle$ and $|v_n, R\rangle$ will not be used and are undefined.)

• The quantum walk on the hypercube preserves the subspace spanned by this set of states:

$$S|\upsilon_k, L\rangle = |\upsilon_{k-1}, R\rangle, \ S|\upsilon_k, R\rangle = |\upsilon_{k+1}, L\rangle,$$

• The quantum walk on the hypercube preserves the subspace spanned by this set of states:

$$S|\upsilon_k, L\rangle = |\upsilon_{k-1}, R\rangle, \ S|\upsilon_k, R\rangle = |\upsilon_{k+1}, L\rangle,$$

• and in the case of the coin operator,

$$(I \otimes C)|\upsilon_k, L\rangle = \left(\frac{2k}{n} - 1\right)|\upsilon_k, L\rangle + \frac{2\sqrt{k(n-k)}}{n}|\upsilon_k, R\rangle$$

$$(I \otimes C)|\upsilon_k, R\rangle = \frac{2\sqrt{k(n-k)}}{n}|\upsilon_k, L\rangle + \left(1 - \frac{2k}{n}\right)|\upsilon_k, R\rangle.$$

• The quantum walk on the hypercube preserves the subspace spanned by this set of states:

$$S|\upsilon_k, L\rangle = |\upsilon_{k-1}, R\rangle, \ S|\upsilon_k, R\rangle = |\upsilon_{k+1}, L\rangle,$$

• and in the case of the coin operator,

$$(I \otimes C)|\upsilon_k, L\rangle = \left(\frac{2k}{n} - 1\right)|\upsilon_k, L\rangle + \frac{2\sqrt{k(n-k)}}{n}|\upsilon_k, R\rangle$$

$$(I \otimes C)|\upsilon_k, R\rangle = \frac{2\sqrt{k(n-k)}}{n}|\upsilon_k, L\rangle + \left(1 - \frac{2k}{n}\right)|\upsilon_k, R\rangle.$$

• This behaviour is similar to the quantum walk on the line, with two differences: first, the direction in which the walker is moving flips with each shift, and second, the coin is different at each position (i.e. depends on *k*).

• The quantum walk on the hypercube preserves the subspace spanned by this set of states:

$$S|\upsilon_k, L\rangle = |\upsilon_{k-1}, R\rangle, \ S|\upsilon_k, R\rangle = |\upsilon_{k+1}, L\rangle,$$

• and in the case of the coin operator,

$$(I \otimes C)|\upsilon_k, L\rangle = \left(\frac{2k}{n} - 1\right)|\upsilon_k, L\rangle + \frac{2\sqrt{k(n-k)}}{n}|\upsilon_k, R\rangle$$

$$(I \otimes C)|\upsilon_k, R\rangle = \frac{2\sqrt{k(n-k)}}{n}|\upsilon_k, L\rangle + \left(1 - \frac{2k}{n}\right)|\upsilon_k, R\rangle.$$

- This behaviour is similar to the quantum walk on the line, with two differences: first, the direction in which the walker is moving flips with each shift, and second, the coin is different at each position (i.e. depends on *k*).
- Based on this reduction, it is easy to plot the behaviour of this quantum walk numerically for small *n*.

Quantum vs. classical walk on the hypercube

• Quantum walks display very different behaviour from classical random walks and are an interesting technique for designing quantum algorithms.

- Quantum walks display very different behaviour from classical random walks and are an interesting technique for designing quantum algorithms.
- They are frequently more difficult to analyse than classical random walks...

- Quantum walks display very different behaviour from classical random walks and are an interesting technique for designing quantum algorithms.
- They are frequently more difficult to analyse than classical random walks...
- Importantly, quantum walks on low-degree graphs can be implemented efficiently on a quantum computer.

- Quantum walks display very different behaviour from classical random walks and are an interesting technique for designing quantum algorithms.
- They are frequently more difficult to analyse than classical random walks...
- Importantly, quantum walks on low-degree graphs can be implemented efficiently on a quantum computer.
- The quantum walk model is quite general: in fact, it turns out that every quantum computation can be interpreted as a quantum walk!
 - "Universal computation by quantum walk", Andrew Childs, arXiv:0806.1972
 - "Universal quantum computation using the discrete time quantum walk", Lovett et al, arXiv:0910.1024

Course summary

- Quantum computers offer new possibilities for information processing which are fundamentally impossible for computers based only on classical physics.
- Significant examples of quantum speed-ups include an efficient algorithm for integer factorisation and a provable quadratic speed-up for unstructured search.
- Quantum computers are not a panacea and one can prove limitations on their power using classical mathematical techniques.
- One of the most important early applications of quantum computers is likely to be the simulation of quantum mechanical systems.

Quantum algorithms we didn't mention

Some exponential speed-ups:

- Extracting information from solutions to linear equations.
- Solving Pell's equation $(x^2 dy^2 = 1)$ in integers.
- Approximating the Jones polynomial of knots on the complex unit circle.
- Testing equality of bit-strings using exponentially less communication.

Quantum algorithms we didn't mention

Some exponential speed-ups:

- Extracting information from solutions to linear equations.
- Solving Pell's equation $(x^2 dy^2 = 1)$ in integers.
- Approximating the Jones polynomial of knots on the complex unit circle.
- Testing equality of bit-strings using exponentially less communication.

And some polynomial speed-ups:

- Computing AND-OR trees with *n* variables in time $O(\sqrt{n})$.
- Determining whether a list contains duplicate elements.
- Finding triangles and other properties of graphs.

Open problems

Unlike many fields of mathematics, the relatively young field of quantum computing has many accessible open problems.

- We know that quantum and classical query complexity of total boolean functions can only be separated by a 6th power. Can this 6 be reduced to a 2?
- Is there any total boolean function which has an exact quantum query algorithm which uses fewer than half the number of queries than the best possible classical algorithm?
- There are exponential query complexity separations for functions with a significant promise on the input (eg. Simon's problem). What about functions with a weaker promise on the input?

Open problems

- Is there a quantum algorithm which can simulate *k*-local Hamiltonians using time $O(t \log(1/\epsilon))$?
- Can we harness the exponentially faster hitting of quantum walks to solve important classical problems?
- Is there an efficient quantum algorithm for the nonabelian hidden subgroup problem? Such an algorithm would solve the graph isomorphism problem.
- More generally, can we find more quantum algorithms?