

Quantum Walks on Graphs

Rachael Alvir, Sophia Dever, Ben Lovitz, James Myer

SUNY Potsdam

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 - Factoring Algorithm (1994 Peter Shor)

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- ★ $|v\rangle$ denotes a column vector and $\langle u|$ denotes a row vector.

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- ★ When a scalar i is placed inside the Dirac brackets, it represents a vector of all zeroes except a single 1 (one) in the i^{th} entry.

$$\langle i| = [0_1 \quad \dots \quad 0_{i-1} \quad 1_i \quad 0_{i+1} \quad \dots \quad 0_n]$$

- ★ Given a graph $G = (V, E)$, we define its *adjacency matrix* $A(G)$ as

$$A_{i,j} = \langle j|A|i\rangle = \begin{cases} 1 & \text{if } (v_i, v_j) \in E(G) \\ 0 & \text{otherwise.} \end{cases}$$

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- ★ We define the *Laplacian matrix* $L(G)$ as

$$L_{i,j} = \langle j|L|i\rangle = \begin{cases} 1 & \text{if } (v_i, v_j) \in E(G) \\ -d(v_j) & \text{if } i = j \\ 0 & \text{otherwise.} \end{cases}$$

More Definitions!

- ★ An adjacency *quantum walk* on a graph G is given by

$$U(t) \equiv e^{-itA} = \sum_{k=0}^{\infty} \frac{(-it)^k}{k!} A^k;$$

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- ★ The *quantum walk* can also be set up physically when the Laplacian is used in place of the adjacency matrix.
- ★ The probability of starting at a vertex a and ending at a vertex b at time \tilde{t} is given by $\left| \langle b | U(\tilde{t}) | a \rangle \right|^2$.

Quantum Walks on Graphs

- ★ **Definition:** Given a graph G , we say there is *perfect state transfer* (*PST*) from vertex a to vertex b if there is a time \tilde{t} such that $|\langle b|U(\tilde{t})|a\rangle|^2 = 1$.

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- ★ We usually evaluate whether a graph exhibits *PST* or *PGST* (or neither) using the **Spectral Decomposition Theorem:** Any n -vertex adjacency (or Laplacian) matrix with eigenvalues λ_k and eigenvectors v_k can be written as the sum
$$A = \sum_{k=0}^n \lambda_k |v_k\rangle \langle v_k|$$

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- ★ The *quantum walk* then becomes $U(t) = \sum_{k=0}^n e^{-it\lambda_k} |v_k\rangle \langle v_k|$

A SAMPLE CALCULATION IN n PARTS ($n \in \mathbb{N}$)

① Why Q2?

② Graph to Matrix

③ Matrix to Eigenstuff

④ Eigenstuff to Quantum Walk

⑤ Quantum Walk to PST (Or not? Spoilers!)



Hypercubes



Figure: Tesseract = Q_4 = 4D hypercube

Hypercubes

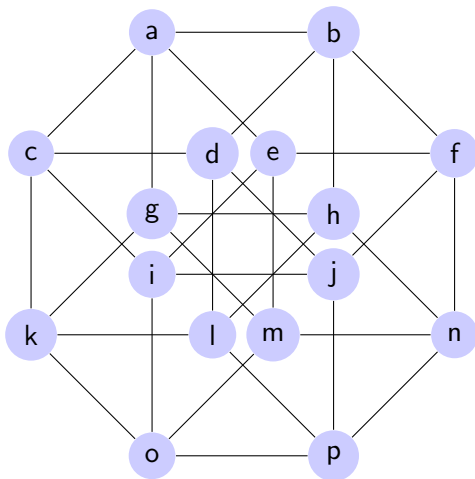


Figure: Tesseract = Q_4 = 4D hypercube

Q2: Graph

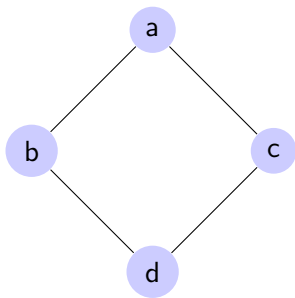


Figure: Q2

Q2: Adjacency Matrix

	<i>a</i>	<i>b</i>	<i>c</i>	<i>d</i>
	↓	↓	↓	↓
<i>a</i> →	—	—	—	—
<i>b</i> →	—	—	—	—
<i>c</i> →	—	—	—	—
<i>d</i> →	—	—	—	—

Q2: Adjacency Matrix

	<i>a</i>	<i>b</i>	<i>c</i>	<i>d</i>
	↓	↓	↓	↓
<i>a</i> →	0	–	–	–
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Q2: Adjacency Matrix

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

Next up: Spectral Decomposition Theorem!

$$\begin{vmatrix} -\lambda & 1 & 1 & 0 \\ 1 & -\lambda & 0 & 1 \\ 1 & 0 & -\lambda & 1 \\ 0 & 1 & 1 & -\lambda \end{vmatrix}$$

$$= \lambda^2(\lambda + 2)(\lambda - 2) = 0$$

$$\rightarrow \lambda = 0, \pm 2$$

Q2: Eigenvectors

$$\begin{pmatrix} -\lambda & 1 & 1 & 0 \\ 1 & -\lambda & 0 & 1 \\ 1 & 0 & -\lambda & 1 \\ 0 & 1 & 1 & -\lambda \end{pmatrix} \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix}$$

$$\lambda = 0: \begin{pmatrix} 0 \\ -1 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} -1 \\ 0 \\ 0 \\ 1 \end{pmatrix}; \lambda = 2: \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}; \lambda = -2: \begin{pmatrix} 1 \\ -1 \\ -1 \\ 1 \end{pmatrix}$$

e^{-itM} = quantum walk on M

$$\frac{1}{2} \begin{pmatrix} \cos(2t) + 1 & -i \sin(2t) & -i \sin(2t) & \cos(2t) - 1 \\ -i \sin(2t) & \cos(2t) + 1 & \cos(2t) - 1 & -i \sin(2t) \\ -i \sin(2t) & \cos(2t) - 1 & \cos(2t) + 1 & -i \sin(2t) \\ \cos(2t) - 1 & -i \sin(2t) & -i \sin(2t) & \cos(2t) + 1 \end{pmatrix}$$

Moment of Truth: PST?

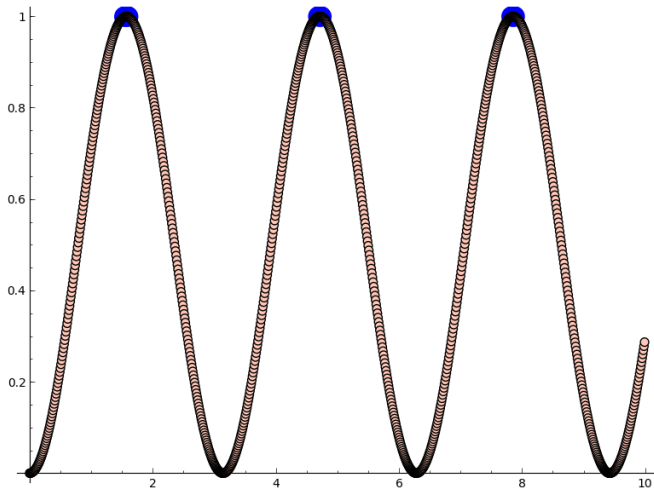


Figure: Quantum walk on Q2

Calculating PST

SO WE HAVE A METHOD! BUT IT'S:

- 1 Hard
- 2 Slow
- 3 Boring
- 4 Involves arithmetic
- 5 Gets exponentially worse on big graphs

WE CAN ALSO USE PROGRAMS. BUT THEY HAVE PROBLEMS TOO:

- 1 Only an approximation
- 2 Hard to differentiate between PST and P(retty Good)ST
- 3 Not a rigorous proof
- 4 Buggy
- 5 Still get exponentially worse on big graphs

SO NOW WHAT?

What if we could turn this...

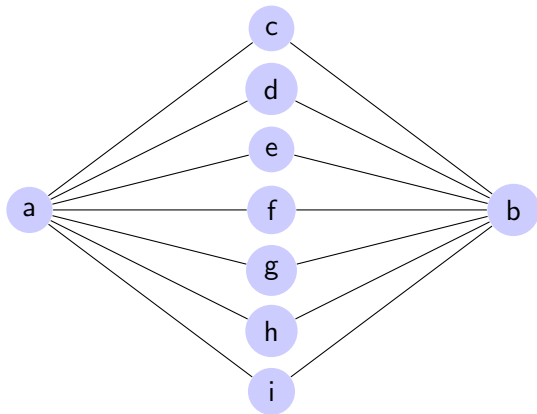


Figure: Ugly Graph

... into this?



Figure: Pretty Graph

A partition is denoted by π (for obvious reasons).



Figure: Partitioning a circle

Partitions

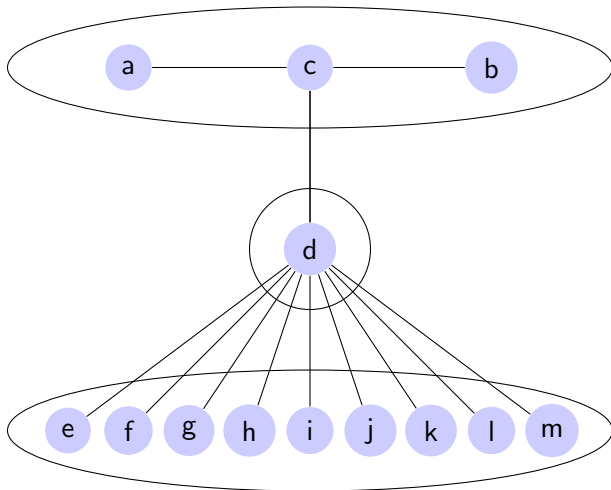


Figure: A sample partition

Almost-Equitable Partition:

$$\forall A, B \text{ partitions, } \forall a_1, a_2 \in A, \\ \sum_{b \in B} \begin{cases} 1 & \text{if } (a_1, b) \in E \\ 0 & \text{otherwise} \end{cases} = \sum_{b \in B} \begin{cases} 1 & \text{if } (a_2, b) \in E \\ 0 & \text{otherwise} \end{cases}$$

Translation: Any two points in the same partition must have the same number of edges going from them into any given other partition.

Equitable Partition

Equitable Partition = almost-equitable + each subgraph is regular

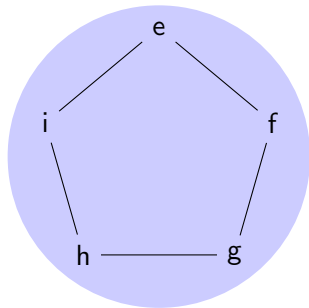
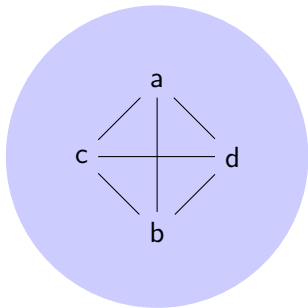


Figure: A sample partition

Almost-Equitable Partitions

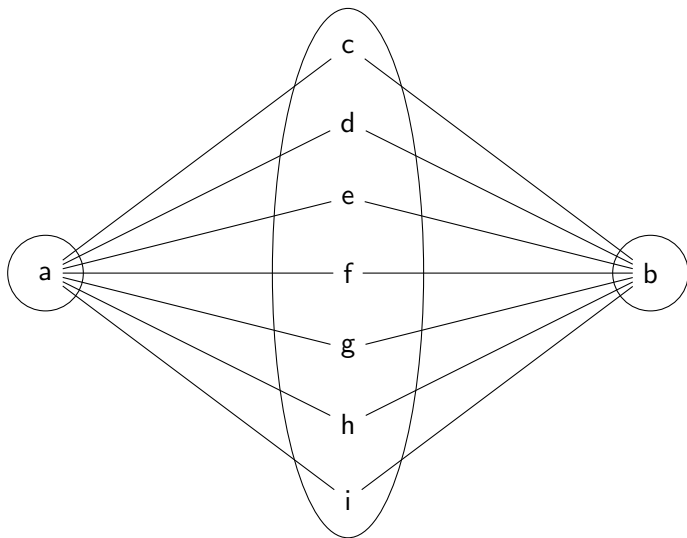


Figure: An almost-equitable partition π

Quotient Graph

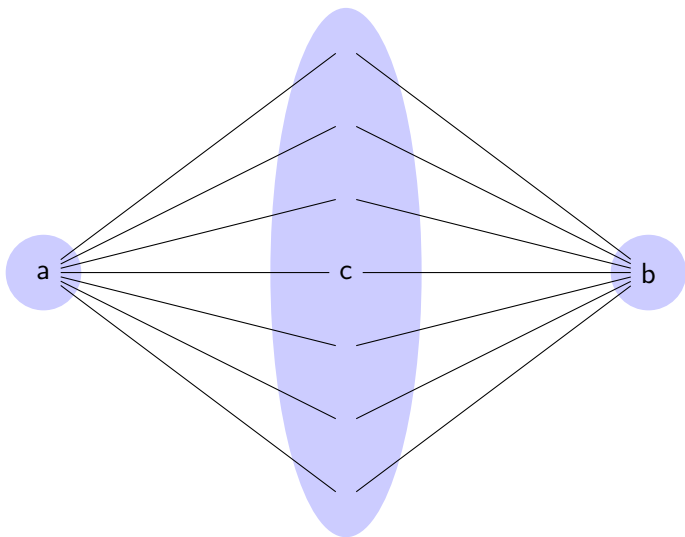


Figure: A quotient graph (almost)

Quotient Graph



Figure: A quotient graph G/π

Theorem. Let H be any graph of n vertices. Let $G = \overline{K_2} + H$.
Let $\pi = \bigcup_k V_k$ be any almost equitable partition of G .
Then, G/π has PST from a to b when analyzed with its Laplacian matrix $L(G/\pi)$ iff $n \equiv 2 \pmod{4}$.

Spectra of $L(G/\pi)$

The Laplacian of G , $L(G/\pi)$, is given by:

$$\begin{bmatrix} n & -\sqrt{n} & 0 \\ -\sqrt{n} & 2 & -\sqrt{n} \\ 0 & -\sqrt{n} & n \end{bmatrix}$$

The eigenvalues of $L(G/\pi)$ include $0, n, n + 2$. The eigenvalue/eigenvector pairs with their respective normalizing constants are:

$$\lambda = 0, \frac{1}{\sqrt{2+n}} \begin{bmatrix} 1 \\ \sqrt{n} \\ 1 \end{bmatrix} ; \lambda = n, \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix} ; \lambda = n+2, \frac{1}{\sqrt{2(n+2)}} \begin{bmatrix} \sqrt{n} \\ -2 \\ \sqrt{n} \end{bmatrix}$$

Quantum Walk on $L(G/\pi)$

By the Spectral Decomposition Theorem, the quantum walk from a to b on $L(G/\pi)$ is given by:

$$\langle b | e^{-itL(G/\pi)} | a \rangle = \frac{1}{2+n} - \frac{e^{-it(n)}}{2} + \frac{ne^{-it(n+2)}}{2(2+n)} = -\frac{e^{-it(n)}}{2} + \frac{2 + ne^{-it(n+2)}}{2(2+n)}.$$

$n \equiv 2 \pmod{4} \implies G/\pi$ has PST from a to b

Since $n \equiv 2 \pmod{4}$, $n = 4k + 2 = 2(2k + 1)$ for some $k \in \mathbb{Z}$.
Choose $t = \frac{\pi}{2}$. Then,

$$e^{-it(n)} = \cos((2k + 1)\pi) + i\sin((2k + 1)\pi) = -1.$$

Also,

$$e^{-it(n+2)} = \cos((2(k + 1))\pi) + i\sin((2(k + 1))\pi) = 1.$$

Since $e^{-it(n)} = -1$ and $e^{-it(n+2)} = 1$,

$$\left| -\frac{e^{-it(n)}}{2} + \frac{2 + ne^{-it(n+2)}}{2(2 + n)} \right| = \left| -\frac{-1}{2} + \frac{2 + n}{2(2 + n)} \right| = 1.$$

G/π has PST from a to $b \implies n \equiv 2 \pmod{4}$

Since G/π has PST from a to b , for some time $t \in \mathbb{R}$,

$$\left| \frac{1}{2+n} - \frac{e^{-it(n)}}{2} + \frac{ne^{-it(n+2)}}{2(2+n)} \right| = 1.$$

Observe that $\frac{1}{2+n} = \frac{1}{2+n} e^{i(2\pi)k}$ for some $k \in \mathbb{Z}$. Then,

$$\left| \frac{1}{2+n} e^{i(2\pi)k} + \frac{e^{i(-nt+\pi)}}{2} + \frac{ne^{i(-t(n+2))}}{2(2+n)} \right| = 1.$$

Since $\{\frac{1}{2+n}, \frac{1}{2}, \frac{n}{2(2+n)}\}$ is a positive set of real numbers such that

$$\frac{1}{2+n} + \frac{1}{2} + \frac{n}{2(2+n)} = 1$$

and $\{(2\pi)k, -(nt + \pi), -t(n+2)\}$ is a set of real numbers such that

$$\left| \frac{1}{2+n} e^{i(2\pi)k} + \frac{e^{i(-nt+\pi)}}{2} + \frac{ne^{i(-t(n+2))}}{2(2+n)} \right| = 1,$$

there exists $\alpha \in \mathbb{R}$ such that

$$\alpha = (2\pi)k = -(nt + \pi) = -t(n+2).$$

Then,

$$\pi = 2t \implies 2(2t)k = -t(n + 2) \implies n = -(4k + 2).$$

Hence, $n \equiv 2 \pmod{4}$.

Theorem. Assume G is a hypercube besides K_2 , and H is an arbitrary graph on n vertices where n is a multiple of 4. Then the join $G + H$ will preserve the Laplacian PST on G with equal periodicity.

THE QUESTION: SUPPOSE A GRAPH G EXHIBITS PST. WHAT CAN WE DO TO PRESERVE PST ON G ?

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- What types of graph operations may we use on G and preserve its PST?
- Can we invent new graph operations or generalize existing graph operations to help answer this question?
- When we experiment with the type of PST which occurs (Laplacian vs. Adjacency), will our results change?

Types of Graph Operations

- 1 The G-Join, $G[G_1, G_2, \dots, G_m]$
- 2 The Weak product
- 3 The Strong product
- 4 The Lexicographic product

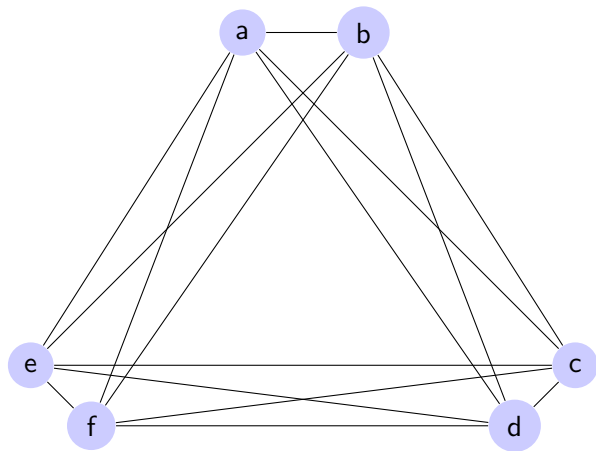


Figure: $C_3[P_2, P_2, P_2,]$

Types of Laplacian Matrices

- 1 The regular laplacian, $L(G) = A - D$ [Join]
- 2 The signless laplacian, $L(G) = A + D$ [Line Graphs]
- 3 The normalized laplacian, $L(G) = D^{-1/2}(A - D)D^{-1/2}$ [Weak/Strong/Lexicographic Product]

Quantum Walks on Line Graphs

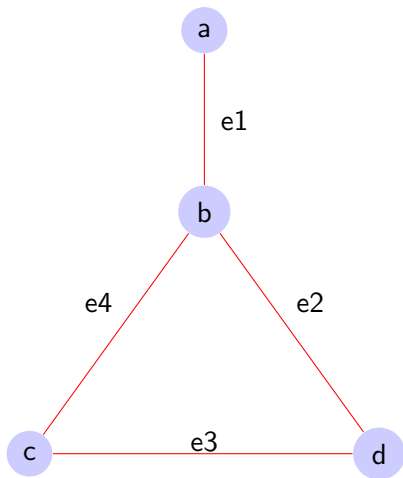


Figure: Original graph

Line Graphs

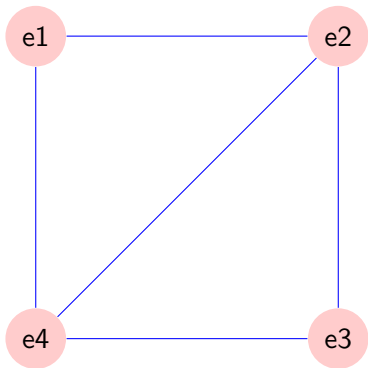


Figure: The Line Graph

There is a relationship between the quantum walk on the Line Graph and the quantum walk on the original graph.

Thanks!

- 1 Dr. Tamon
- 2 Dr. Foisy
- 3 Clarkson, SUNY Potsdam
- 4 The NSF