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Quantum Walks and Graph Coloring

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Tuesday

Outline of the Mini-course

- Review on graph coloring
- **Coined quantum walks on graphs**
- Staggered quantum walks on graphs
- Spatial search algorithm
- Equivalence of discrete-time QWs

Today's Outline

- Coined quantum walks on class-2 graphs
- Coined quantum walks on class-1 graphs
- Locality
- Quasi-periodicity
- Limiting probability distribution
- Mixing time
- Interesting problems

Coined Quantum Walks on Graphs

Definition of the standard version: $U = S \cdot C$ or $U = S \cdot (I \otimes C)$

Note for coined quantum walks:

1. For a class-1 graph G, the walk is defined on G or $D(G)$ (symmetric digraph).
2. For a class-2 graph G, the walk must be defined on the associated symmetric digraph $D(G)$ using the *arc notation*.

Since coined quantum walks on both class-1 and class-2 graphs can be defined on the associated symmetric digraph $D(G)$, we start by this general definition.

Definition of the Standard Coined Quantum Walk [1,2]

1. Let $\mathcal{H}_A$ be the Hilbert space associated with the symmetric digraph $D(G)$. The computational basis is

$$\mathcal{H}_A = \text{span}\{|a\rangle : a \in A(D(G))\}, \quad \dim(\mathcal{H}_\mathcal{A}) = |A| = 2|E|.$$

   The walker steps on arcs (not on vertices).
2. The evolution operator is $U = SC$.
3. The flip-flop shift operator is $S|a\rangle = |\bar{a}\rangle$, where $\bar{a}$ is the reversed arc of a. S is a permutation and involutory ($S^2 = I$)
4. C is the coin operator. The Grover coin is

$$C|a\rangle = \sum_{\substack{b\in A \\ \text{tail}(b)=\text{tail}(a)}} \left(\frac{2}{d^+(\text{tail}(a))} - \delta_{a,b} \right) |b\rangle \qquad (a \in A).$$

[1] Severini, Hancock et.al, Krovi&Brun, Konno et.al, ...
[2] R. Portugal. Quantum Walks and Search Algorithms, 2nd edition, Springer, 2018.

Continuation of the definition

5. The state of the walk at time t (integer) is

$$|\psi(t)\rangle = U^t|\psi(0)\rangle,$$

   where $|\psi(0)\rangle$ is the initial state.
6. The probability of finding the walker on an arc a after t steps is

$$p_a(t) = \left|\langle a|\psi(t)\rangle\right|^2.$$

7. The probability of finding a vertex v after t steps is

$$p_v(t) = \sum_{\substack{a\in A\\ \text{tail}(a)=v}} \left|\langle a|\psi(t)\rangle\right|^2.$$

Notes on the definition

1. The sum over arcs in the definition

$$p_v(t) = \sum_{\substack{a \in A \\ \mathrm{tail}(a)=v}} \left|\langle a|\psi(t)\rangle\right|^2$$

   is equivalent to adding up over all coin values (see class 1).
2. If the walker is on any arc whose tail is v, we have enough information to find v. We cannot additionally consider the arcs whose heads are v because that would introduce an indeterminacy.
3. The coin need not be the Grover coin (Fourier coin, Hadamard coin, ...)
4. S can be persistent (non flip-flop)

$$S|v, w\rangle = |w, v'\rangle.$$

   S is a permutation but is not involutory.

Alternative notation - still arc notation

1. Let $\mathcal{H}_A$ be the Hilbert space associated with the symmetric graph $D(G)$. The computational basis is

$$\mathcal{H}_A = \text{span}\{|v, w\rangle : (v, w) \in A(D(G))\},$$

where $|v, w\rangle$ is equivalent to $|(v, w)\rangle$.

2. The evolution operator is $U = SC$.
3. The flip-flop shift operator is $S|v, w\rangle = |w, v\rangle$, where $(v, w) \in A(D(G))$.
4. C is the coin operator. The Grover coin is

$$C|v, w\rangle = \sum_{v' \in N^+(v)} \left(\frac{2}{d^+(v)} - \delta_{w,v'} \right) |v, v'\rangle,$$

where $(v, w) \in A(D(G))$.

Continuation of the alternative notation

5. The state of the walk at time t (integer) is
$$|\psi(t)\rangle = U^t|\psi(0)\rangle,$$
where $|\psi(0)\rangle$ is the initial state.
6. The probability of finding the walker on an arc (v, w) after t steps is
$$p_{(v,w)}(t) = \left|\langle v, w|\psi(t)\rangle\right|^2.$$
7. The probability of finding a vertex v after t steps is
$$p_v(t) = \sum_{w \in N^+(v)} \left|\langle v, w|\psi(t)\rangle\right|^2.$$

Note: The alternative notation cannot be used for multigraphs because (v, w) denotes only one arc.

Matrix Representation of the Operators S and C

The matrix representation depends on the order of the computational basis $\mathcal{CB}$:

1. Take $\mathcal{CB} = \{(v_1, w_1), (w_1, v_1), (v_2, w_2), (w_2, v_2), \ldots\}$. Then

$$S = \begin{pmatrix} X & & \\ & X & \\ & & \ddots \end{pmatrix}$$

   S is block-diagonal but C is not.

2. Take $\mathcal{CB} = \{(v_1, w_1), \ldots, (v_1, w_k), (w_1, w_1'), \ldots, (w_1, w_\ell'), \ldots\}$. Then

$$C = \begin{pmatrix} C_1 & & \\ & C_2 & \\ & & \ddots \end{pmatrix}$$

   C is block-diagonal but S is not. S is a permutation matrix.

Implementation of Coined Walks in Python

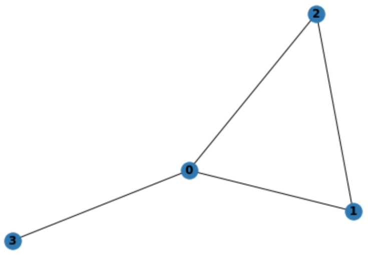
A is the adjacency matrix of a graph (no multiple edges)

```
def ShiftOperator(AdjMatrix):
    n = AdjMatrix.shape[0]
    CB = [[v,w] for v in range(n) for w in range(n) if AdjMatrix[v,w]==1]
    N = len(CB)
    S = sp.sparse.csr_matrix((N, N))
    for j in range(N):
        S[j,CB.index([CB[j][1],CB[j][0]])] = 1
    return S

from scipy.linalg import block_diag
def CoinOperator(AdjMatrix):
    n = AdjMatrix.shape[0]
    G = networkx.from_numpy_matrix(AdjMatrix)
    L = [GroverOperator(G.degree(i)) for i in range(n)]
    return block_diag(*L)

def GroverOperator(N):
    return sympy.Rational(2,N)*sympy.ones(N)-sympy.eye(N)

def EvolutionOperator_CoinedModel(AdjMatrix):
    return ShiftOperator(AdjMatrix)*CoinOperator(AdjMatrix)
```

Implementation of Coined Walks in Python

In [1]:
```
import numpy as np
import scipy as sp
import scipy.linalg
import networkx
import sympy
import matplotlib.pyplot as plt
```

In [2]:
```
#G = networkx.complete_graph(4)
G = networkx.Graph()
G.add_nodes_from([0,1,2, 3])
G.add_edge(0, 1)
G.add_edge(0, 2)
G.add_edge(1, 2)
G.add_edge(0, 3)
networkx.draw(G,with_labels=True, font_weight='bold')
```



In [6]:
```
A = networkx.linalg.graphmatrix.adjacency_matrix(G) # Sparse matrix
```

Implementation of Coined Walks in Python

In [9]:
```
S = ShiftOperator(A)
sympy.Matrix(S.todense())
```

Out[9]:

$$\begin{bmatrix} 0 & 0 & 0 & 1.0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.0 \\ 1.0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1.0 & 0 \\ 0 & 1.0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1.0 & 0 & 0 & 0 \\ 0 & 0 & 1.0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

In [10]:
```
C = CoinOperator(A)
sympy.Matrix(C)
```

Out[10]:

$$\begin{bmatrix} -\frac{1}{3} & \frac{2}{3} & \frac{2}{3} & 0 & 0 & 0 & 0 & 0 \\ \frac{2}{3} & -\frac{1}{3} & \frac{2}{3} & 0 & 0 & 0 & 0 & 0 \\ \frac{2}{3} & \frac{2}{3} & -\frac{1}{3} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

Coined Walks on Class-1 Graphs

Let G be a simple graph and let $\{M_1, .., M_\Delta\}$ be a partition of $E(G)$ into matchings, where $\Delta = \chi'(G)$. Colors are c=1,...,Δ.

1. The Hilbert space of the coined model is $\mathcal{H} = \mathcal{H}_V \otimes \mathcal{H}_C$ in the position-coin notation. The computational basis is

$$\mathcal{H} = \text{span}\big\{|v, c\rangle : v \in V(G),\, c \in \{1, ..., \Delta\}\big\}.$$

2. The evolution operator is $U = SC$.
3. The flip-flop shift operator is $S|v, c\rangle = |v', c\rangle$, where c is the color of edge $\{v, v'\}$.
4. C is the coin operator. The Grover coin is

$$C|v, c\rangle = |v\rangle \otimes \sum_{c' \in \mathcal{C}_v} \left(\frac{2}{d(v)} - \delta_{c,c'} \right) |c'\rangle,$$

where $c \in \mathcal{C}_v$ and $\mathcal{C}_v$ is the set of colors of the edges incident to v.

Continuation of Coined Walks on Class-1 Graphs

5. The state of the walk at time t (integer) is

$$|\psi(t)\rangle = U^t|\psi(0)\rangle,$$

where $|\psi(0)\rangle$ is the initial state.

6. The probability of finding the walker on a vertex v after t steps is

$$p_v(t) = \sum_{c \in \mathcal{C}_v} \left| \left\langle v, c \middle| \psi(t) \right\rangle \right|^2,$$

$\mathcal{C}_v$ is the set of colors of the edges incident to v.

Note: The definition can be used for multigraphs if we consider multigraphs with $\chi' = \Delta$.

Coined Walks on Δ-regular Class-1 Graphs

Let $\{M_1, .., M_\Delta\}$ be a partition of $E(G)$ into perfect matchings, where $\Delta = \chi'(G)$.

We can simplify the definition of the coin operator:

Definition

1. The evolution operator is $U = S \cdot (I \otimes C)$.
2. $I \otimes C$ is the coin operator. The Grover coin is

$$C = 2|u\rangle\langle u| - I_\Delta, \quad \text{where} \quad |u\rangle = \frac{1}{\sqrt{\Delta}} \sum_{c'=1}^{\Delta} |c'\rangle.$$

   Equivalently

$$C|c\rangle = \sum_{c'=1}^{\Delta} \left(\frac{2}{\Delta} - \delta_{c,c'} \right) |c'\rangle.$$

3. The remaining items are the same as before.

Uniquely-defined Coined Quantum Walks

- From graph theory: There are graphs that are uniquely k-edge-colorable
- (Thomason [1]) For $k \neq 3$, only paths, cycles and stars are uniquely k-edge-colorable.
- (Tutte, Belcastro&Haas [2]) There are infinitely many uniquely 3-edge colorable cubic non-planar triangle-free graphs.
- (Greenwell&Kronk [3]) For every uniquely k-edge colorable graph $G \neq K_3$, $\chi'(G) = \Delta(G) = k$.
- The uniquely-defined QWs are QWs on uniquely k-edge-colorable class-1 graphs using the flip-flop shift and Grover coin.

[1] A. Thomason, Hamiltonian cycles and uniquely edge colourable graphs, Annals Disc. Math. 3 (1978), 259-268.
[2] S.M. Belcastro and R. Haas, Triangle-free uniquely 3-edge colorable cubic graphs, arXiv:1508.06934.
[3] D. Greenwell and H.V. Kronk, Uniquely line-colorable graphs, Canad. Math. Bull 16 (1973), 525-529.

Locality

Intuitively, the walker must move only to neighboring vertices (class 1) or neighboring arcs (class 2).

Class-1 graphs (assume the walker in on a vertex):

- The coin operator is local because does not shift the walker (action only on the internal space).
- The shift operator is local because it follows the adjacency matrix.

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Class-2 graphs $\big($assume the walker is on the arc $(v, v')\big)$:

- The coin operator spreads the walker's position over the arcs whose tails are v.
- The shift operator shift the walker to (v', v).

Note: In the arc notation, the action of the coin is visible.

Locality – Formal definition in the arc notation

Definition

An operator A on the Hilbert space $\mathcal{H}_A$ is *local* when $\langle a_1 | A | a_2 \rangle \neq 0$ only if the pair of arcs a_1 and a_2 are adjacent.

Adjacent arcs: $\bullet \overset{\times}{\underset{*}{\leftrightarrow}} \bullet$, $\overset{\times}{\leftarrow} \bullet \overset{*}{\rightarrow}$, $\overset{\times}{\rightarrow} \bullet \overset{*}{\rightarrow}$, $\overset{\times}{\rightarrow} \bullet \overset{*}{\leftarrow}$

Non-adjacent arcs: $\overset{\times}{\rightarrow} \bullet \rightarrow \bullet \overset{*}{\rightarrow}$

Note 1: The shift S and the coin C are local operators.

Note 2: The evolution operator U is nonlocal in the arc notation.
U is local if S is flip-flop.

Periodicity of QWs on Finite Graphs

Definition

The quantum walk dynamic is *periodic* if there is a *fundamental period* $t_0 \in \mathbb{Z}^+$ and a real parameter α such that $U^{t_0} = \mathrm{e}^{2\pi \mathrm{i}\alpha} I$.

It follows that $\left|\langle\psi(0)\middle|\psi(nt_0)\rangle\right|^2 = 1$ for all positive integer n and for any choice of the initial state $|\psi(0)\rangle$.

Theorem

The discrete-time quantum-walk dynamic on finite graphs with evolution operator U is periodic if the arguments of the eigenvalues of U are rational multiples of 2π.

Periodicity is rare.

Periodicity in cycles and 2D cyclic lattices (Kendon et.al), bipartite graphs (Kubota), some negative results (Saito)

Quasi-Periodicity of QWs on Finite Graphs

Definition

The quantum walk dynamic is *quasi-periodic* if for any fixed positive number ϵ there is a time step t such that $\left\| U^t - I \right\| \leq \epsilon$.

The norm of operator U is

$$\|U\| = \max_{\left\langle \psi \middle| \psi \right\rangle = 1} \left| \langle \psi | U | \psi \rangle \right|$$

Theorem

Discrete-time quantum-walk dynamics on finite graphs are quasi-periodic.

Lemma

Given a positive number ϵ and unit complex numbers $\mathrm{e}^{i\theta_k}$ for $1 \leq k \leq N$ and $N \in \mathbb{Z}^+$, there exists $t \in \mathbb{Z}^+$ such that

$$\max_k \left| \mathrm{e}^{it\theta_k} - 1 \right| \leq \epsilon.$$

Limiting Probability Distribution

- The limit $\lim_{t\to\infty} p_v(t)$ usually doesn't exit.
- The *average probability distribution* is defined as

$$\bar{p}_v(T) = \frac{1}{T}\sum_{t=0}^{T-1} p_v(t).$$

- The limiting probability distribution is

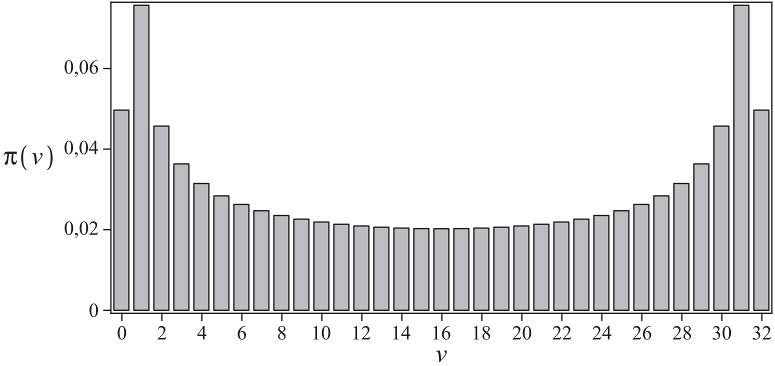
$$\pi(v) = \lim_{T\to\infty} \bar{p}_v(T).$$

Fact

- *The limit exists for all graphs.*
- *Usually the limiting probability depends on the initial state*

Limiting Probability Distribution

Example: limiting probability distribution of a coined QW as function of the Hamming weight on the hypercube with $N = 2^{32}$ ($|\psi(0)\rangle = |0\rangle$).



Quantum mixing time [1]

The *quantum mixing time* is

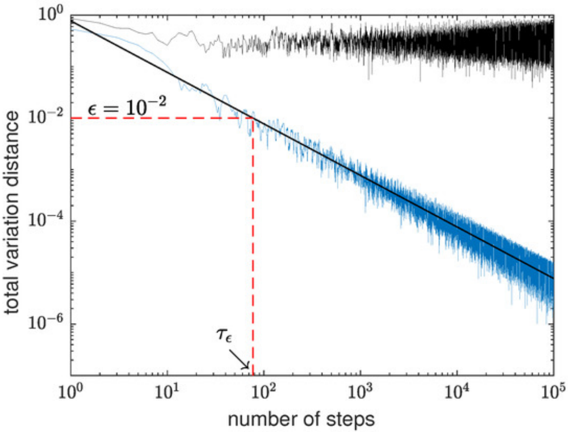
$$\tau_\epsilon = \min\left\{T \mid \forall t \geq T, \left\|\bar{p}_v(t) - \pi_v\right\| \leq \epsilon\right\},$$

where

$$\left\|p - q\right\| = \frac{1}{2}\sum_{v=1}^{N} \left|p_v - q_v\right|.$$

[1] D. Aharonov et al. Quantum Walks on Graphs. Proceedings of ACM-STOC'01, 50-59, 2001.

Example: Quantum mixing time on cycles



Blue curve: $\left\|\bar{p}_v(t) - \pi_v\right\|$ as a function of t (usually $1/t$)

Black curve: $\left\|p_v(t) - \pi_v\right\|$ as a function of number of steps t

Quantum and classical mixing time

Comparing quantum mixing time with classical:

τ_ϵ	N-cycle	2D lattice	Hypercube
Quantum	$O\left(\frac{N\log N}{\epsilon}\right)$	$O\left(\frac{\sqrt{N\log N}}{\epsilon}\right)$	$O\left(\frac{\log N}{\epsilon}\right)$
Classical	$O\left(N^2\log\frac{1}{\epsilon}\right)$	$O\left(N\log\frac{1}{\epsilon}\right)$	$O\left(\log N\log\frac{\log N}{\epsilon}\right)$

QW on Graphs: Interesting Problems

- Determine the limiting probability distribution π_v on graphs
- Analyze the mixing time and related times
- Find graphs with periodic evolution

It is also interesting (we have not discussed the details):

- Analyze the evolution of the standard deviation of $p_v(t)$ and other statistics
- Find graphs with perfect state transfer and fractional revival
- Find graphs with instantaneous uniform mixing
- Find algorithmic applications: searching and other problems

Final comments

- We have formally defined coined QWs
- The arc notation can be used for any multigraph
  - The locations of the walker are the arcs
- Class-2 graphs may use the position-coin notation
  - The locations of the walker are the vertices
  - The coin space is an internal (hidden) space
- It is easy to implement the coined model in Python
- We have defined:
  - Locality
  - Quasi-periodicity
  - Limiting probability distribution
  - Mixing time
- Tomorrow the focus will be on the staggered model

Thank you

Questions?

Questions can be sent by email to `Portugal@Lncc.Br`