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Quantum walks on quantum computers

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Quantum states, Dirac's bra - ($\langle x|$) and ket ($|x\rangle$) notations

1) ket $|\cdot\rangle$

- quantum states are 'ket': $|\psi\rangle$
- linearity (superpositions): complex linear combinations of states are states $c_1 |\psi_1\rangle + c_2 |\psi_2\rangle$, $c_i \in \mathbb{C}$.

2) bra $\langle\cdot|$

- inner product is defined: $\langle\phi|\psi\rangle \in \mathbb{C}$, 'a bracket'
- quantum states are kets $|\psi\rangle$ with unit norm $\| |\psi\rangle \|^2 := \langle\psi|\psi\rangle = 1$
- fix $|\phi\rangle$, a linear functional: $\ell_\phi(|\psi\rangle) := \langle\phi|\psi\rangle$ is called 'bra' $\langle\phi|$
- all possible bras $\langle\phi|$ form a linear space (dual to the space of kets)

3) Quantum states $|x\rangle \in \mathcal{H}$

- $\mathcal{H}$ is a Hilbert space
- inner product of elements $|x\rangle$, $|y\rangle$ is $\langle x|y\rangle$

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Consider finite dimensional state space

Theorem

Every n-dimensional complex Hilbert space is isomorphic to $\mathbb{C}^n$ (with the standard inner product)

$\rightarrow$ We can work in an abstract vector space ($\mathbb{C}^n$): ket is a column vector and bra is a row vector:

$$|\psi\rangle \in \mathbb{C}^n \text{ or } |\psi\rangle = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix} \text{ and } \langle\psi| = (c_1^*, c_2^*, \dots, c_n^*)$$

$$\langle\phi|\psi\rangle = (d_1^*, d_2^*, \dots, d_n^*) \cdot \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix} = d_1^* c_1 + d_2^* c_2 + \dots + d_n^* c_n$$

Norm: $\| |\psi\rangle \|^2 = \langle\psi|\psi\rangle = \sum_i |c_i|^2$

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Linear operator A

is a linear function, $A : \mathbb{C}^n \rightarrow \mathbb{C}^n$, and $A(\sum_i c_i |\psi_i\rangle) = \sum_i c_i A |\psi_i\rangle$
Let $\{|\psi\rangle_i\}$ be an orthonormal basis in state space matrix of A is defined by

$$A|\psi_i\rangle := |a_i\rangle,\ |a_i\rangle = \begin{pmatrix} a_{1i} \\ a_{2i} \\ \vdots \\ a_{ni} \end{pmatrix}$$

$$A = \left(|a_1\rangle, |a_2\rangle, \ldots, |a_n\rangle\right) = \begin{pmatrix} a_{11}, a_{12}, \ldots, a_{1n} \\ a_{21}, a_{22}, \ldots, a_{2n} \\ \vdots \\ a_{n1}, a_{n2}, \ldots, a_{nn} \end{pmatrix},$$

e.g. $A|\psi_1\rangle := A \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} = \begin{pmatrix} a_{11} \\ a_{21} \\ \vdots \\ a_{n1} \end{pmatrix}$

$A(\sum_i c_i |\psi_i\rangle) = \sum_i c_i A |\psi_i\rangle = \sum_i c_i |a_i\rangle$

Examples

If we know $A\left|\psi_i\right\rangle := \left|a_i\right\rangle$, we get i-th column of the matrix of A.
Unit operator I: for all $\left|\psi\right\rangle$, $I\left|\psi\right\rangle = \left|\psi\right\rangle$, as a result for any orthonormal basis $\{\left|\psi\right\rangle_i\}$: $I = (\left|\psi_1\right\rangle, \cdots, \left|\psi_n\right\rangle) = \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1 \end{pmatrix}$

Or: $I = \left|\psi_1\right\rangle\left\langle\psi_1\right| + \left|\psi_2\right\rangle\left\langle\psi_2\right| + \cdots + \left|\psi_n\right\rangle\left\langle\psi_n\right|$
Eigenvectors: $M\left|\psi_i\right\rangle = \lambda_i\left|\psi_i\right\rangle$,

$$M = (\lambda_1\left|\psi_1\right\rangle, \cdots, \lambda_n\left|\psi_n\right\rangle) = \begin{pmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \lambda_n \end{pmatrix}$$

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Adjoint-operator $A^\dagger$ of an operator A

Let A be a matrix of an operator in orthonormal basis $\{|\psi_i\rangle\}$:

$$A = \begin{pmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ r_{21} & r_{22} & \cdots & r_{2n} \\ \vdots & & & \\ r_{n1} & r_{n2} & \cdots & r_{nn} \end{pmatrix}$$

By definition, matrix of adjoint-operator $A^\dagger$ of A has the matrix which is conjugate transpose of A:

$$A^\dagger = \begin{pmatrix} r_{11}^* & r_{21}^* & \cdots & r_{n1}^* \\ r_{12}^* & r_{22}^* & \cdots & r_{n2}^* \\ \vdots & & & \\ r_{1n}^* & r_{2n}^* & \cdots & r_{nn}^* \end{pmatrix}$$

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Some relations

Ket is a one-column matrix and we have: If $|\psi\rangle = \begin{pmatrix} c_1 \\ \vdots \\ c_n \end{pmatrix}$, then $|\psi\rangle^\dagger = \langle\psi|$ is:

$$\begin{pmatrix} c_1 \\ \vdots \\ c_n \end{pmatrix}^\dagger = (c_1^*, \cdots, c_n^*),$$ and

$$\langle\psi|\psi\rangle = (c_1^*, \cdots, c_n^*) \begin{pmatrix} c_1 \\ \vdots \\ c_n \end{pmatrix} = |c_1|^2 + |c_2|^2 + \cdots + |c_n|^2$$

$|\phi\rangle \langle\psi|$ is an operator acting according to: $(|\phi\rangle \langle\psi|) |\cdot\rangle = |\phi\rangle \langle\psi|\cdot\rangle$ for any $|\cdot\rangle$

We have: $(|\phi\rangle \langle\psi|)^\dagger = (\langle\psi|)^\dagger (|\phi\rangle)^\dagger = |\psi\rangle \langle\phi|$

Self-adjoint operators

A linear operator is self-adjoint if: $M^\dagger = M$.
Eigenvalues of an self-adjoint operator are real and eigenvector with different eigenvalues are orthogonal Self-adjoint operators $M^\dagger = M$,

- real eigenvalues -possible outcomes of measurements
- orthonormal eigenvectors - squares of absolute values of coordinates -> probability distribution of outcomes
- $M\left|\lambda_i\right\rangle = \lambda_i \left|\lambda_i\right\rangle$, $\left|\psi\right\rangle = \sum_i c_i \left|\lambda_i\right\rangle \rightarrow \mathbb{P}(M \rightarrow \lambda_i | \left|\psi\right\rangle) = |c_i|^2$
- expectation of M in state $\left|\psi\right\rangle$ is $\left\langle\psi\right| M \left|\psi\right\rangle = \sum_i \lambda_i |c_i|^2$

Unitary operators

- U is a unitary operator iff $U^\dagger U = I$, or $U^\dagger = U^{-1}$
  - $\| U |\psi\rangle \|^2 = (U|\psi\rangle)^\dagger U |\psi\rangle = \langle\psi| U^\dagger U |\psi\rangle = \langle\psi|\psi\rangle = \| |\psi\rangle \|^2$
  - unitary transformation preserves norm of a vector
  - evolution of state vector $|\psi(t)\rangle$ is a unitary transformation $|\psi(t)\rangle = U(t)|\psi(0)\rangle$, t is 'time'
  - eigenvectors $|\theta\rangle$, $U|\theta\rangle = e^{i\theta}|\theta\rangle$
  - quantum computer realises unitary transformation using 'quantum gates'

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Example I: Not-gate X

X-gate

- permutation of basis states in $\mathbb{C}^2$, $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$
  - $X : |0\rangle \rightarrow |1\rangle$
  - $X : |1\rangle \rightarrow |0\rangle$
  - $X = |1\rangle \langle 0| + |0\rangle \langle 1|$
  - $X(c_0 |0\rangle + c_1 |1\rangle) = c_0 |1\rangle \langle 0|0\rangle + c_1 |0\rangle \langle 1|1\rangle = c_0 |1\rangle + c_1 |0\rangle$

Example II: A permutation operator

Proposition

A permutation of basis states defines a unitary operator

- Assume a finite orthonormal basis $\{|i\rangle\}_{i=1}^{n}$
- A bijection $\pi : \{1, 2, \cdots, n\} \to \{1, 2, \cdots, n\}$ (a permutation)
- define a permutation operator S:
- $S = |\pi(1)\rangle\langle 1| + |\pi(2)\rangle\langle 2| + \cdots + |\pi(n)\rangle\langle n|$
  - for a given state-vector, S permutes its coordinates
- $S^\dagger = |1\rangle\langle\pi(1)| + |2\rangle\langle\pi(2)| + \cdots + |n\rangle\langle\pi(n)|$
- $SS^\dagger =$ $|\pi(1)\rangle \langle 1|1\rangle \langle\pi(1)| + |\pi(2)\rangle \langle 2|2\rangle \langle\pi(2)| + \cdots + |\pi(n)\rangle \langle n|n\rangle \langle\pi(n)| =$ $|\pi(1)\rangle\langle\pi(1)| + |\pi(2)\rangle\langle\pi(2)| + \cdots + |\pi(n)\rangle\langle\pi(n)| = |1\rangle\langle 1| + \cdots + |n\rangle\langle n| = I_n,$

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Tensor products of Hilbert spaces

Let H_1 and H_2 be two Hilbert spaces describing two quantum systems - how to create state space of a quantum system which has such two parts, $H_1 \otimes H_2$?

- if $\{|\psi_i\rangle\}$ and $\{|\phi_i\rangle\}$ are orthonormal baseses of H_1 and H_2, then $\{|\psi_i\rangle |\phi_j\rangle := |\psi_i\rangle \otimes |\phi_j\rangle\}$ is a basis in $H_1 \otimes H_2$
- a generic element in $H_1 \otimes H_2$ has a form: $|\Psi\rangle = \sum_{ij} c_{ij} |\psi_i\rangle |\phi_j\rangle$, $c_{ij} \in \mathbb{C}$
- define inner product of an element $|\psi_1\rangle |\psi_2\rangle$ as: $|\psi_1\rangle |\phi_1\rangle \cdot |\psi_2\rangle |\phi_2\rangle = \langle\phi_1|\phi_2\rangle \langle\psi_1|\psi_2\rangle$
- inner product is denoted $|\psi_1\rangle |\phi_1\rangle \cdot |\psi_2\rangle |\phi_2\rangle = \langle\psi_1, \phi_1|\psi_2, \phi_2\rangle$
- continue inner product by linearity to all elements of $H_1 \otimes H_2$
- operators M_1, M_2 acting in H_1, H_2 act in $H_1 \otimes H_2$ as $M_1 \otimes M_2 |\psi_i\rangle \otimes |\phi_j\rangle = (M_1 |\psi_i\rangle) \otimes (M_2 |\phi_j\rangle)$

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Qubits

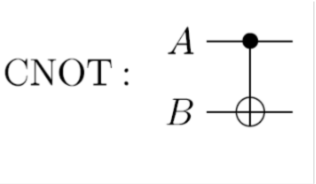
One qubit states - two dimensional space $\mathbb{C}^2$ spanned by:
$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$
An element in $\mathbb{C}^2$, $|\psi\rangle = c_0 |0\rangle + c_1 |1\rangle = \begin{pmatrix} c_0 \\ c_1 \end{pmatrix}$, $|c_0|^2 + |c_1|^2 = 1$

Many qubit space

- tensor product of more than 2 Hilbert spaces: by induction
- one qubit space is $\mathbb{C}^2$, two qubit space is $\mathbb{C}^2 \otimes \mathbb{C}^2 = \mathbb{C}^4$ and so on
- take basis vectors in each one qubit space: $|0\rangle, |1\rangle$, computational bases
- computational basis in n-qubit space ($\mathbb{C}^{2^n}$) is formed by all possible combinations:
  - $|x_1\rangle \otimes |x_2\rangle \otimes \cdots \otimes |x_n\rangle = |x_1\rangle |x_2\rangle \cdots |x_n\rangle = |x_1, x_2, \cdots, x_n\rangle$, $x_i \in \{0, 1\}$
  - ordering of basis: $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$ (and similarly for more than 2 qubits)
  - $|x_1, x_2, \cdots, x_n\rangle = |x\rangle$, in which $x \in \{0, \cdots, 2^n - 1\}$ is integer corresponding to its binary representation $(x_1, \cdots, x_n) = \sum_i x_i 2^{i-1}$
  - so: $|00\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, |01\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, |10\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, |11\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$

Gates I

- Evolution of quantum state is unitary
- manipulation of qubits - unitary oprators
- gates are unitary operations
- Example controlled-NOT: if the control qubit is in $|1\rangle$ reverses the target qubit, otherwise does not change anyting
  - $U_{CN}|00\rangle = |00\rangle, U_{CN}|01\rangle = |01\rangle, U_{CN}|10\rangle = |11\rangle, U_{CN}|11\rangle = |10\rangle$
  - in matrix form $U_{CN} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$

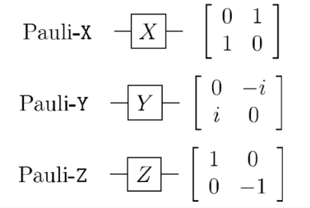


Gates II

- Any unitary operation can be represented by C-NOT gates and one-qubit gates

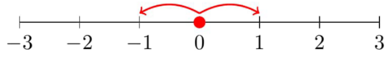
Some important 1-qubit gates: Hadamar gate: $H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$,
$H|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$

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



Random walk on $\mathbb{Z}$

- classical random walk on $\mathbb{Z}$: start from the point 0, at each discrete time step ($t = 0, 1, 2, \cdots$) step flip a fair coin C, if $C = 0$, move one step to the right, otherwise move one step to the left.
- result a probability distribution of finding the walker at position $n \in \mathbb{Z}$ at the moment of time t, $p(t, n)$
- say, if $p(0, 0) = 1$, then $p(1, -1) = p(1, 1) = \frac{1}{2}$
- for large t, $p(t, n) \sim \frac{2}{\sqrt{2\pi t}} e^{-\frac{n^2}{2t}}$
  - $\mathbb{E}n(t) = 0$, $\sigma(t) = \sqrt{\mathbb{E}n(t)^2} = \sqrt{t}$

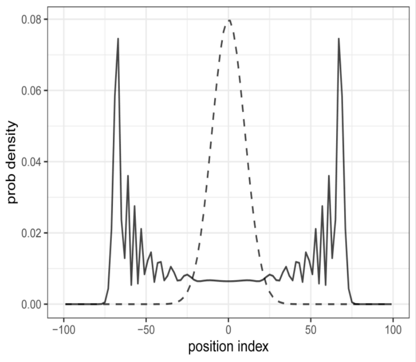


Quantum walk on $\mathbb{Z}$, basic definitions

- state space: ℓ_2 with orthonormal basis $\{|k\rangle\}_{k\in\mathbb{Z}}$
  - a generic state: $|\psi\rangle = \sum_{i\in\mathbb{Z}} c_i |i\rangle$, $\sum_i |c_i|^2 = 1$
  - state $|\psi\rangle = |i\rangle$ means that the walker is at the position $i \in \mathbb{Z}$
  - $|c_i|^2$ is the probability of finding the walker in position i
- quantum coin state $|\phi\rangle \in \mathbb{C}^2$ with basis $\{|0\rangle, |1\rangle\}$
- quantum walk state space is $\ell_2 \otimes \mathbb{C}^2$
- shift to the right operator: $S_0 := \sum_{i\in\mathbb{Z}} |i+1\rangle\langle i|$
- shift to the left operator: $S_1 := \sum_{i\in\mathbb{Z}} |i-1\rangle\langle i|$
- coin flip operator Hadamar H
- unitary operator of a quantum walk step:
  $U := S_0 \otimes (|0\rangle\langle 0| H) + S_1 \otimes (|1\rangle\langle 1| H)$
- U is unitary because both S_0 and S_1 are permutations ($S_i S_i^\dagger = I_{\ell_2}$):
  - $UU^\dagger = S_0 S_0^\dagger \otimes (|0\rangle\langle 0| HH^\dagger |0\rangle\langle 0|) + S_1 S_1^\dagger \otimes (|1\rangle\langle 1| HH^\dagger |1\rangle\langle 1|) =$
    $I_{\ell_2} \otimes (|0\rangle\langle 0| + |1\rangle\langle 1|) = I_{\ell_2} \otimes I_2 = I$

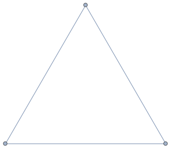
Quantum walk on $\mathbb{Z}$

- quantum state of the quantum walk at time $t \in \{0, 1, 2, \cdots\}$ with initial state $|\psi(0)\rangle$ is: $|\psi(t)\rangle = U^t |\psi(0)\rangle$
- take, for instance, $|\psi(0)\rangle = |n = 0\rangle \otimes \left(\frac{|0\rangle - i|1\rangle}{\sqrt{2}}\right)$
- we get a linear stretch of distribution
- at $t = 100$, probability of position - solid line. Dashed - line random walk



A simple graph

- let $G(E, V)$ be a simple graph with set of links E and set of n vertices V
- adjacency matrix of $G(E, V)$, A is indicator of links
  - A is $n \times n$ symmetric binary matrix with $A_{ij} = 1$ if $\{i, j\} \in E$ or if $\{i, j\}$ is a link, otherwise $A_{ij} = 0$
  - A simple graph: no self-loops ($A_{ii} = 0$), no multiple links ($A_{ij} \in \{0, 1\}$)
- an example K_3 a triangle



$$A = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

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Quantum walk on a finite graphs

- vertex set $V = \{1, \cdots, N\}$, position of a walker $|v\rangle, v \in V$.
- a quantum walk unitary operator U defines evolution of the state
- $|\psi(t)\rangle = U^t |\psi(0)\rangle, t = 1, 2, \cdots$
- U may involve coin-operator
- $p(v, t)$ denotes the probability of finding walker in node v at time t
  - $p(v, t)$ does not converge as $t \to \infty$
  - depends on initial state $|\psi(0)\rangle$
  - $p(v, t)$ is quasi-periodic, because U is unitary
  - average probability distribution: $p_v(T) := \frac{1}{T} \sum_{i=0}^{T-1} p(v, t)$
  - sampling: take uniformly at random $t \in \{0, T - 1\}$, measure $|\psi(t)\rangle$, probability of finding $v = p_v(T)$
  - $\pi(v) = \lim_{T \to \infty} p_v(T)$, exists, though convergence may be slow (power-laws has been seen)
  - $\pi(v) = \frac{1}{N}$, may happen when all eigenvalues of U are distinct

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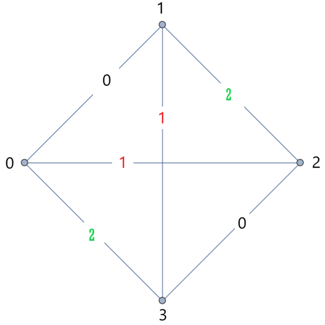
Quantum walk on a $d-$regular graph with even number of vertices

- assume a simple graph $G_d(V,E)$ with $|V| = N$ even number of vertices and with constant degrees $= d$ of all nodes (a class 1 graph).
- such a graph has an edge coloring with d colors (each edge is assigned a color in such a way that all edges adjacent to a node have different colors)
- take a d-dimensional coin space, $\mathbb{C}^d$
- take a N-dimensional position space $\mathbb{C}^N$
- take a edge coloring with d-colors, for a color a and vertex $v \in V$, denote $v(a)$ neighbor of v sharing an edge with color a.
- basis states are denoted: $|a,v\rangle \in \mathbb{C}^d \otimes \mathbb{C}^N$, $a \in \{0,1,\cdots,d-1\}$ and $v \in \{1,\cdots,N\}$
- Quantum walk is defined by an operator $U = S(C \otimes I_N)$
  - C is unitary coin operator
  - $S\,|a,v\rangle = |a,v(a)\rangle$

K_4-example



- for each edge color $a \in \{0, 1, 2\}$ $S(a)$ defines a permutation of vertices
- for instance for a color $= 0$: $S(0) = (|0\rangle\langle 1| + |1\rangle\langle 0| + |3\rangle\langle 2| + |2\rangle\langle 3|)$
- $S(0)S(0)^{\dagger} = (|0\rangle\langle 0| + |1\rangle\langle 1| + |2\rangle\langle 2| + |3\rangle\langle 3|) \otimes |0\rangle\langle 0|) = I_3$
- that is why $U = \sum_{a=0}^{2} S(a) \otimes |a\rangle\langle a| (C \otimes I_N)$ is unitary

Continuous time quantum walk on a graph

- $n \times n$ adjancency matrix A of a simple graph G is a binary and symmetric matrix and as a result Hermitian
- A is a 'Hamiltonian'
- e^{-iAt}, $t \in \mathbb{R}$ is a unitary operator
- take a Hilbert space $H_A = \mathbb{C}^n$ in which an orthonormal basis correspond to nodes of the graph
- continuous time quantum walk on G starting from $|\psi\rangle \in H_A$ corresponds to the evolution: $|\psi(t)\rangle = e^{-iAt} |\psi\rangle$
- instead of A we could have taken the 'graph Laplacian' as an Hamiltonian (- degrees on diagonal and A entries outside the diagonal)

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Hypercube

- take n qubits
- take 2^n nodes
- a node with number k is mapped to the computational basis state $|k\rangle$
- the binary string corresponding to $|k\rangle$ is taken as coordinates of an vertex of n - hypercube
- denote by σ_x^i the X-gate acting on a qubit i ($X|0\rangle = |1\rangle, X|1\rangle = |0\rangle$)
- Claim: matrix of $H := \sum_{i=1}^{n} \sigma_x^i$ is adajcency matrix of the corresponding hypercube
- indeed, $\langle k| H |k'\rangle = 1$ only if the bit strings k and k' differ exactly by a one binary digit, which is the adjacency rule for the hypercube
- say, for $n = 3$, $\langle 001| H |000\rangle = \langle 001| \sigma_x^1 |000\rangle = \langle 001|001\rangle = 1$

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Quantum walk on a hypercube

- as a result, we have a unitary for quantum walk on the hypercube: $U_{HC}(t) = e^{-itH} = \prod_{j=1}^{n} e^{-i\sigma_x^j t}$
- or in other words: $U_{HC}(t) = \bigotimes_{j=1}^{n} \begin{pmatrix} \cos(t) & -i\sin(t) \\ -i\sin(t) & \cos(t) \end{pmatrix}$
- U_{HC} has one-qubit implementation with standard gates: $U_{HC}(t) = \bigotimes_{j=1}^{n} RX(2t)$

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Quantum approximate optimization algorithm (QAOA)

QAOA imitates quantum adiabatic evolution: start from a known ground state of a trivial Hamiltonian, then slowly change the Hamiltonian, the state remains in the ground state all the time, at the end read the ground state of the final Hamiltonian which solves an optimization problem.

QAOA Hamiltonians:

- solutions of the problem are encoded as bit strings of constant length n, $x = (x_1, \cdots, x_n)$ with cost function $c(x)$ taking real values
- task is to find $x^* = \arg\min_x c(x)$
- take quantum register with n qubit
- Define a 'problem Hamiltonian' C
- C is diagonal in computational basis and $C\,|x\rangle = c(x)\,|x\rangle$
- 'trivial Hamiltonian' $H_0 = -\sum_{i=1}^{n} \sigma_x^i$, ground state is $|\psi\rangle = \frac{1}{2^{n/2}} \sum_x |x\rangle = \frac{1}{2^{n/2}}(|0\rangle + |1\rangle)(|0\rangle + |1\rangle)\cdots(|0\rangle + |1\rangle)$
- $H_0\,|\psi\rangle = -n\,|\psi\rangle$, because $\sigma_x(|0\rangle + |1\rangle) = |0\rangle + |1\rangle$

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QAOA

- define $U(t, \tau) = e^{-iH_0 t} e^{-iC\tau}$
- and for $p = 1, 2, \cdots$,
  $|(t_1, \tau_1), \cdots, (t_p, \tau_p)\rangle = U(t_p, \tau_p) \cdots U(t_1, \tau_1) |\psi\rangle$
- parameters are chosen from the condition $((t_1, \tau_1), \cdots, (t_p, \tau_p)) = \arg\min \langle (t_1, \tau_1), \cdots, (t_p, \tau_p)| C |(t_1, \tau_1), \cdots, (t_p, \tau_p)\rangle$
- note: $e^{-iH_0 t}$ is unitary of the quantum walk on the corresponding hypercube

Quantum walk assisted QAOA

S. Marsh and J. B. Wang, Quantum Inf Process 18, 61 (2019)

- QAOA needs modifications when not all vertices of the hypercube correspond to a solution
- for instance the problem of minimal vertex cover of a graph
  - a vertex cover is a subset of vertices such that any edge of the graph has an endpoint in it
- a graph with n nodes: take n qubits, a cover can be described as one of the basis vectors $|x_1, \cdots, x_n\rangle$ in which $x_i = 1$ iff node i is in the cover
- not all basis states are covers, say, $|0\rangle$ corresponds to the empty vertex set, which can not cover any graph
- a solution instead of quantum walk $e^{-iH_0 t}$, take a quantum walk on the solution subspace avoiding states which are not possible solutions
- efficient gate implementations exist if the problem instances can be decided efficiently (NP optimization problems)

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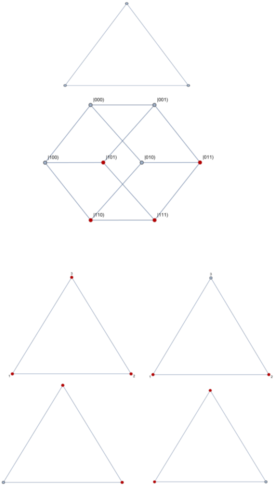
Example: triangle

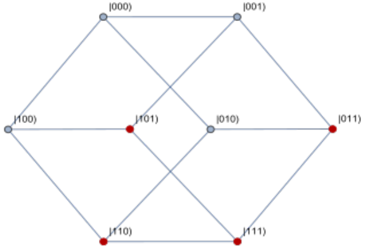
Covering a triangle (K_3) and the corresponding hypercube. Red vertices indicate valid covers



Quantum walk on a solution subspace

In case of K_3 vertex cover, quantum walk should be only among red vertices

- Take an adjacency matrix A which connects only red nodes (like the complete graph K_4 in this case)
- instead of $e^{-iH_0 t}$, use e^{-iAt} in the QAOA algorithm
- in more general case one needs an indexing unitary which permutes basis states so that red vertices are in a canonical order
- a good idea is to use so caled 'circular graphs' in the corresponding solution space (a complete graph is an example)



Solving minimum vertex cover for K_3

- four possible covers, take 4-dimensional vector space $\mathbb{C}^4$
- a circulant graph K_4 with adjacency matrix $A_4 = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}$
- first 3 dimensions correspond to covers with two nodes, the last to the cover with 3 nodes
- take the cost matrix as $C = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$
- the initial state $|s\rangle = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$

Optimal solution for QAOA

- Let $|\psi\rangle$ is the state after QAOA transformation
- target is to find $|\psi^*\rangle = \arg\max_{|\psi\rangle} \langle\psi| C |\psi\rangle$, which maximizes expectation of C,
- achieved with e.g. $|\psi^*\rangle = \frac{1}{\sqrt{3}}\begin{pmatrix}1\\1\\1\\0\end{pmatrix}$ and $\langle\psi^*| C |\psi^*\rangle = 2$
- Claim: $|\psi^*\rangle$ can be found with one round of QAOA

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Solution of cover problem for K_3 with one step of quantum walk assisted QAOA

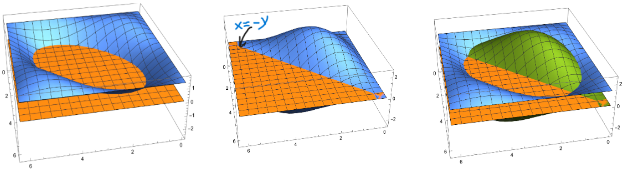
Using Wolfram Mathematica (or analytics):

- $|\psi\rangle = e^{-iA_4 t} e^{i\tau C} |s\rangle = \frac{e^{-3it+i\tau}}{8} \begin{pmatrix} c \\ c \\ c \\ c' \end{pmatrix}$
- $c = 1 - e^{4it} + 3e^{i\tau} + e^{i(4t+\tau)}$
- and $c' = 1 + 3(e^{4it} + e^{i\tau} - e^{i(4t+\tau)})$
- $|\psi\rangle = |\psi^*\rangle$ iff $c' = 0$ (because $\langle\psi|\psi\rangle = 1$)
- solving numerically:
- $c' = -1.56986 * 10^{-9} + 1.98889 * 10^{-10} i$ for $t = 3.449332507981935$ and $\tau = 5.0522258895115755$
- probabilty of wrong answer is $|c'|^2/64 = 3.91251 * 10^{-20}$

VTT

Perfect solution for QAOA exists: a sketch of proof

- A solution of $c' = 0$ is a point in which 3 functions intersect:
- 1) $z(x,y) = 0$, 2) $z(x,y) = \cos x + \cos y - \cos(x+y) + \frac{1}{3}$ and 3)$z(x,y) = \sin x + \sin y - \sin(x+y)$, ($z(x,y) = 0$, when $x = -y$)



1) and 2) 1) and 3) All

Figure: $z(x,y) = 0$ orange-plot

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Circulant graphs

- Circulat graph is agraph with circulant adjacency matrix
- For instance any complete graph

Circulant matrix has rows and columns which are ordered cyclic permutations of each other:

$$C = \begin{pmatrix} c_0 & c_{n-1} & \cdots & c_2 & c_1 \\ c_1 & c_0 & \cdots & c_3 & c_2 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ c_{n-2} & c_{n-3} & \cdots & c_0 & c_{n-1} \\ c_{n-1} & c_{n-2} & \cdots & c_1 & c_0 \end{pmatrix}$$

Has closed form spectra: $\omega := \exp\left\{\frac{2\pi i}{n}\right\}$, eigenvectors are $|v_j\rangle = \frac{1}{\sqrt{n}}\begin{pmatrix}1 & \omega^j & \omega^{2j} & \ldots & \omega^{(n-1)j}\end{pmatrix}^T$,
with eigenvalues:

$$\lambda_j = c_0 + c_{n-1}\omega^j + c_{n-2}\omega^{2j} + \cdots + c_1\omega^{(n-1)j}$$

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Circulant graphs and quantum Fourier transformation

- if A is circulant, then $e^{iAt}\left|v_j\right\rangle = e^{it\lambda_j}\left|v_j\right\rangle$
- spectral decomposition: $e^{iAt} = \sum_j e^{i\lambda_j t}\left|v_j\right\rangle\left\langle v_j\right|$
- quantum Fourier transformation of a orthonormal basis:
  $F(|j\rangle) = \sum_k \frac{1}{\sqrt{n}} e^{2\pi ikj/n}|k\rangle = \sum_k \frac{1}{\sqrt{n}}\omega^{jk}|k\rangle = \left|v_j\right\rangle$
- as a result $F = \sum_j \left|v_j\right\rangle\langle j|$
- and $F^{-1} = F^{\dagger} = \sum_j |j\rangle\left\langle v_j\right|$
- F is a transformation of one orthonormal basis to another one

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A sketch of gate implementation of a quantum walk on circulant graphs

- Let A be an adjacency matrix of a circulant graph
- we need gates for $e^{iAt}\left|\psi\right\rangle$, for an arbitrary quantum register state $\left|\psi\right\rangle$
- expand $\left|\psi\right\rangle = \sum_j c_j \left|v_i\right\rangle$
- then $e^{iAt}\left|\psi\right\rangle = \sum_j e^{i\lambda_j t} c_j \left|v_j\right\rangle$
- let $e^{i\Lambda t}$ be a diagonal matrix with $e^{i\lambda_j t}$ at as the jth diagonal element
- $F^\dagger \left|\psi\right\rangle = \sum_j c_j F^\dagger \left|v_j\right\rangle = \sum_j c_j \left|j\right\rangle$
- $e^{i\Lambda t} F^\dagger \left|\psi\right\rangle = \sum_j c_j e^{i\Lambda t} \left|j\right\rangle = \sum_j c_j e^{i\lambda_j t} \left|j\right\rangle$
- $F e^{i\Lambda t} F^\dagger \left|\psi\right\rangle = \sum_j c_j e^{i\lambda_j t} F \left|j\right\rangle = \sum_j e^{i\lambda_j t} c_j \left|v_j\right\rangle = e^{iAt}\left|\psi\right\rangle$
- as a result: $e^{iAt} = F e^{i\Lambda t} F^\dagger$

Staggered quantum walk

- Discrete walk on a graph G
- select a set, $\mathcal{T}_i$, of complete subgraphs of G covering all vertices
- take several such 'tesselations' $\mathcal{T} = (\mathcal{T}_1, \cdots, \mathcal{T}_n)$, until $\mathcal{T}$ covers all edges of G
- $\mathcal{T}$ is called tesselation cover of G
- for all complete graphs $K_\alpha(i)$ constituting $\mathcal{T}_i$, make equal superposition of vertex states $|D_\alpha(i)\rangle$
- make a Hamiltonian $H_i = 2\sum_\alpha |D_\alpha(i)\rangle \langle D_\alpha(i)| - I$
- unitary $U(t_1, \cdots, t_n) = \exp\{it_n H_n\} \cdots \exp\{it_1 H_1\}$ with real parameters $t_1, \cdots, t_n$, defines a staggered quantum walk on G

Staggered quantum walk assisted QAOA?

- For a solution space graph find tesselation cover $\mathcal{T}$
- find corresponding Hamiltonians H_i and $U_S(t) = U(t, \cdots, t)$
- use $U_S(t)$ in quantum walk assisted QAOA
- works for minimum vertex cover problem in K_3, with one step
- tesselation cover used:

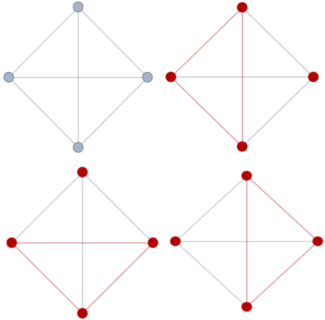


Figure: 3 tesselation of K_4 shown in red

Amplitude of non-optimal vertex cover of K_3 using QAOA with staggered QW

By tuning two real parameters, probability of sub-optimal vertex covers can be adjusted to almost zero $\sim 10^{-7}$:

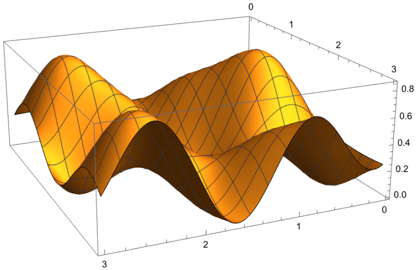


Figure: Probability (vertical) of finding non-optimal vertex cover as a function of two real parameters of QAOA

Non-backtracking quantum walk: background

M. Bolla, H. Reittu, and F. Abdelkhalek, "Clustering the Nodes of Sparse Edge-Weighted Graphs via Non-Backtracking Spectra", to appear

- a hot topic in graph based data mining
- a so called non-backtracking matrix is involved - describes non-backtracking walk on a graph
- is there a quantum version?
- Application: spectral clustering based on non-backtracking matrix of a graph/matrix, see:

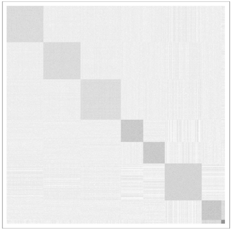
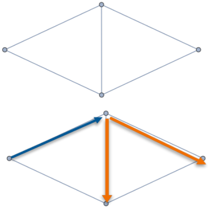


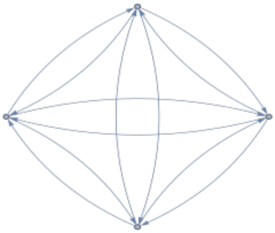
Figure: Clustering of a 7600 node chemical network

Non-backtracking classical walk on a graph: one step forward and no step back

A step (blue) and all possible next steps (orange) - no backtracking

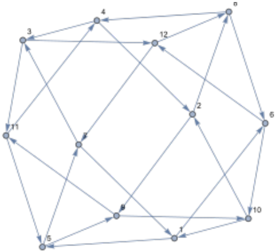


Directed graph associated with the non-backtracking walk



K_4

$\rightarrow$



Directed graph

The adjacency matrix of the directed graph = Non-backtracking matrix

$$
\begin{pmatrix}
0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\
0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\
1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0
\end{pmatrix}
$$

A coined non-backtracking quantum walk; condition of existence

Ashley Montanaro, Quantum walks on directed graphs, Quantum Information Computation vol. 7 no. 1, pp. 93-102, 2007, quant-ph/0504116

- Consider a directed graph (links are ordered pairs of vertices, 'a link from a to b= (a,b)'
- link a $\rightarrow$ b is reversible if there is a path from b to a
- A graph is reversible if all its links are reversible
- Theorem: A discrete-time coined quantum walk can be defined on a finite directed graph G if and only if G is reversible
- A Corollary: Quantum walk on a non-backtracking graph is possible iff the non-backtracking graph is reversible

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Generic recipe (Montanaro, ibid.)

- In reversible directed graph G choose a set C of elementary cycles (no repeated nodes) such that every link (a, b) is at least in one cycle from C
- a cycle is an ordered sequence of vertices $(v_1, v_2, \cdots, v_k)$, such that every $(v_i, v_{i+1}), 1 \leq i \leq k-1$ and (v_k, v_1) is a link
- make bijection of nodes to orthonormal states $|\cdot\rangle$
- each cycle $c_i \in C$ defines a permutation operator $S(c_i) = \sum_{(a,b) \in c_i} |b\rangle \langle a| + \sum_{k \notin c_i} |k\rangle \langle k|$
- choose $|C|$ orthonormal coin states and a unitary coin operator F
- quantum walk operator is $W = (\sum_i |i\rangle \langle i| \otimes S(c_i))(F \otimes I_{|C|})$

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Cycles in NB-graph

- need to choose set of cycles from a NB-graph so that every link is at least in one cycle
- e.g. could take 8 cycles each a directed triangle
- needs 12 orthonormal states to represent vertices

  4 qubits and use first 12 basis states ($|0000\rangle, \cdots, |1011\rangle$ as vertices)
- to switch among 8 cycles, take a coin space with 8 basis states
  - 3 qubit space, $|000\rangle, \cdots, |111\rangle$ representing cycles
- in total needs 7 qubits

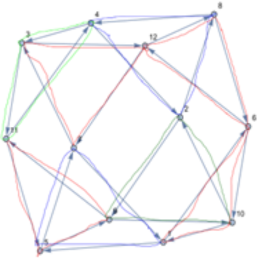


Figure: 8 cycles of the NB-graph

Graphical view of one of S_i

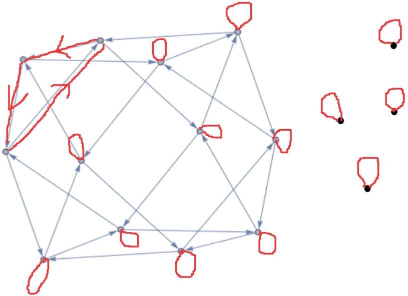
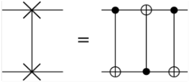


Figure: A permutation corresponding to a cycle, self-loops correspond to I_2

Cycle as a sequence of 'swaps'

- any n-cycle can is equivalent to $n-1$ subsequent transpositions (2-cycles)
- a cycle $(a, b, c, \cdots, d, g)$ is a permutation: $\begin{pmatrix} a & b & c & \cdots & g \\ g & a & b & \cdots & d \end{pmatrix}$
- can be decomposed into transpositions $(a, b), (b, c), \cdots, (d, g)$
- each transposition (i,j) is like $(|i\rangle\langle j| + |j\rangle\langle i| + \sum_{k\neq i,j}|k\rangle\langle k|)$,
- a SWAP gate, implemented as 3 CNOT gates:



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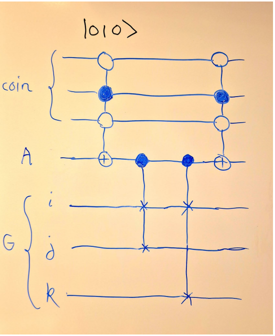
Quantum circuit for a cycle

A quantum circuit for a cycle (ijk) controlled by a coin state $|010\rangle$ for a NB-graph G using one ancilla qubit A.



Non-backtracking classical walk on K_3

- classical random walk on K_3 (triangle)
- first coin toss decides: go clockwise or counter clockwise

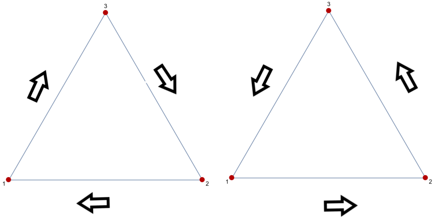


Figure: Clockwise or counter clockwise

Quantum non-backtracking walk on K_3

- The non-backtracking graph is a set of two triangles (see Fig.)
- has two unique 3-cycles
- needs coin with two states $|0\rangle$ and $|1\rangle$ to switch between cycles
- 6 orthonormal vectors for position $|1\rangle, |2\rangle, \cdots, |6\rangle$

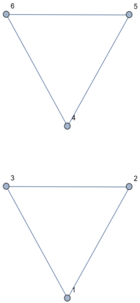


Figure: Non-backtracking graph for K_3

Unitary for NB on K_3

- shift operator: $S = |0\rangle\langle 0| S_1 + |1\rangle\langle 1| S_2$
  - $S_1 = |2\rangle\langle 1| + |3\rangle\langle 2| + |1\rangle\langle 3|$
  - $S_2 = |5\rangle\langle 4| + |6\rangle\langle 5| + |4\rangle\langle 6|$
- unitary operator using Hadamar-coin: $U = S \otimes H$
- S_1 is diagonal in Fourier-basis: $(|1\rangle, |2\rangle, |3\rangle) \to (|\alpha_1\rangle, |\alpha_2\rangle, |\alpha_3\rangle)$
  - $|\alpha_1\rangle = \frac{1}{\sqrt{3}}(|1\rangle + |2\rangle + |3\rangle)$
  - $|\alpha_2\rangle = \frac{1}{\sqrt{3}}(|1\rangle + \omega|2\rangle + \omega^2|3\rangle)$, $\omega := \exp(2\pi i/3)$
  - $|\alpha_3\rangle = \frac{1}{\sqrt{3}}(|1\rangle + \omega^2|2\rangle + \omega|3\rangle)$, $(\omega^3 = 1)$
- similarly S_2 is diagonal in Fourier basis: $(|4\rangle, |5\rangle, |6\rangle) \to (|\beta_1\rangle, |\beta_2\rangle, |\beta_3\rangle)$
- $S_1|\alpha_i\rangle = \lambda_i|\alpha_i\rangle$, $\lambda_1 = 1, \lambda_2 = \omega^{-1}, \lambda_3 = \omega^{-2}$
- $S_2|\beta_i\rangle = \lambda_i|\beta_i\rangle$
- U is not diagonal in the Fourier basis $\{|\alpha_i\rangle, |\beta_j\rangle\}$ if using $(|0\rangle, |1\rangle)$-basis for the coin

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Diagonalizing K_3 NB-walk unitary operator

- for fixed i, $S \otimes H \left|0\right\rangle \left|\alpha_i\right\rangle = \frac{1}{\sqrt{2}} S(\left|0\right\rangle + \left|1\right\rangle) \left|\alpha_i\right\rangle = \frac{1}{\sqrt{2}}(\lambda_i \left|0\right\rangle + \left|1\right\rangle) \left|\alpha_i\right\rangle$
- and $S \otimes H \left|1\right\rangle \left|\alpha_i\right\rangle = \frac{1}{\sqrt{2}} S(\left|0\right\rangle - \left|1\right\rangle) \left|\alpha_i\right\rangle = \frac{1}{\sqrt{2}}(\lambda_i \left|0\right\rangle - \left|1\right\rangle) \left|\alpha_i\right\rangle$
- for generic coin state $\left|\alpha\right\rangle$,U $\left|\alpha\right\rangle \left|\alpha_i\right\rangle = u(i) \left|\alpha\right\rangle \left|\alpha_i\right\rangle$
  - with $u_\alpha(i) = \frac{1}{\sqrt{2}} \begin{pmatrix} \lambda_i & \lambda_j \\ 1 & -1 \end{pmatrix}$
  - find orthonormal eigenvectors of $u_\alpha(i)$, $\left|a_i^1\right\rangle$ and $\left|a_i^2\right\rangle$, with eigenvalues a_i^1, a_i^2
- similarly for states $\left|\beta_i\right\rangle$ we get matrix $u_\beta(i) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ \lambda_i & -\lambda_i \end{pmatrix}$, and the spectra is denoted as vectors $\left|b_i^1\right\rangle$ and $\left|b_i^2\right\rangle$ with eigenvalues b_i^1, b_i^2.
- U is diagonal in basis $\{(\left|a_i^k\right\rangle \left|\alpha_i\right\rangle, \left|b_j^k\right\rangle \left|\beta_j\right\rangle)\}$, $k = 1, 2$
- $U = \sum_i \{(a_i^1 \left|a_i^1\right\rangle \left\langle a_i^1\right| + a_i^2 \left|a_i^2\right\rangle \left\langle a_i^2\right|) \left|\alpha_i\right\rangle \left\langle\alpha_i\right| + (b_i^1 \left|b_i^1\right\rangle \left\langle b_i^1\right| + b_i^2 \left|b_i^2\right\rangle \left\langle b_i^2\right|) \left|\beta_i\right\rangle \left\langle\beta_i\right|\}$

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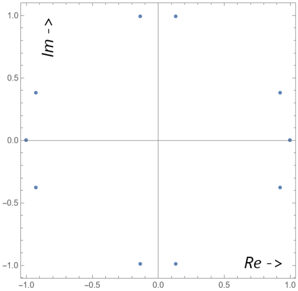
Eigenvalues of NB-walk on K_3

- U has 12 eigenvectors
- All eigenvalues are distinct, except for eigenvalues ± 1, which are doubly degenerate both
- they correspond to case: $u_\alpha(1) = u_\beta(1) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$
- eigenvalues (dots) of U on complex plane:



K_4 example: needed resources

- a complete quantum circuit consists of 8 blocks for cycles
- needs 8 qubits
- each block has two generalized Toffoli-gates (for coin) with 3 controls
- each block has 2 controlled SWAP-gates (Fredkin-gates)
- CNOT count
  - for generalized Toffoli gates -needs 1 ancilla qubit and $3 \times 6 = 18$ CNOT gates
  - Each Fredkin-gate needs 18 CNOT-gates
  - in total need 9 qubits and $8 \times 5 \times 18 = 720$ CNOT-gates
  - generally CNOT-count $\sim 12|C| \log_2 |C| + 18 \sum_i (|c_i| - 1)$

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