From Markov chains to quantum information

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1. First Links in the Markov Chain
2. Quantum walk versus random walk
3. Jacobi operators on graphs and perfect quantum state transfer
4. Grover search algorithm and continuous-time quantum walk
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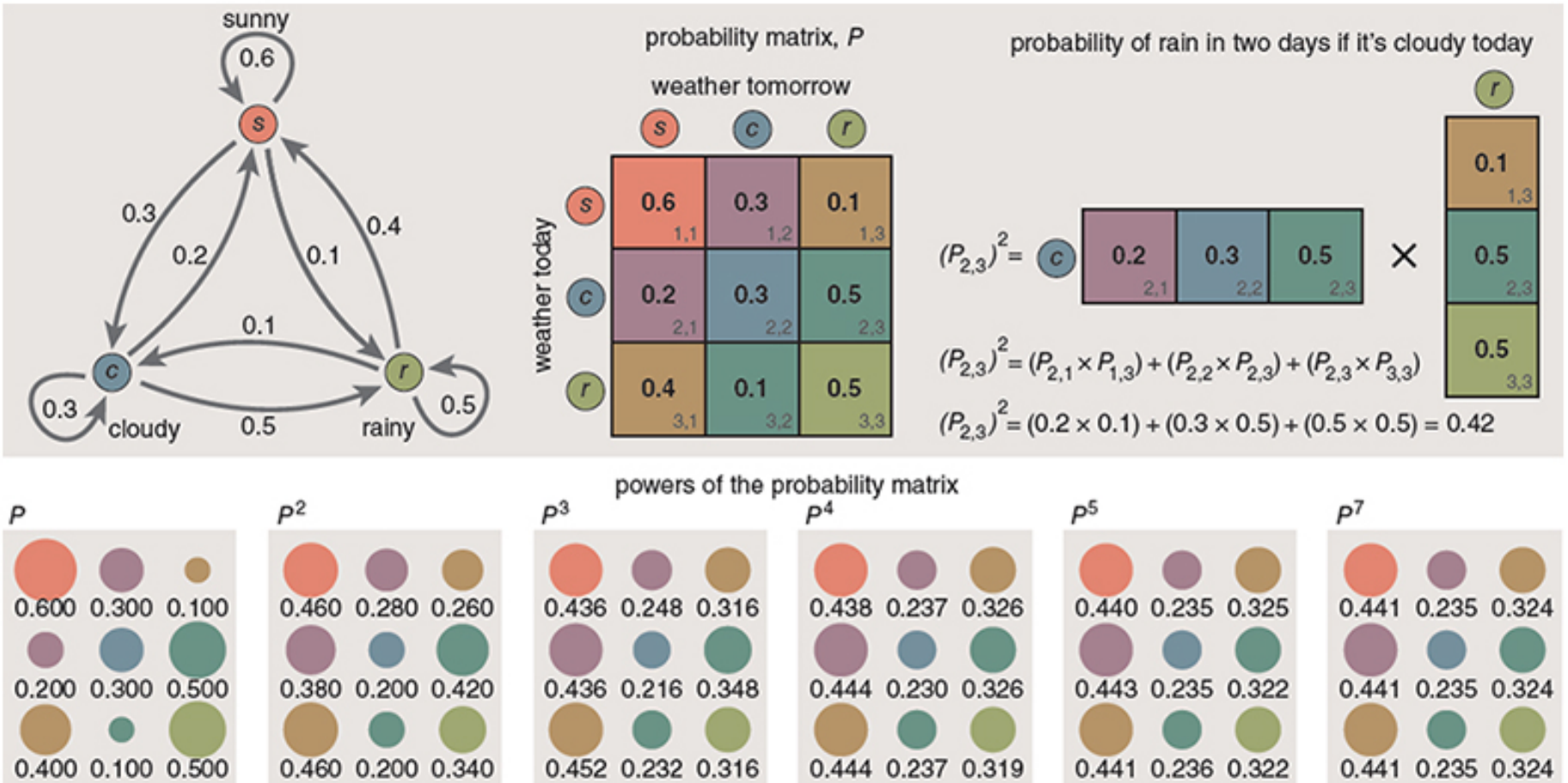
Outline

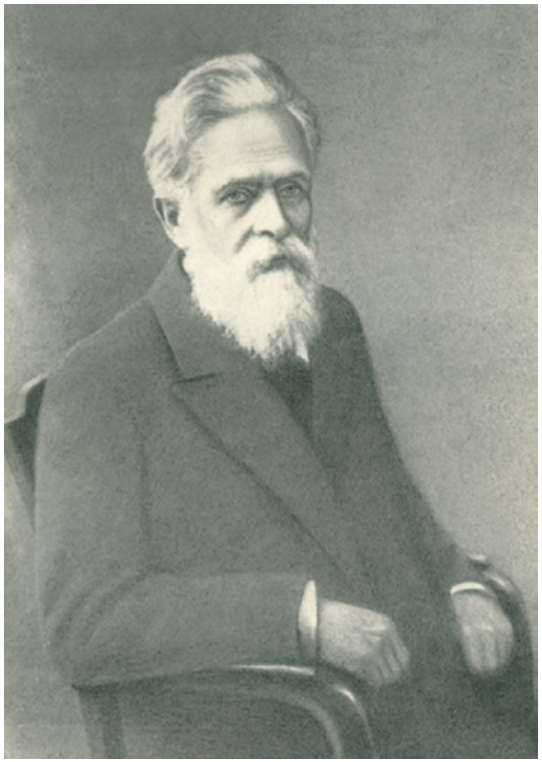
Past, Present and Future

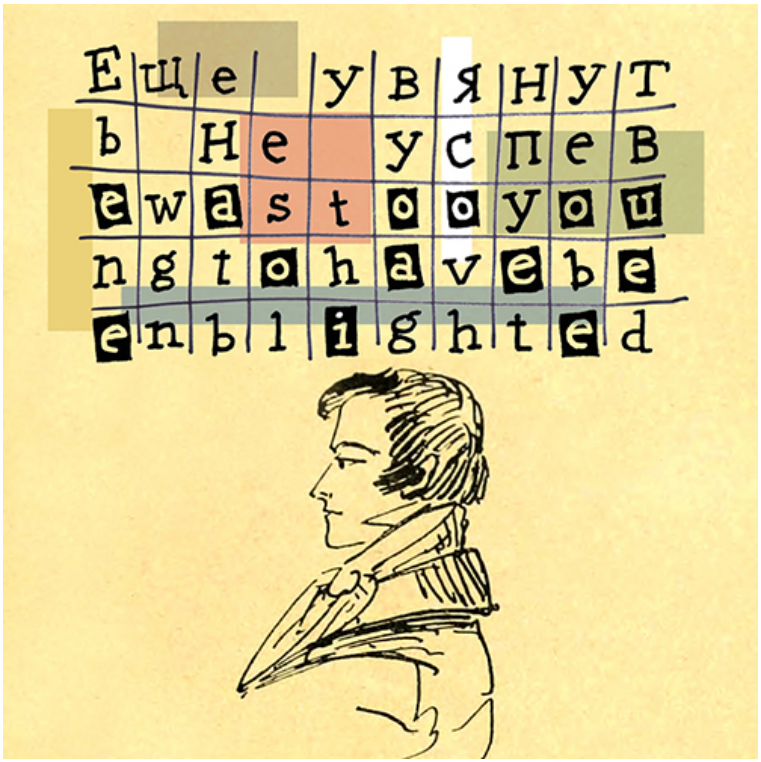


by Hayes, Brian. American Scientist 101.2 (2013): 252.
https://www.americanscientist.org/article/first-links-in-the-markov-chain

First Links in the Markov Chain

Probability and poetry were unlikely partners in the creation of a computational tool





When the Russian church excommunicated Leo Tolstoy, Markov asked that he be expelled also. (The request was granted.) In 1902, the leftist writer Maxim Gorky was elected to the Academy, but the election was vetoed by Tsar Nicholas II. In protest, Markov announced that he would refuse all future honors from the tsar.

In 1913, when the tsar called for celebrations of 300 years of Romanov rule, Markov responded by organizing a symposium commemorating a different anniversary: the publication of *Ars Conjectandi* [by Jacob Bernoulli] 200 years before.

In a paper published in 1902 Nekrasov injected the law of large numbers into the centuries-old theological debate about free will versus predestination. His argument went something like this: Voluntary acts – expressions of free will – are like the independent events of probability theory, with no causal links between them. The law of large numbers applies only to such independent events. Data gathered by social scientists, such as crime statistics, conform to the law of large numbers. Therefore the underlying acts of individuals must be independent and voluntary.

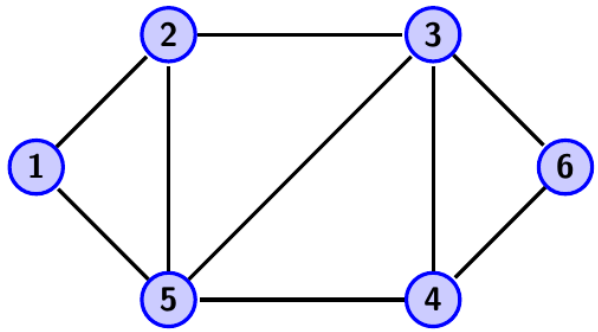
Markov first addressed the issue of dependent variables and the law of large numbers in 1906. ... Nekrasov assumed that the law of large numbers requires the principle of independence. Although this notion had been a commonplace of probability theory since the time of Jacob Bernoulli, Markov set out to show that the assumption is unnecessary. The law of large numbers applies perfectly well to systems of dependent variables if they meet certain criteria.

Outline

Quantum mechanics on graphs

- Let $G = (V, E)$ be a finite (possibly directed) graph.
- We assume that G has N vertices, i.e. $|V| = N$.
- Equip V with a measure μ.
- Define a Hilbert space

$$\ell^2(G) = \{\psi : V \to \mathbb{C}\} = \mathbb{C}^N,$$
$$\langle \psi, \varphi \rangle = \sum_{x \in V} \psi(x)\overline{\varphi(x)}\mu(x),$$



- The *volume* of the graph G is then given by $vol(G) := \sum_{x \in V} \mu(x)$.

Quantum mechanics on graphs

- A quantum state is represented by a normalized vector $\psi \in \ell^2(G)$.
- A physical quantity (i.e. observable) is represented by a self-adjoint operator A acting on $\ell^2(G)$, i.e.

$$\langle \psi, A\varphi \rangle = \langle A\psi, \varphi \rangle \quad \forall \psi, \varphi \in \ell^2(G)$$

- The energy is represented by a self-adjoint operator called a Hamiltonian H.
- The time dependence of a state is governed by the Schrödinger equation

$$i\frac{\partial}{\partial t}\psi(t) = H\psi(t)$$

Probabilistic interpretation

- Let $\delta_1, \ldots, \delta_N$ be the canonical basis of $\mathbb{C}^N$, i.e.

$$\delta_x = \begin{cases} 1 & , \text{ on vertex } x, \\ 0 & , \text{ on the vertices } V \backslash \{x\} \end{cases}$$

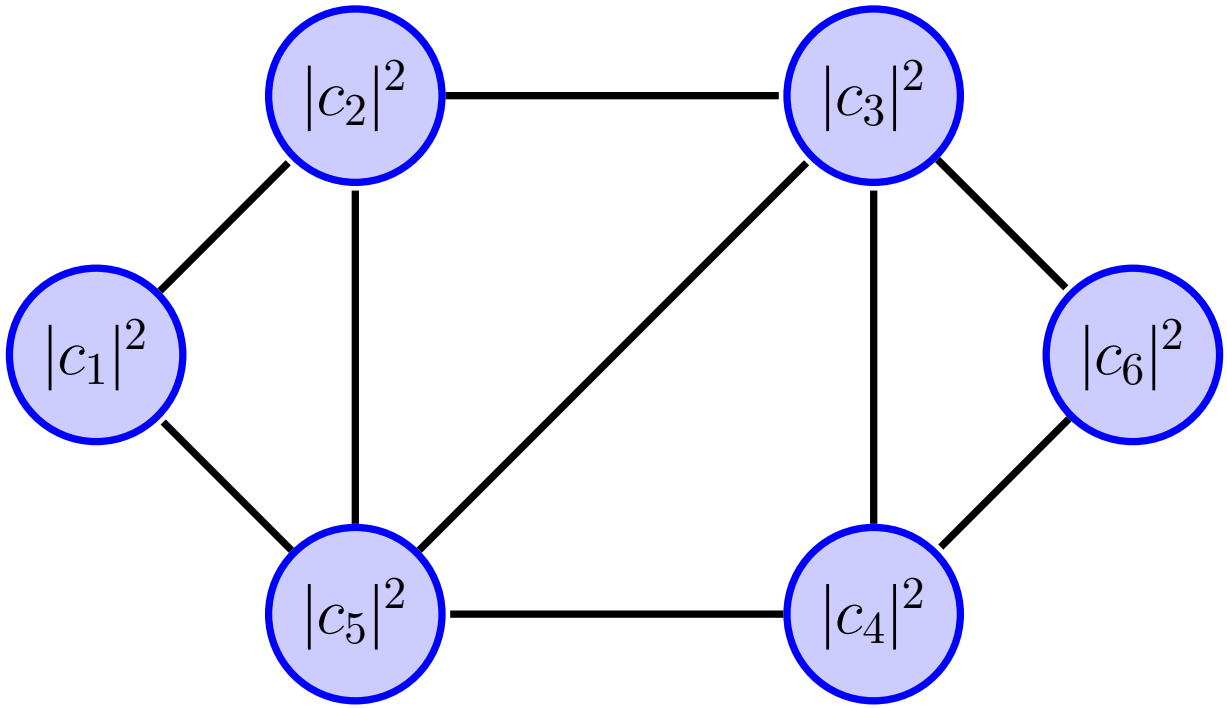
- The normalized vector of δ_x is $e_x := \dfrac{1}{\sqrt{\mu(x)}} \delta_x$.
- Write $\psi \in \ell^2(G)$ as a linear combination

$$\psi = \sum_x c_x e_x$$

where the $c_x \in \mathbb{C}$ satisfy $\sum_x |c_x|^2 = 1$ (because $\langle \psi, \psi \rangle = 1$).

A probability distribution

- Probabilistic interpretation: $\psi = \sum_x c_x e_x$ is in the state e_x with probability $|c_x|^2$.



The time-evolution operator

- H is assumed to be time-independent.
- The Schrödinger equation is solved by

$$\psi(t) = U(t)\psi(0), \quad U(t) := \exp(-itH).$$

- $U(t)$ is unitary.
- $U(t)$ is called a time-evolution operator.

Example: discrete-time quantum walk

- Discrete time $t \in \mathbb{N}$. For $t = n$, we have

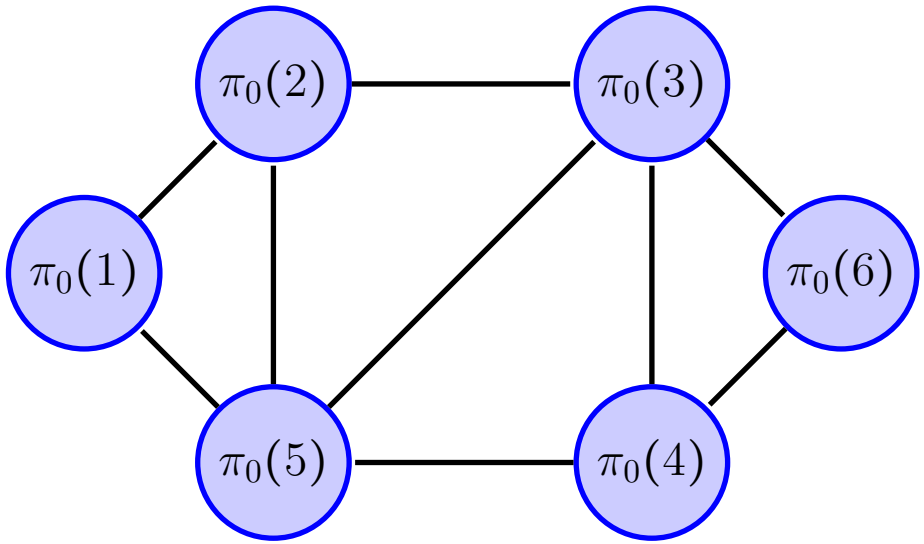
$$U(n) = \exp(-inH) = \exp(-iH)\cdots\exp(-iH)$$
$$= U(1)\cdots U(1) = \big(U(1)\big)^n$$

- We write $U := U(1)$.
- One step of a discrete-time quantum walk is described by U, i.e.

$$\psi(0) \xrightarrow{U} \psi(1) \xrightarrow{U} \psi(2) \xrightarrow{U} \psi(3) \xrightarrow{U} \dots$$

Markov chain comparison

- We start with an initial probability distribution $\pi_0 \in \mathbb{R}^N$.



- Classical random walk: initial probability distribution $\{\pi_0(x)\}_{x\in V}$.
- Quantum walk: probability distribution of initial state $\psi(0)$ via $\{|c_x|^2\}_{x\in V}$.

Markov chain comparison

- Discrete-time classical random walk on N-vertex graph can be represented by a stochastic $N \times N$-matrix P, i.e. $\sum_{j=1}^{N} P_{jk} = 1$.
- The entry P_{jk} represents the probability of making a transition to k from j.
- The initial probability distribution π_0 becomes $P\pi_0$ after one step of the walk, i.e.

$$\pi_0 \to P\pi_0 \to P^2\pi_0 \to P^3\pi_0 \to \dots$$

- Compare to discrete-time quantum walk:

$$\psi(0) \xrightarrow{U} \psi(1) \xrightarrow{U} \psi(2) \xrightarrow{U} \psi(3) \xrightarrow{U} \dots$$

Outline

Motivation

Kempton, Mark, Gabor Lippner, and Shing-Tung Yau. **Perfect state transfer on graphs with a potential**. *Quantum Information and Computation* (2017). **Pretty good quantum state transfer in symmetric spin networks via magnetic field**. *Quantum Information Processing* (2017).

... for paths of length greater than three, there is no potential on the vertices of the path for which perfect state transfer between the endpoints can occur ... this answers a question raised by Godsil ...
... if a graph has two vertices that share a common neighborhood, then there is a potential on the vertex set for which perfect state transfer will occur between those two vertices
... numerous examples where perfect state transfer does not occur without the potential, but adding a potential makes perfect state transfer possible.
... investigate perfect state transfer on graph products, which gives further examples where perfect state transfer can occur.

Jacobi operators on graphs

Definition

A Jacobi operator on a graph $G = (V(G), E(G))$ is a matrix $\mathbf{J} = \big(\mathbf{J}(x,y)\big)_{x,y\in V(G)}$ indexed by the vertices $V(G)$, such that $\mathbf{J}(x,y) = 0$ whenever $(x,y) \notin E(G)$ and $x \neq y$.

- Generalization of graph Laplacians and adjacency matrices.
- Adequate to simulate physical models and define "Hamiltonian operators".

[0] N. Avni, J. Breuer, and B. Simon. Periodic Jacobi matrices on trees. Adv. Math., 370:107241, 42, 2020.

$\mathbb{Z}$-graded Graphs

We refer to the triple $G = (V(G), E(G), \mathbf{\Pi})$ as a $\mathbb{Z}$-graded graph[1], where

1. $(V(G), E(G))$ is a connected combinatorial graph with a countable set of vertices $V(G)$ and a set of edges $E(G)$.
2. There exists a (rank) function $\mathbf{\Pi} : V(G) \to \mathbb{Z}$, such that for an edge $(x, y) \in E(G)$, we have $\mathbf{\Pi}(y) = \mathbf{\Pi}(x) + 1$
3. For $n \in \mathbb{Z}$, we call $\mathbf{\Pi}^{-1}(n)$ the n-th transversal layer.

[1] Richard P. Stanley. *Differential Posets*. J. Amer. Math. Soc., 1(4):919961, 1988. Sergey Fomin. *Duality of graded graphs*. J. Algebraic Combin., 3(4):357404, 1994 1,4.

$\mathbb{Z}$-graded Graphs

The rank function relates a $\mathbb{Z}$-graded graph G to an auxiliary path graph $(V(\mathbb{Z}), E(\mathbb{Z}))$.

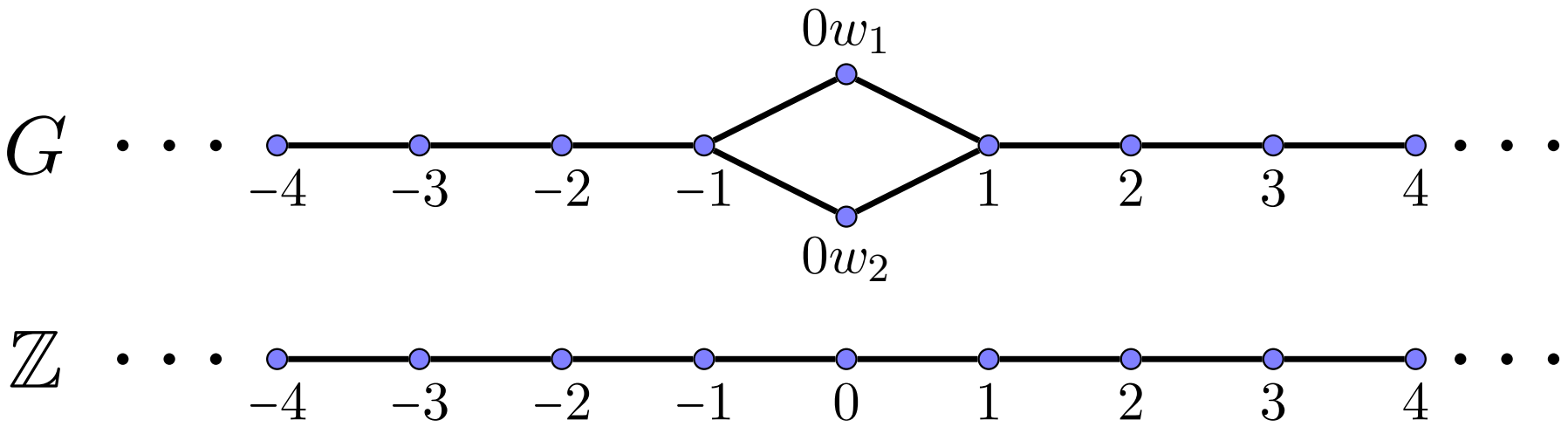


Figure: One of the simplest nontrivial $\mathbb{Z}$-graded graphs G. The rank function provides a transversal decomposition[3], i.e. $V(G) = \bigcup_{n\in\mathbb{Z}} \mathbf{\Pi}^{-1}(n)$.

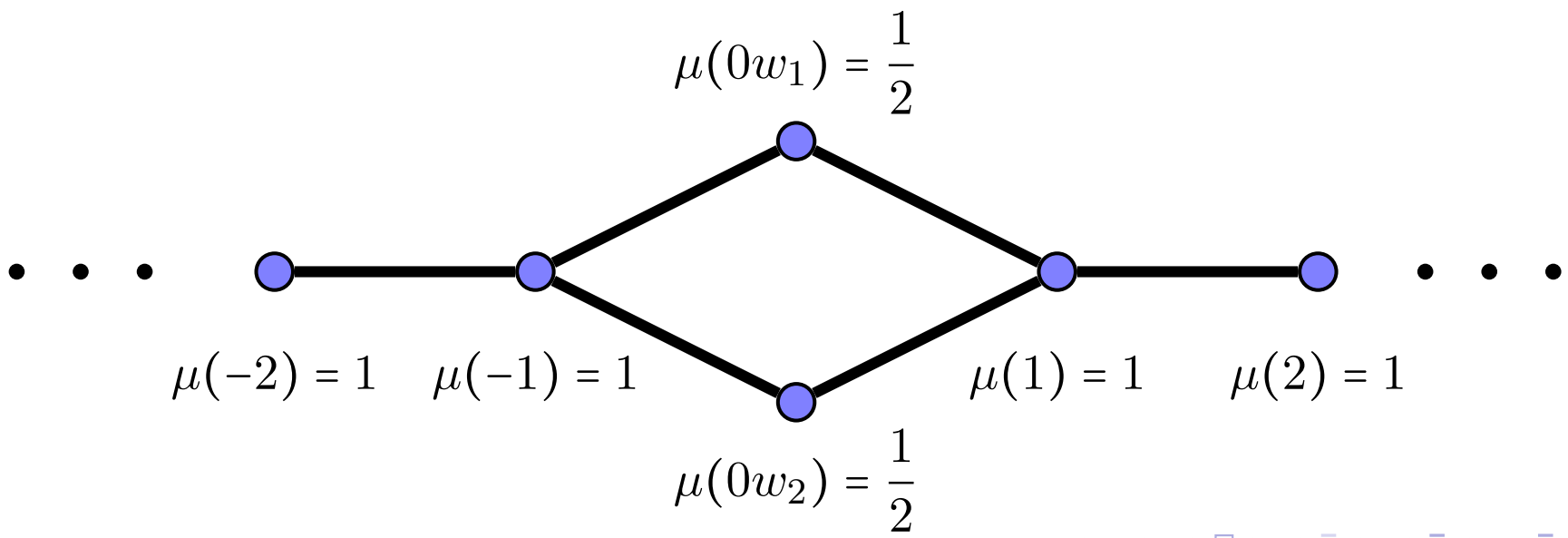
[3] *stratification of a graph"* in *Quantum probability and spectral analysis of graphs*. Hora, A. and Obata, N., Springer, Berlin, 2007.

Measures on $V(G)$

Given $G = (V(G), E(G), \mathbf{\Pi})$ a $\mathbb{Z}$-graded graph. We equip $V(G)$ with a measure, $\mu_V : V(G) \to [0, \infty]$.

Assumption (1)

We assume $\mu_V(x) > 0$ for all $x \in V(G)$ and that the restriction of μ_V to a transversal layer is a probability measure, i.e , $\mu(\mathbf{\Pi}^{-1}(n)) = 1$, $\forall\ n \in \mathbb{Z}$.

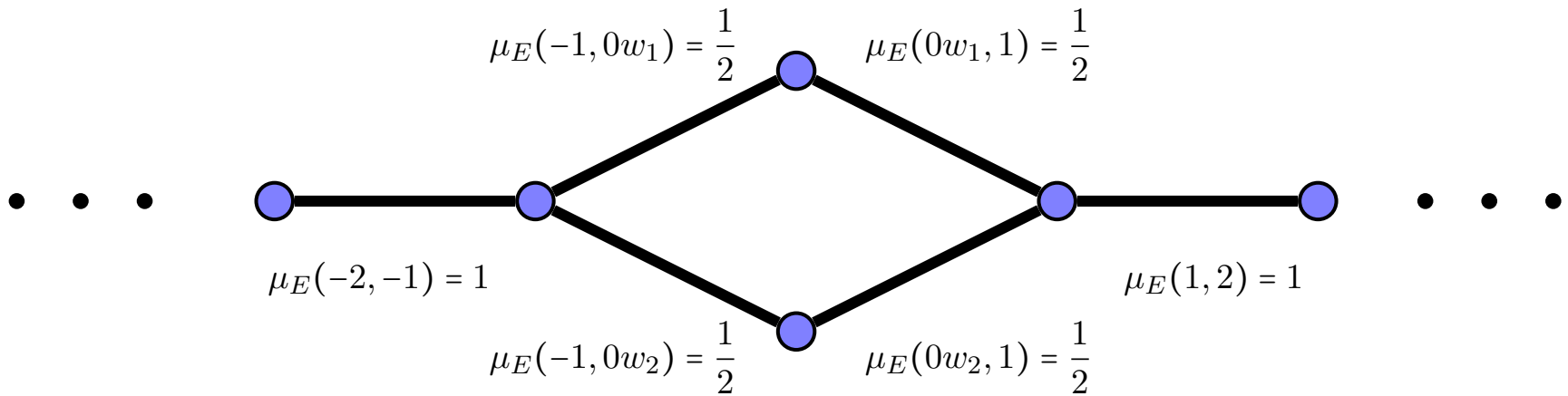


Measures on $E(G)$

We equip the set of edges with a measure $\mu_E : E(G) \to [0, \infty]$, $(x, y) \mapsto \mu_E(x, y)$.

Assumption (2)

We assume $\mu_E(x, y) > 0$ for all $(x, y) \in E(G)$ and that the restriction of μ_E to a transversal layer of edges is a probability measure.

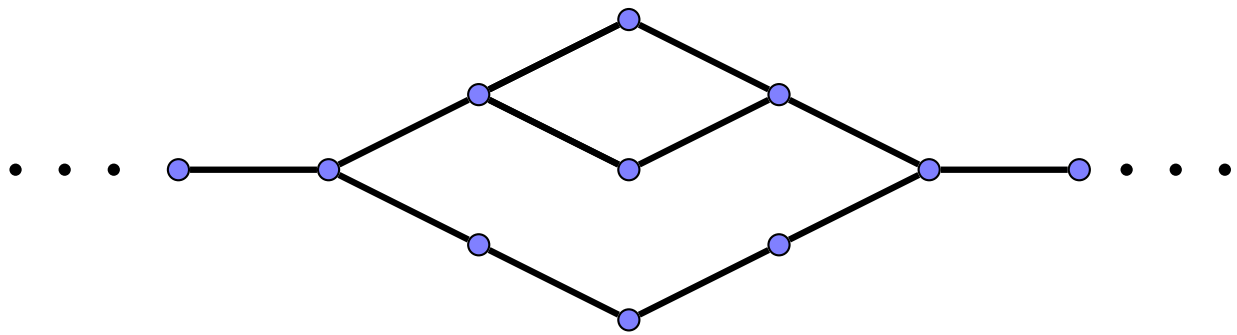


Measure balance assumption

Assumption (3)

Let $x \in V(G)$. We assume that the following identities hold:

$$\mu_V(x) = \sum_{(x,y)\in E(G)} \mu_E(x,y), \qquad \mu_V(x) = \sum_{(y,x)\in E(G)} \mu_E(y,x).$$



Hilbert spaces

We introduce the following Hilbert spaces:

$$\ell^2(G) = \{\psi : V(G) \to \mathbb{C} \mid \langle \psi, \psi \rangle_V < \infty\},$$
$$\langle \psi, \varphi \rangle_V = \sum_{x \in V(G)} \psi(x)\overline{\varphi(x)}\mu_V(x),$$
$$\ell^2(\mathbb{Z}) = \{\psi : \mathbb{Z} \to \mathbb{C} \,|\, \langle \psi, \psi \rangle < \infty\},$$
$$\langle \psi, \varphi \rangle = \sum_{n \in \mathbb{Z}} \psi(n)\overline{\varphi(n)}.$$

Radial functions and the Averaging Operator $\widetilde{\Pi}$

Given $G = (V(G), E(G), \mathbf{\Pi})$ a $\mathbb{Z}$-graded graph.

Definition

- The subspace of radial functions is defined as $\ell^2_{rad}(G) = \{\psi \in \ell^2(G) \mid \psi(x) = \psi(y) \text{ if } \mathbf{\Pi}(x) = \mathbf{\Pi}(y)\}$.
- We define the averaging operator as the following mapping

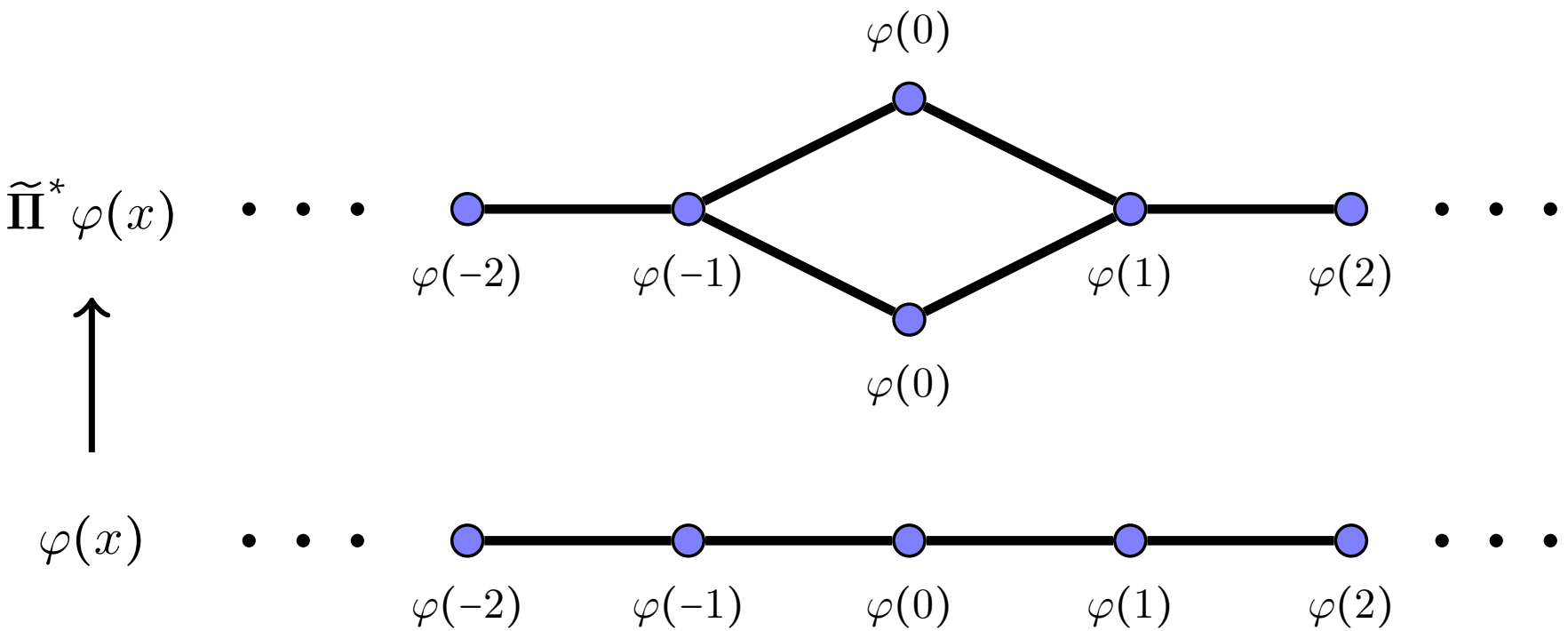
$$\widetilde{\mathbf{\Pi}} : \ell^2(G) \to \ell^2(\mathbb{Z}), \quad \psi \mapsto \widetilde{\mathbf{\Pi}}\psi(n) := \sum_{x \in \mathbf{\Pi}^{-1}(n)} \psi(x)\mu_V(x).$$

We show: $Ker\widetilde{\mathbf{\Pi}} = \ell^2_{rad}(G)^{\perp}$.
Radial-"Angular" decomposition: $\ell^2(G) = \ell^2_{rad}(G) \oplus Ker\widetilde{\mathbf{\Pi}}$.

The adjoint operator of $\widetilde{\Pi}$

Proposition

The averaging operator $\widetilde{\Pi}$ *is bounded with* $||\widetilde{\Pi}|| = 1$. *Let* $\widetilde{\Pi}^*$ *be the adjoint operator of* $\widetilde{\Pi}$, *then* $\widetilde{\Pi}^*$ *is given by* $\widetilde{\Pi}^* : \ell^2(\mathbb{Z}) \to \ell^2(G)$,
$\varphi \mapsto \widetilde{\Pi}^* \varphi(x) = \varphi(\Pi(x))$.



Lifting an Operator

Definition

Let $A : \ell^2(G) \to \ell^2(G)$ be bounded, such that:

- A is a Jacobi operator on a graph G, i.e. it reflects the adjacency relation of the graph G, in the sense that its off-diagonal elements $(A(x,y))_{x \neq y}$ are zero whenever they correspond to non-adjacent vertices.
- We define $B : \ell^2(\mathbb{Z}) \to \ell^2(\mathbb{Z})$ such that $B = \widetilde{\Pi} A \widetilde{\Pi}^*$.

We say, the operator A *lifts* B.

$$\begin{array}{ccc} \ell^2(G) & \xrightarrow{\quad A \quad} & \ell^2(G) \\ \uparrow{\scriptstyle \widetilde{\Pi}^*} & & \downarrow{\scriptstyle \widetilde{\Pi}} \\ \ell^2(\mathbb{Z}) & \xrightarrow{\quad B \quad} & \ell^2(\mathbb{Z}) \end{array}$$

Spectral separation assumption

Definition (Spectral separation assumption)

A bounded linear operator $\mathbf{H} : \ell^2(G) \to \ell^2(G)$ is said to satisfy the spectral separation assumption, if the following hold:

1. $\mathbf{H}(Ker\widetilde{\Pi}) \subset Ker\widetilde{\Pi}$, i.e., the subspace $Ker\widetilde{\Pi}$ is **H**-invariant,
2. $\mathbf{H}(\ell^2_{rad}(G)) \subset \ell^2_{rad}(G)$, i.e., the subspace $\ell^2_{rad}(G)$ is **H**-invariant.

Result: Lifting a tridiagonal Jacobi Matrix

Theorem

Given $G = (V(G), E(G), \mathbf{\Pi})$ a $\mathbb{Z}$-graded graph. Under the Assumptions (1), (2) and (3), for a symmetric tridiagonal Jacobi matrix **J** *there exists a Jacobi operator* **H** *on G that lifts* **J**, *i.e.*

$$\mathbf{J} = \widetilde{\mathbf{\Pi}}\mathbf{H}\widetilde{\mathbf{\Pi}}^{*}.$$

H *can be explicitly computed (next two slides), shown to be self-adjoint on $\ell^2(G)$ and satisfies the spectral separation assumption, i.e.*

- $\mathbf{H}(Ker\widetilde{\mathbf{\Pi}}) \subset Ker\widetilde{\mathbf{\Pi}}$, *i.e., the subspace $Ker\widetilde{\mathbf{\Pi}}$ is* **H**-*invariant,*
- $\mathbf{H}(\ell^2_{rad}(G)) \subset \ell^2_{rad}(G)$, *i.e., the subspace $\ell^2_{rad}(G)$ is* **H**-*invariant.*

Symmetric tridiagonal Jacobi matrix

Let $\mathbf{J} : \ell^2(\mathbb{Z}) \to \ell^2(\mathbb{Z})$, be the following *symmetric tridiagonal Jacobi matrix*

$$\mathbf{J} = \begin{pmatrix} & \ddots & \vdots & \vdots & \vdots & \iddots \\ \ddots & b(n-1) & a(n-1,n) & 0 & 0 & \dots \\ \dots & a(n-1,n) & b(n) & a(n,n+1) & 0 & \dots \\ \dots & 0 & a(n,n+1) & b(n+1) & a(n+1,n+2) & \dots \\ & \iddots & \vdots & \vdots & \ddots & \end{pmatrix}$$

The Jacobi matrix $\mathbf{J}$ is bounded and self-adjoint on $\ell^2(\mathbb{Z})$.

Jacobi operator on G

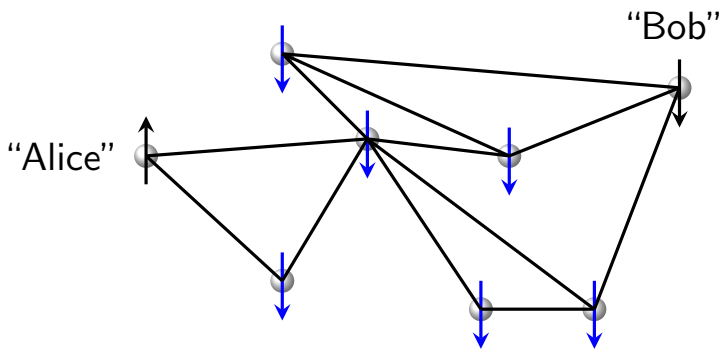
We define $\mathbf{H} = [\mathbf{H}(x,y)]_{x,y\in V(G)}$ with the following matrix elements.

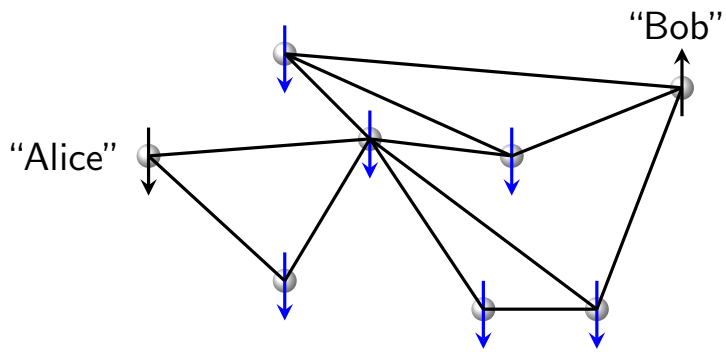
$$\mathbf{H}(x,y) = \begin{cases} b(n) & \text{, if } x = y \text{ and } \mathbf{\Pi}(x) = n, \\ \dfrac{\mu_E(x,y)}{\mu_V(x)} a(n,n+1) & \text{, if } (x,y) \in E(G) \text{ and } \mathbf{\Pi}(x) = n, \\ \dfrac{\mu_E(y,x)}{\mu_V(x)} a(n-1,n) & \text{, if } (y,x) \in E(G) \text{ and } \mathbf{\Pi}(y) = n-1, \\ 0 & \text{, otherwise.} \end{cases}$$

Perfect Quantum State Transfer (PQST)

- PQST on one dimensional Spin Networks[4] is well understood.
- More general Spin Networks? graph properties?
- Transfer of $|A\rangle$ to $|B\rangle$ as PQST? Hamiltonian operator (spin-spin interactions)?

$$|A\rangle \qquad e^{i\phi}|B\rangle = e^{iT\,\mathbf{H}}|A\rangle$$



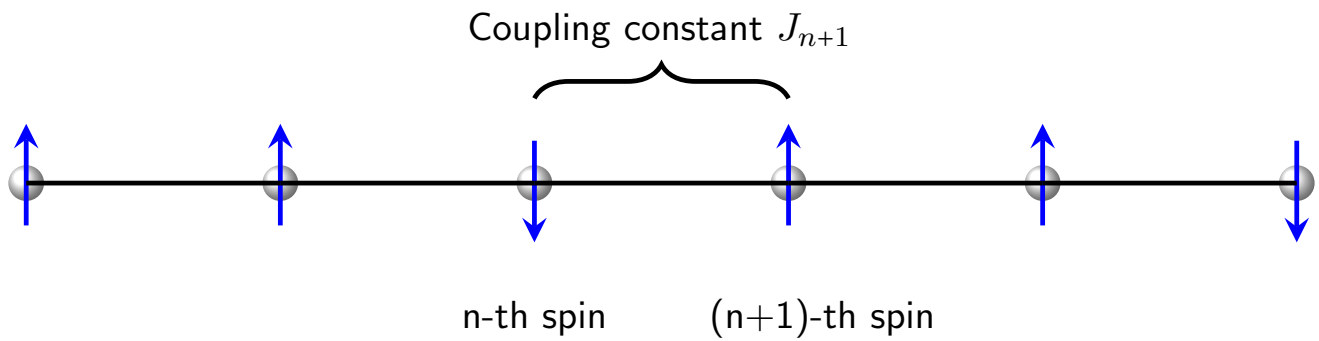


[4] Sougato Bose. *Quantum communication through an unmodulated spin chain*. Physical Review Letters, 91(20):207901, 2003.

1D Spin Chains

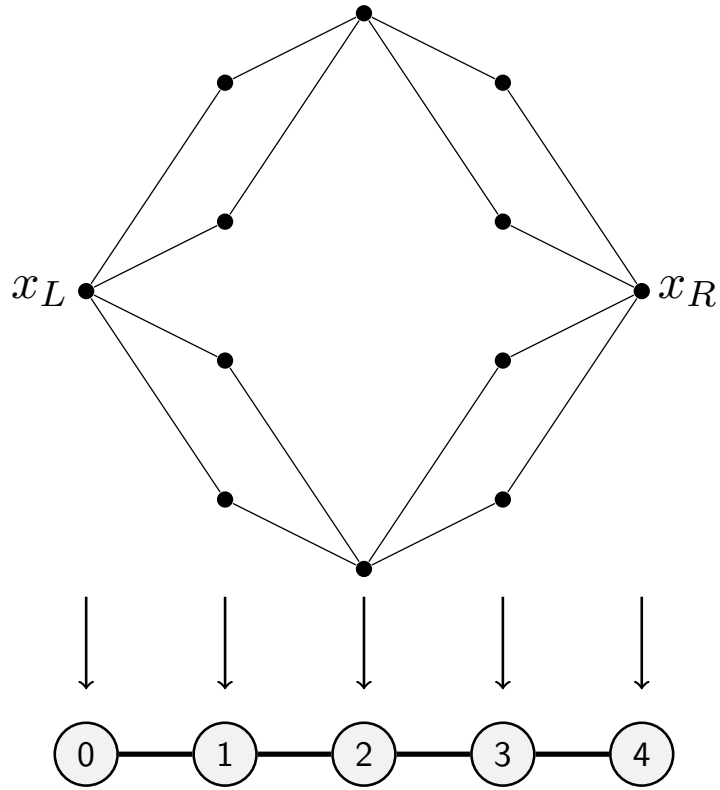
- One dimensional Hamiltonians of the XX-type with nearest-neighbor interactions reduced to the following Jacobi matrix.

$$\mathbf{J} = \begin{pmatrix} B_0 & J_1 & & & \mathbf{0} \\ J_1 & B_1 & J_2 & & \\ & J_2 & B_2 & \ddots & \\ & & \ddots & \ddots & J_N \\ \mathbf{0} & & & J_N & B_N \end{pmatrix}.$$



Example: Berker lattice

- *Transversal decomposition* of finite graphs, then the range of rank function $\mathbf{\Pi}$ is $\mathbb{Z} \bigcap [0, n]$ for some $n \in \mathbb{N}$.
- The left-hand side degree $\deg_- : V(G) \to \mathbb{N}$, $x \in \Pi^{-1}(n)$, then $\deg_-(x)$ assigns the vertex x the number of edges that connect x to vertices in $\Pi^{-1}(n-1)$ (Similarly, we define $\deg_+$).



Special case

Corollary

Let $G = (V(G), E(G), \mathbf{\Pi})$ be a $\mathbb{Z}$-graded graph. For $x_1, y_1, x_2, y_2 \in V(G)$ such that both x_1, y_1 and x_2, y_2 are adjacent, we assume

$$\mu_E(x_1, y_1) = \mu_E(x_2, y_2), \text{ if } \mathbf{\Pi}(x_1) = \mathbf{\Pi}(x_2) \text{ and } \mathbf{\Pi}(y_1) = \mathbf{\Pi}(y_2).$$

Then the lifted Jacobi matrix takes the form

$$\mathbf{H}(x,y) = \begin{cases} b(n) & \text{if } x = y \text{ and } \mathbf{\Pi}(x) = n, \\ \dfrac{1}{\mathbf{deg}_+(x)} a(n, n+1) & \text{if } (x,y) \in E(G) \text{ and } \mathbf{\Pi}(x) = n, \\ \dfrac{1}{\mathbf{deg}_-(x)} a(n-1, n) & \text{if } (y,x) \in E(G) \text{ and } \mathbf{\Pi}(y) = n-1, \\ 0 & \text{otherwise.} \end{cases}$$

Graph properties

Theorem

Assume that the mappings $\mathbf{deg}_+$ *and* $\mathbf{deg}_-$ *are constant on a transversal layer, i.e., for* $x, y \in \Pi^{-1}(n)$ *we have*

$$\mathbf{deg}_+(x) = \mathbf{deg}_+(y), \quad \mathbf{deg}_-(x) = \mathbf{deg}_-(y).$$

If a PQST on the 1D chain is achieved, i.e. there exists $T > 0$ *such that*

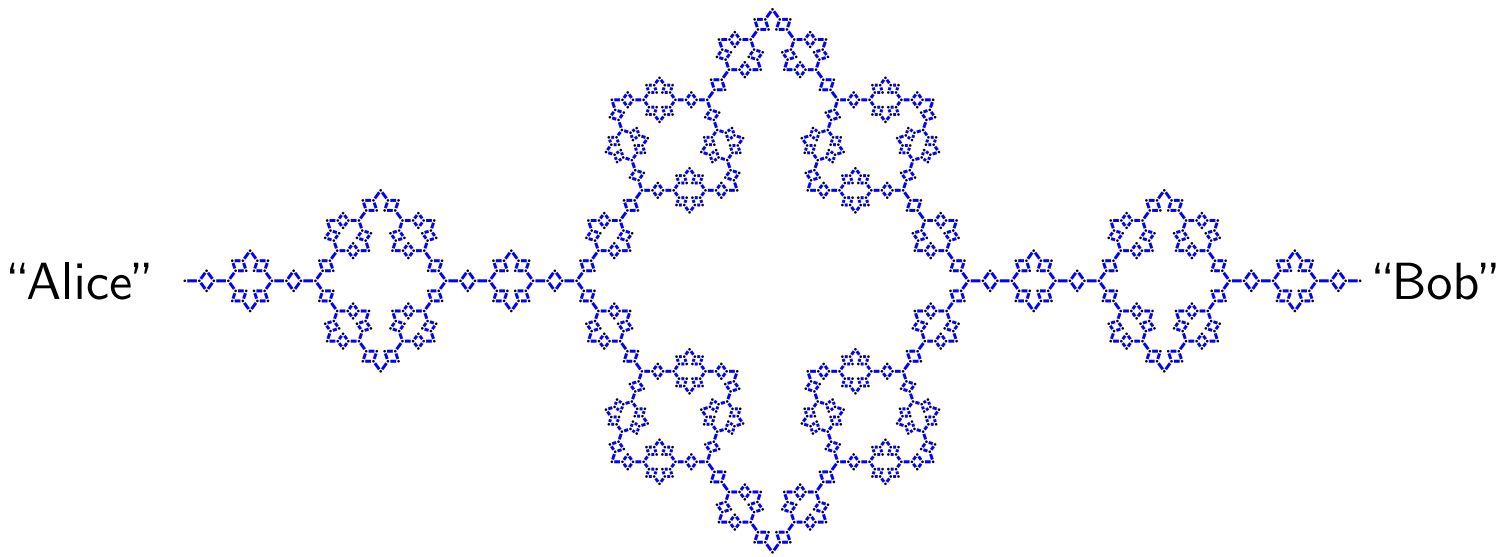
$$e^{iT\mathbf{J}} |0\rangle = e^{i\phi} |N\rangle$$

for some phase ϕ*, then the PQST on* G *is also achieved with the same time* T *and phase* ϕ*, i.e.*

$$e^{iT\mathbf{H}} |A\rangle = e^{i\phi} |B\rangle \quad \text{and} \quad e^{iT\mathbf{H}} |B\rangle = e^{i\phi} |A\rangle .$$

Diamond fractal-type graphs

- In particular, we proved that PQST can be achieved on a large class of fractal-type graphs (Diamond Fractals[5]).



[5] Urs Lang and Conrad Plaut. *Bilipschitz embeddings of metric spaces into space forms*. Geom. Dedicata, 87(1-3):285307, 2001.
E. Akkermans, G. Dunne, and A. Teplyaev, Physical Consequences of Complex Dimensions of Fractals, 2009 EPL 88.

Outline

Continuous-time quantum walk

- Traced back to Edward Farhi and Sam Gutmann[6].
- The database is modeled by a $G = (V, E)$.
- We associate to each element of the database a standard vector e_x.
- We denote the target vertex by w and the corresponding state $e_w \in \ell^2(G)$.

[6] Farhi, E. and Gutmann, S.. *Quantum computation and decision trees*. Physical Review A. American Physical Society (APS). 58 (2): 915928 (1998).

Continuous-time quantum walk

- The initial state is given by (the ground state of the Laplacians introduced below)

$$s = \frac{1}{\sqrt{vol(G)}} \sum_{x \in V} \delta_x.$$

- Time-evolution operator:

$$\exp(-itH)s = c_1(t)e_1 + \cdots + c_w(t)e_w + \cdots + c_N(t)e_N$$

- The probability that $\exp(-itH)s$ evolves into the target state e_w is

$$|c_w(t)|^2 = |\langle e_w, \exp(-itH)s\rangle|^2.$$

- The *success probability* at time t is given by

$$\pi_w(t) := |\langle e_w, \exp(-itH)s\rangle|^2.$$

Continuous-time quantum walk

- Goal: Find a Hamiltonian H such that for some (preferably small) t, we have

$$\pi_w(t) = |\langle e_w, \exp(-itH)s\rangle|^2 = 1.$$

- How do we define H? there are different approaches.
- Standard form of a Hamiltonian: $H = \Delta + U$, sum of a Laplacian Δ and a potential operator U.
- Context of graphs: Δ_G is a graph Laplacian, adjacency matrix or probabilistic graph Laplacian of G.

Childs-Goldstone approach

- Childs and Goldstone proposed the following family of Hamiltonians[7]

$$\begin{cases} H_\gamma := \gamma \Delta_G - V_w, \\ V_w f := \langle e_w, f \rangle e_w, \quad f : V \to \mathbb{C} \end{cases}$$

  where $\gamma \in (0, \infty)$ is a tunable parameter.
- H_γ is a rank-one perturbation of a scaled graph Laplacian.
- The potential $V_w f := \langle e_w, f \rangle e_w$ is an orthogonal projection onto $span\{e_w\}$.

[7] A. Childs and J. Goldstone. Spatial search by quantum walk. Phys. Rev. A, 70:022314, Aug 2004.

Probabilistic graph Laplacians

- Let $\{p(x,y)\}_{(x,y)\in E}$ be a sequence of weights assigned to the edges.
- $p(x,y)$ is a transition probability of a random walker from x to y, i.e.

$$\begin{cases} (x,y) \in E \Leftrightarrow 0 < p(x,y) \leq 1 \\ (x,y) \notin E \Leftrightarrow p(x,y) = 0 \\ \sum_{y:(x,y)\in E} p(x,y) = 1, \ \forall \ x \in V. \end{cases}$$

- A *probabilistic graph Laplacian* on G is then defined by

$$\Delta_G f(x) = f(x) - \sum_{y:(x,y)\in E} p(x,y) f(y),$$

- We assume there exists a Hilbert space $\left(\mathcal{H}, \langle .,. \rangle\right)$ such that Δ_G is self-adjoint,

$$\langle \Delta_G \psi, \phi \rangle = \langle \psi, \Delta_G \phi \rangle, \quad \mu(x) := \langle \delta_x, \delta_x \rangle.$$

Childs-Goldstone approach

- Is there a systematic approach to determine the value γ_{opt} for which $H_{\gamma_{opt}}$ leads to optimal search outcomes, i.e. $\pi_w^{\gamma_{opt}}(t)$ is maximal in the shortest time possible?
- Childs and Goldstone[8]elaborated on the interplay between the success probability and the overlap probabilities

$$|\langle s, \psi_0\rangle|^2,\ |\langle e_w, \psi_0\rangle|^2,\ |\langle s, \psi_1\rangle|^2,\ |\langle e_w, \psi_1\rangle|^2$$

where ψ_0 (resp. ψ_1) refer to the ground (resp. first excited) state of H_γ.

[8] A. Childs and J. Goldstone. Spatial search by quantum walk. Phys. Rev. A, 70:022314, Aug 2004.

Childs-Goldstone approach

- We will consider the following parameters

$$\begin{cases} \gamma_s := \inf_{\gamma\in(0,\infty)} \left\{\gamma \;\middle|\; \text{such that } |\langle s,\psi_0\rangle|^2 = |\langle s,\psi_1\rangle|^2\right\}. \\ \gamma_w := \inf_{\gamma\in(0,\infty)} \left\{\gamma \;\middle|\; \text{such that } |\langle e_w,\psi_0\rangle|^2 = |\langle e_w,\psi_1\rangle|^2\right\}. \\ \gamma_E := \inf_{\gamma\in(0,\infty)} \left\{\gamma \;\middle|\; \text{such that } E_0 = -E_1\right\}. \end{cases}$$

  where ψ_0 (resp. ψ_1) refer to the ground (resp. first excited) state of H_γ corresponding to the eigenvalue E_0 (resp. E_1).
- Our first result:
  1) establishes a relationship between the overlap probabilities and the eigenvalues E_0, E_1.
  2) provides sufficient conditions to approximate these eigenvalues by the square root of the graph's volume.

First result

Theorem

Assume that there exist $\gamma \in (0, \infty)$ *and* $\epsilon > 0$ *such that*

$$\left| |\langle s, \psi_0 \rangle|^2 - |\langle e_w, \psi_0 \rangle|^2 \right| \leq \epsilon. \tag{1}$$

Then

$$\left| E_0^2 - \frac{\langle \delta_w, \delta_w \rangle}{vol(G)} \right| \leq \epsilon.$$

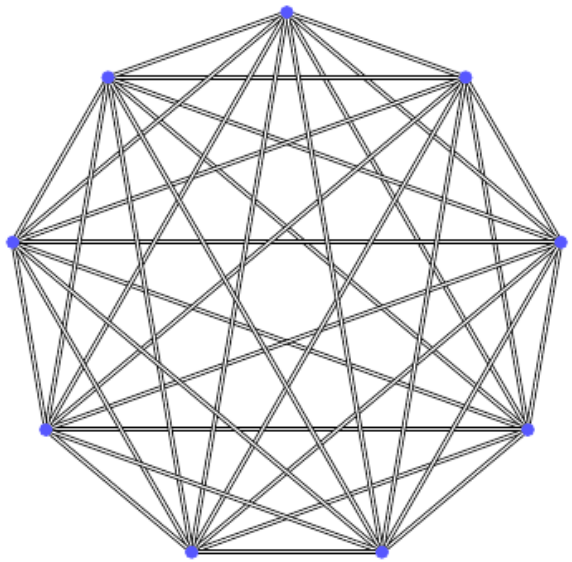
Similarly, if the inequality (1) holds for ψ_1*, then*

$$\left| E_1^2 - \frac{\langle \delta_w, \delta_w \rangle}{vol(G)} \right| \leq \left(1 + \frac{\langle \delta_w, \delta_w \rangle}{vol(G)} \frac{\left| |\langle s, \psi_1 \rangle|^2 - |\langle s, \psi_0 \rangle|^2 \right|}{|\langle s, \psi_1 \rangle|^2 |\langle s, \psi_0 \rangle|^2} \right) \epsilon$$

Example: Complete graphs

- Let $G = (V, E)$ be a complete graph.
- We assume that G has N vertices, i.e. $|V| = N$.
- Probabilistic graph Laplacian

$$\Delta_G = \begin{pmatrix} 1 & -\frac{1}{N-1} & \cdots & \cdots & -\frac{1}{N-1} \\ -\frac{1}{N-1} & 1 & -\frac{1}{N-1} & \cdots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 1 & -\frac{1}{N-1} \\ -\frac{1}{N-1} & \cdots & \cdots & -\frac{1}{N-1} & 1 \end{pmatrix}$$



Example: Complete graphs

- If set $\gamma = \dfrac{N-1}{N}$, then a direct computation of the overlap probabilities gives

$$\begin{cases} |\langle s, \psi_0\rangle|^2 = |\langle e_w, \psi_0\rangle|^2 = \frac{\sqrt{N}+1}{2\sqrt{N}} \\ |\langle s, \psi_1\rangle|^2 = |\langle e_w, \psi_1\rangle|^2 = \frac{\sqrt{N}-1}{2\sqrt{N}} \end{cases}$$

- The sufficient conditions in our Theorem are satisfied for any $\epsilon > 0$.
- Hence, the eigenvalues are given by

$$E_0 = -\frac{1}{\sqrt{N}}, \quad E_1 = \frac{1}{\sqrt{N}}, \tag{2}$$

- Note that for Complete graphs, $vol(G) = N$ is nothing else but the number of vertices.

Second result

- For complete graphs, the Theorem implies that $E_0 = -E_1$ and hence $\gamma_E = \dfrac{N-1}{N}$.

Proposition

Suppose that there exists $\gamma \in (0,\infty)$ such that $E_0 = -E_1$, then

$$\frac{|\langle e_w, \psi_1\rangle|^2}{|\langle s, \psi_1\rangle|^2} = \frac{|\langle e_w, \psi_0\rangle|^2}{|\langle s, \psi_0\rangle|^2}.$$

Consequently, we have $\overline{\langle \psi_1, s\rangle}\langle e_w, \psi_0\rangle = -e^{i2\theta}\overline{\langle \psi_0, s\rangle}\langle e_w, \psi_1\rangle$ for some phase $\theta \in [0,\pi)$. Moreover, the success probability reduces to

$$\pi_w^\gamma(t) = 4|\langle s, \psi_0\rangle|^2\ |\langle e_w, \psi_1\rangle|^2 \sin^2(E_1 t + \theta) + C + R(t)$$

where C, and $R(t)$ are given on the next slide.

Second result

Proposition

C and $R(t)$ are given by

$$\begin{cases} C := |\langle e_w, \psi_0\rangle|^2 |\langle s, \psi_0\rangle|^2 + |\langle e_w, \psi_1\rangle|^2 |\langle s, \psi_1\rangle|^2 - 2|\langle s, \psi_0\rangle|^2 \ |\langle e_w, \psi_1\rangle|^2 \\ R(t) := 2Re\big(A(t)\overline{r(t)}\ \big) + |r(t)|^2 \end{cases}$$

with

$$\begin{cases} A(t) := \langle e_w, \psi_0\rangle\langle \psi_0, s\rangle \exp(-iE_0 t) + \langle e_w, \psi_1\rangle\langle \psi_1, s\rangle \exp(-iE_1 t) \\ r(t) := \sum_{a\geq 2} \langle e_w, \psi_a\rangle\langle \psi_a, s\rangle \exp(-iE_a t) \end{cases}$$

Example: Complete graphs

- For complete graphs, the eigenvalues E_0, E_1 can be computed explicitly for each γ.
- Solving $E_0 = -E_1$ for γ, we obtain $\gamma_E = \dfrac{N-1}{N}$.
- Is any of the parameters γ_s,γ_w and γ_E detecting the optimal case γ_{opt}?
- For a complete graph of N vertices, we have $\gamma_E = \gamma_{opt}$ for all N.
- Using our Proposition, we can compute the optimal success probability explicitly:

$$\pi_w^{\gamma_{opt}}(t) = \left(\frac{N-1}{N}\right)\sin^2\left(\frac{t}{\sqrt{N}}\right) + \frac{1}{N}. \tag{3}$$

- Quadratic speedup at $t_{opt} = \dfrac{\pi}{2}\sqrt{N}$

Starting questions of our project

- Does the equality $\gamma_{opt} = \gamma_E$ hold for other graphs?
- Is it possible to construct a graph such that the following properties hold:
  1) A graph with variable volume $vol(G)$.
  2) E_1 is well approximated by $\frac{\sqrt{\langle \delta_w, \delta_w \rangle}}{\sqrt{vol(G)}}$. In particular, E_1 is tunable via $vol(G)$.
  3) The optimal success probability is well approximated by

$$\pi_w^{\gamma}(t) = 4|\langle s, \psi_0 \rangle|^2 \, |\langle e_w, \psi_1 \rangle|^2 \sin^2(E_1 t + \theta) + C + R(t) \qquad (4)$$

- Goal: tunable optimal time in Grover's algorithm via $vol(G)$.

Comments on other works

- E. Agliari et al. studied the parameter γ_s on graphs of different topologies[9].
- Used graph Laplacian $D - A$, where D (resp. A) is the degree (resp. adjacency) matrix of the graph.
- For complete graphs, we observe

$$\gamma_s \leq \gamma_E = \gamma_{opt} = \frac{N-1}{N} \leq \gamma_w,$$

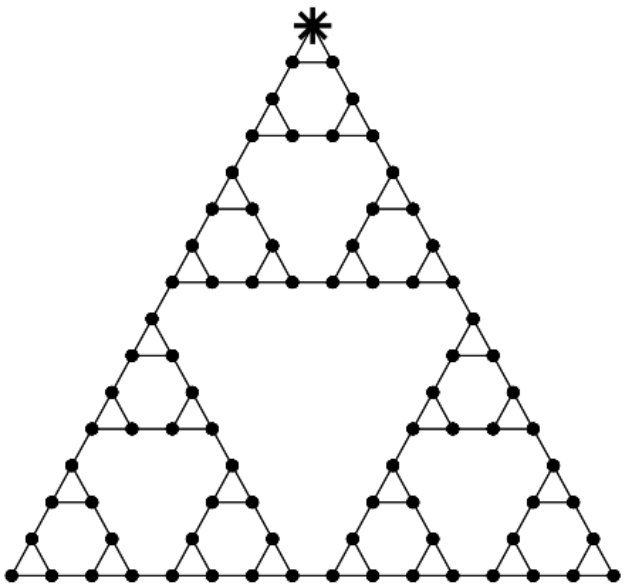
- For a complete graph of two vertices, i.e. $N = 2$ we have $\gamma_s = 0$ and $\gamma_w = \infty$, while for large N, we see that

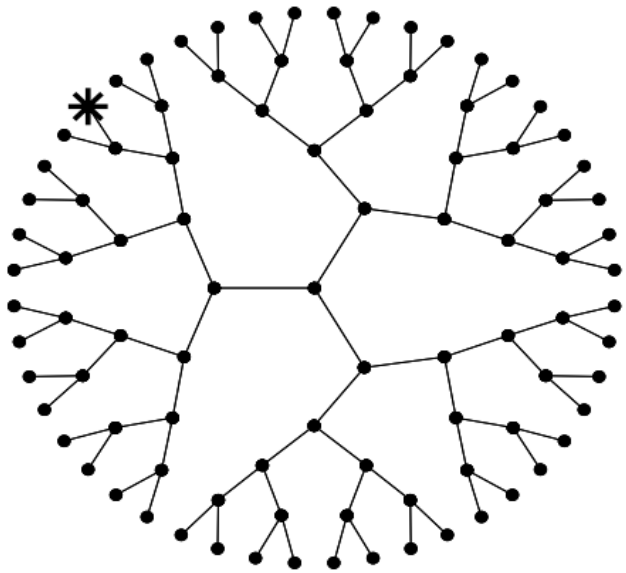
$$\gamma_s \approx \gamma_E \approx \gamma_w \approx 1. \tag{5}$$

[9] E. Agliari, A. Blumen, and O. Mulken. Quantum-walk approach to searching on fractal structures. Phys. Rev. A, 82:012305, Jul 2010.

Self-similar database structures

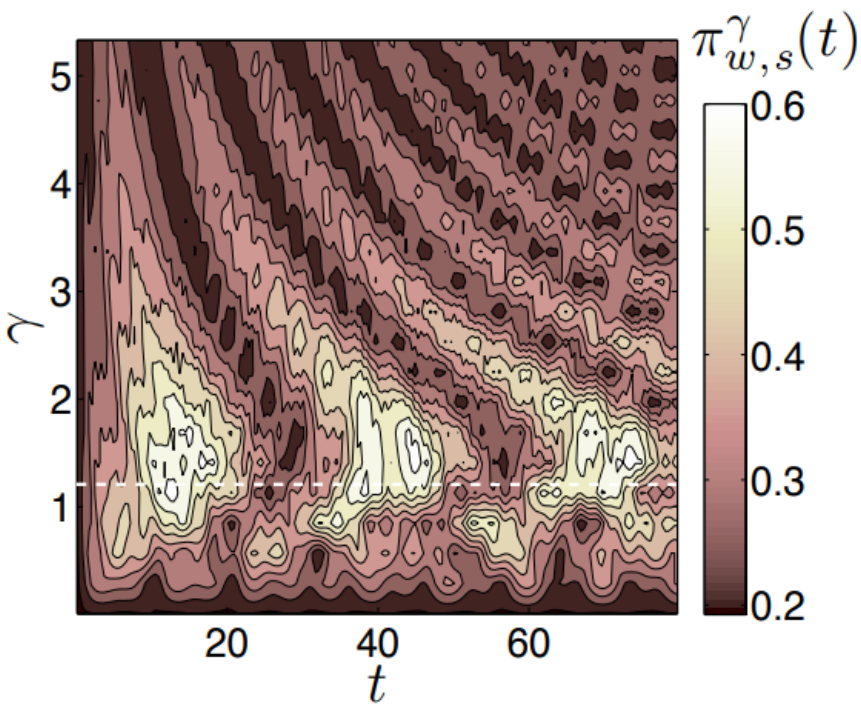
- Examples[10]: Quantum walk on Hanoi graphs and Cayley trees.

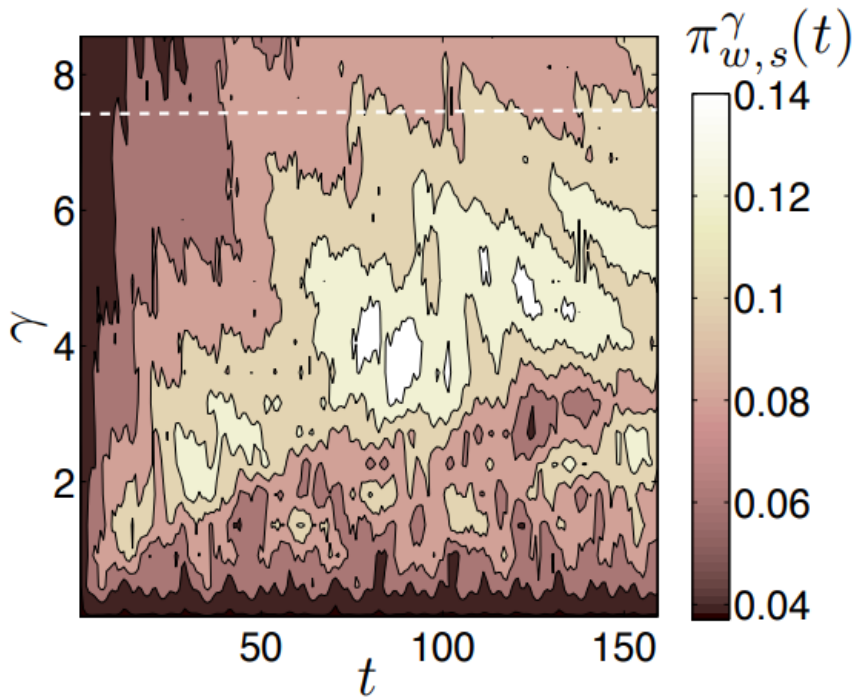




[10] E. Agliari, A. Blumen, and O. Mulken. Quantum-walk approach to searching on fractal structures. Phys. Rev. A, 82:012305, Jul 2010.

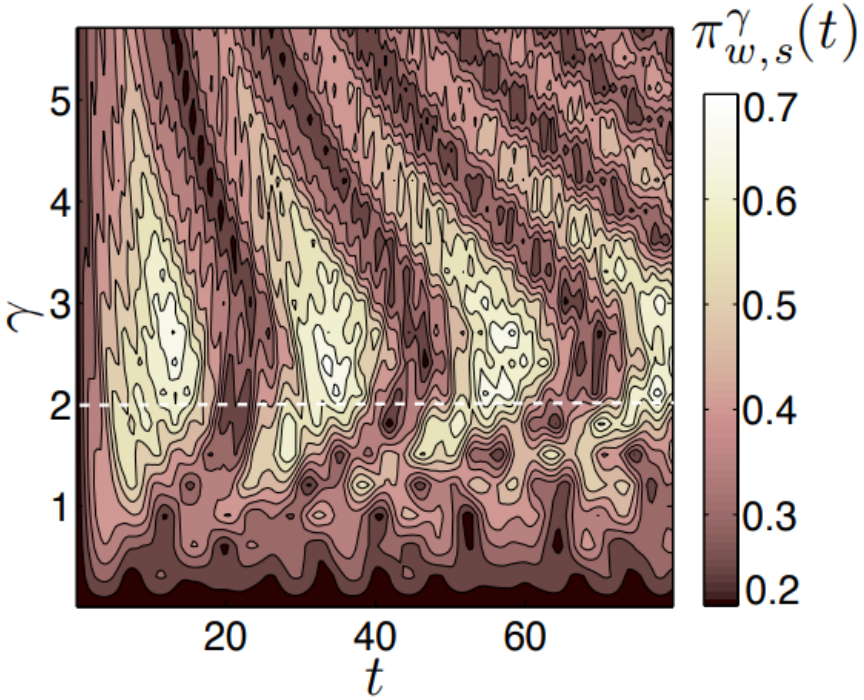
Hanoi graphs level 3 and 6

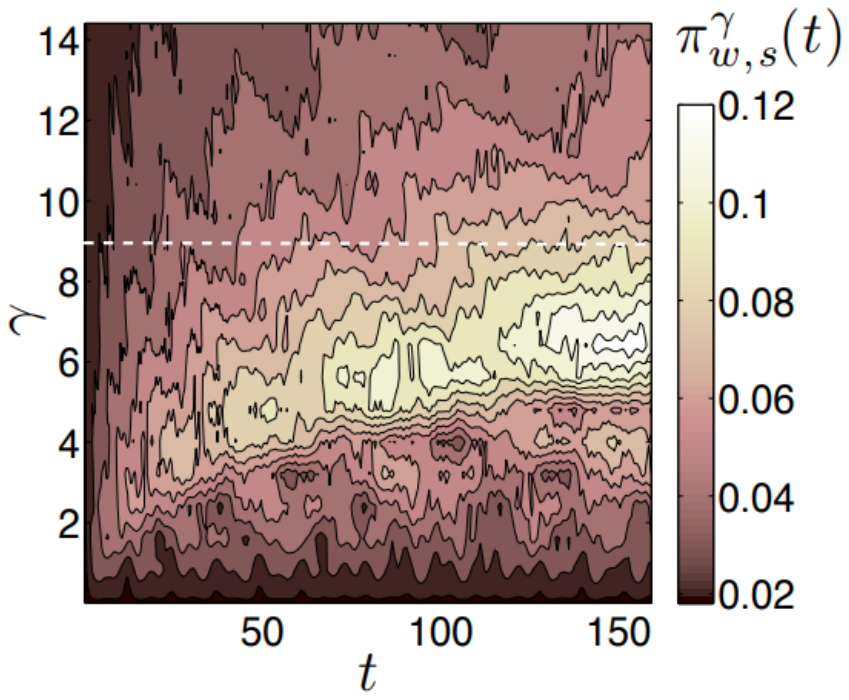




[10] E. Agliari, A. Blumen, and O. Mulken. Quantum-walk approach to searching on fractal structures. Phys. Rev. A, 82:012305, Jul 2010.

Cayley trees level 3 and 10





[10] E. Agliari, A. Blumen, and O. Mulken. Quantum-walk approach to searching on fractal structures. Phys. Rev. A, 82:012305, Jul 2010.

Subsection 1

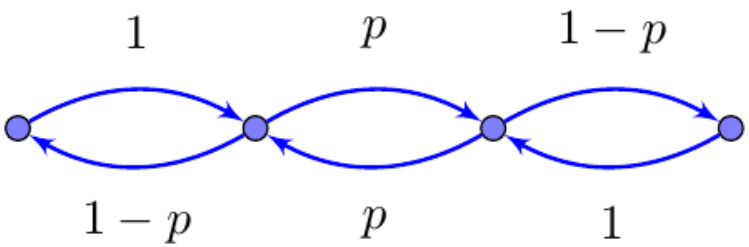
Varying analytical structure

Alternative approach

- Instead of finding specific graph topologies convenient for the related quantum walk, we fix the graph topology and vary the underlying graph Laplacians.
- In other words, we search for the most appropriate analytical structure on graphs yielding better search outcomes.
- Concrete: we vary the transition probabilities $\{p(x,y)\}_{(x,y)\in E}$ of a random walker on G. By doing so, we are effectively varying Δ_G.

Example: Hypercubic lattices

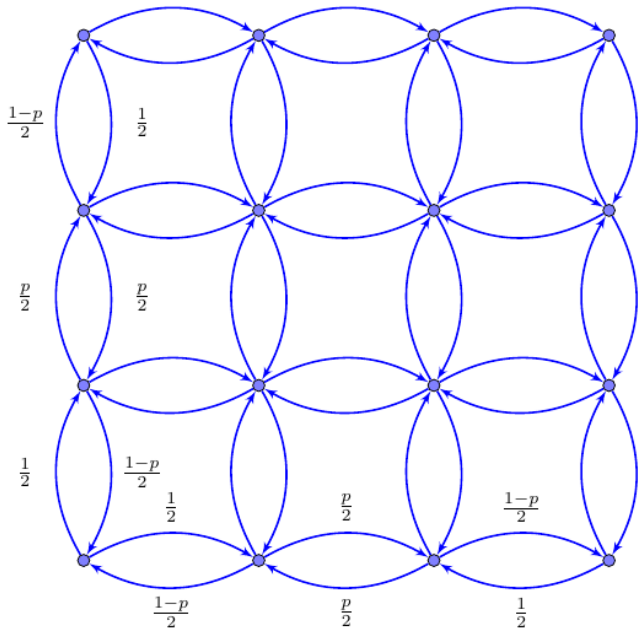
- Let $G = (V, E)$ be a directed path graph of 4 vertices.
- The probabilistic graph Laplacian Δ_G is given by the transition probability $p \in (0, 1)$.
- When $p = 1/2$, Δ_G becomes the standard probabilistic graph Laplacian.
- Homogeneity versus non-homogeneity of the database, i.e., $p = 1/2$ versus $p \neq 1/2$.



$$\Delta_G = \begin{pmatrix} 1 & -1 & 0 & 0 \\ p-1 & 1 & -p & 0 \\ 0 & -p & 1 & p-1 \\ 0 & 0 & -1 & 1 \end{pmatrix}.$$

d-dimensional hypercubic lattice

A *d-dimensional hypercubic lattice* is constructed as the d-fold Cartesian product of finite directed path graphs $G_d = G \times G \times .. \times G$.



For example, a Laplacian on G_2 is a (normalized) Kronecker sum, i.e.

$$\Delta_{G_2} = \frac{1}{2}\left(\Delta_G \otimes I + I \otimes \Delta_G\right)$$

where I is an identity matrix.

The setting

- Numerical results on the Grover's search algorithm on the graph G_5.
- The number of vertices is $|V(G_5)| = 1024$.
- The target vertex $w \in V(G_5)$ is assumed to be one of the corners of G_5.
- Our focus is to analyze the search algorithm based on the homogeneity versus non-homogeneity of the database, i.e., $p = 1/2$ versus $p \neq 1/2$.

Overlap probabilities for different transition probabilities p

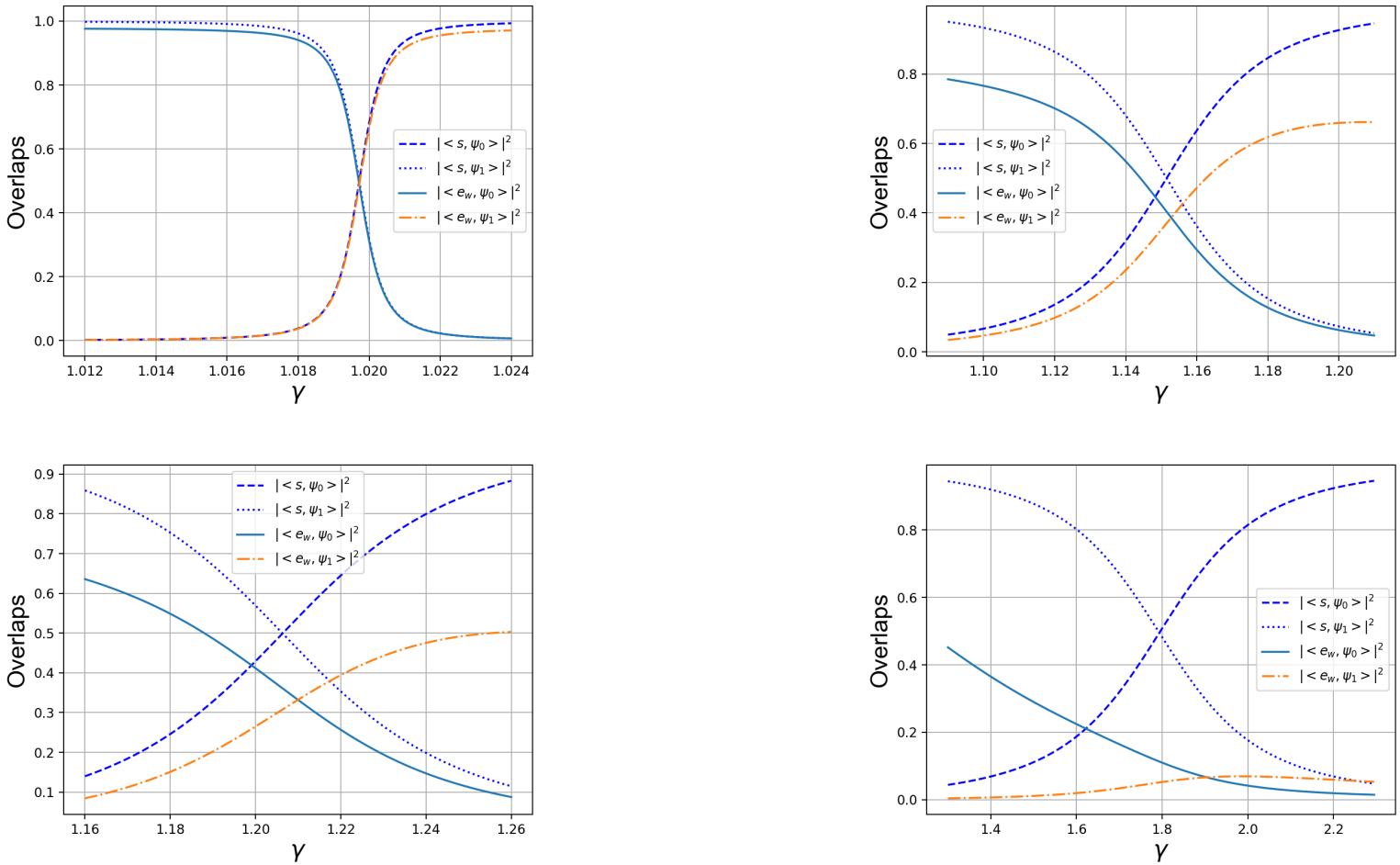


Figure: Overlap probabilities as a function of γ for G_5: (top, left) $p = 0.91$, (top, right) $p = 0.5$, (bottom, left) $p = 0.4$, (bottom, right) $p = 0.1$.

Success probabilities for different transition probabilities p

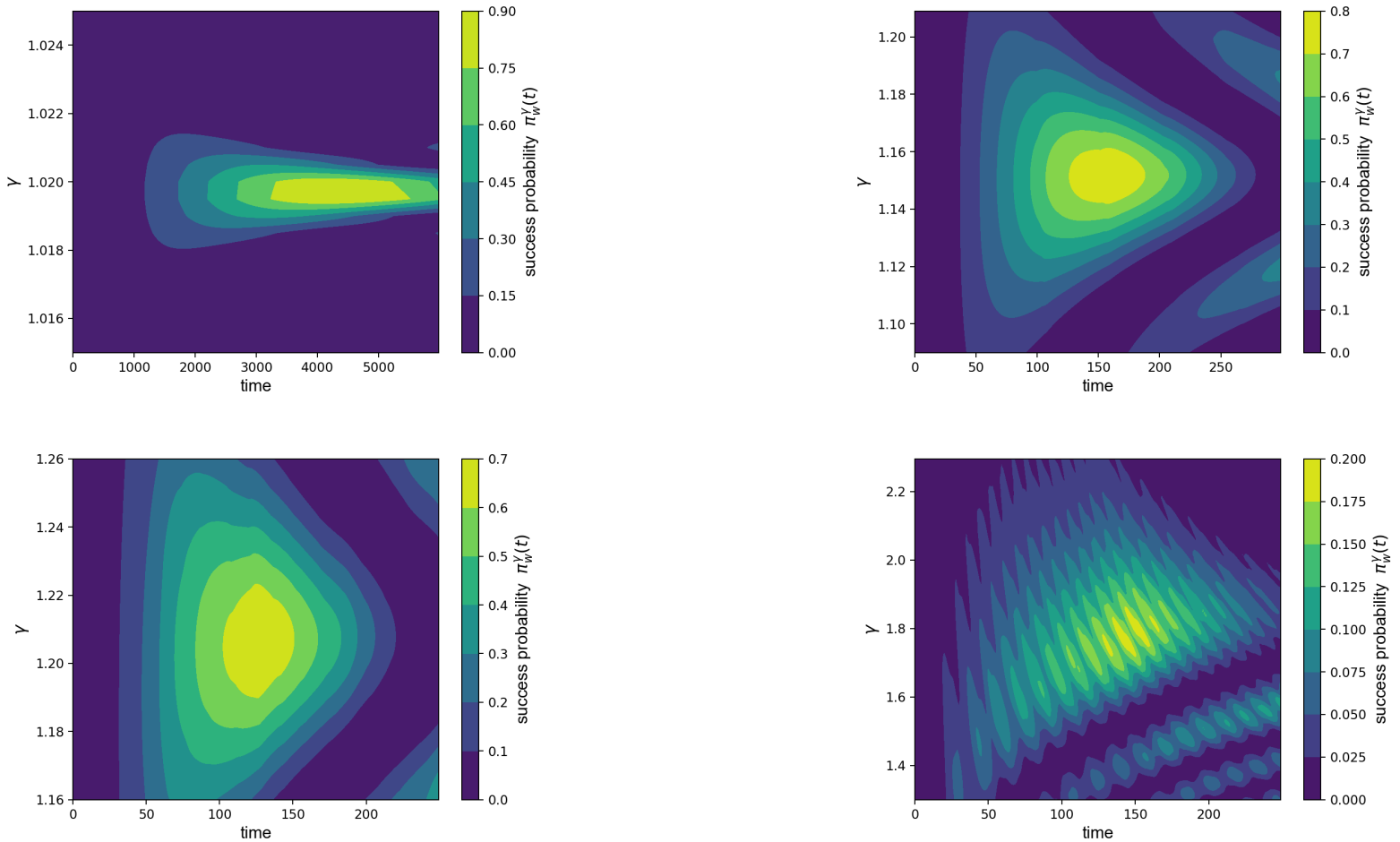


Figure: Contour plot of the success probability $\pi_w^\gamma(t)$ as a function of the time t and γ for G_5: (top, left) $p = 0.91$, (top, right) $p = 0.5$, (bottom, left) $p = 0.4$, (bottom, right) $p = 0.1$.

Observations

- We numerically determine γ_s,γ_w, γ_E and γ_{opt} and observe that in all cases

$$\gamma_s \leq \gamma_E \leq \gamma_w,$$

  where for larger p, γ_E is increasingly squeezed between γ_s and γ_w.
- For $p = 0.91$, we have $\gamma_{opt} \approx \gamma_E \approx \gamma_s \approx \gamma_w$.
- The case $p = 0.91$ is particularly interesting and is qualitatively similar to the results for the complete graphs.
- For $p = 0.91$, the optimal success probability is in very good agreement with the analytical formula (see next slide)

$$\pi_w^{\gamma_{opt}}(t) \approx 0.89 \sin^2(E_1 t).$$

Optimal success probabilities for different p

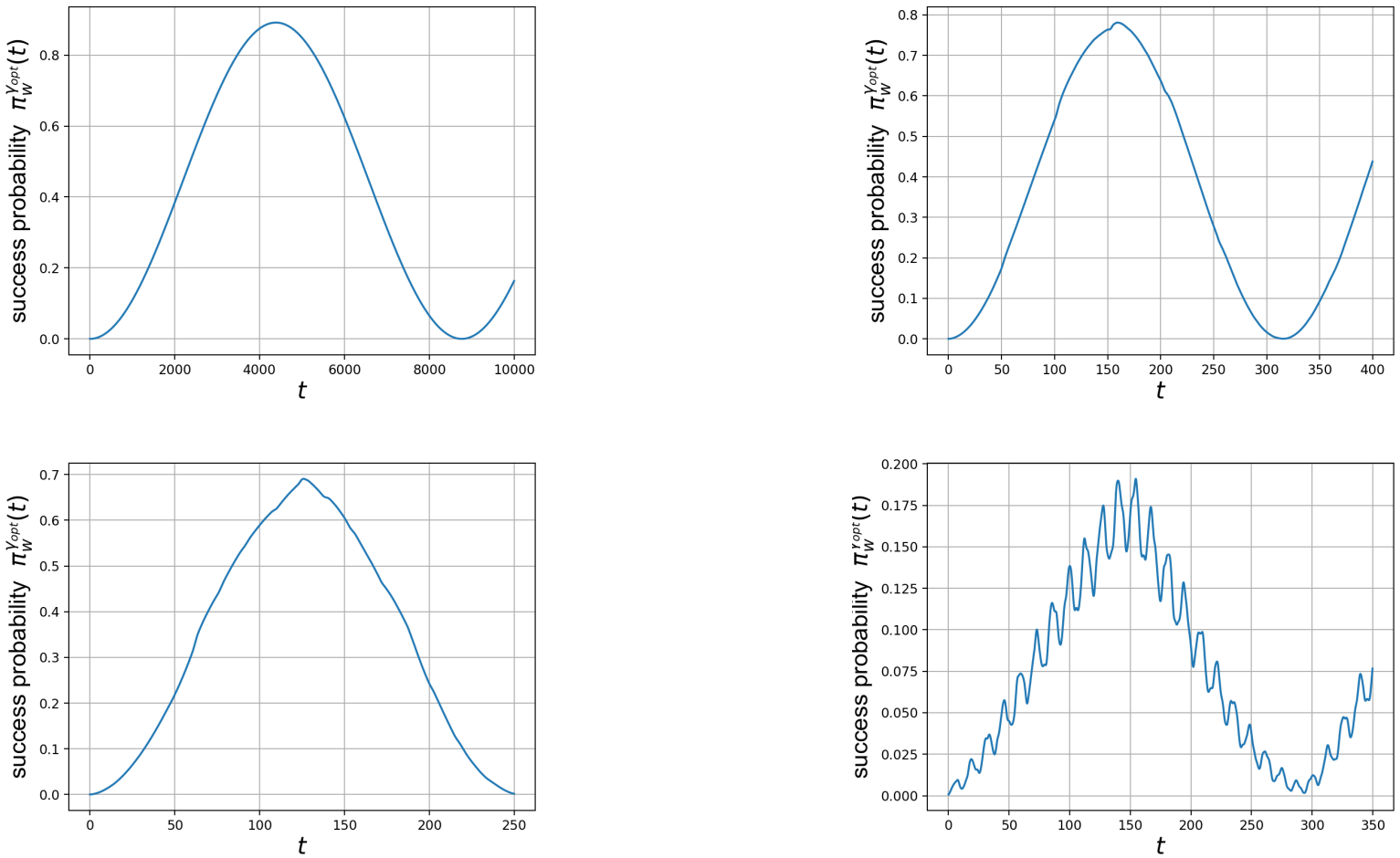


Figure: Plot of the success probability $\pi_w^{\gamma}(t)$ as a function of time t for G_5. We set $\gamma = \gamma_{opt}$ in all panels: (top, left) $p = 0.91$, (top, right) $p = 0.5$, (bottom, left) $p = 0.4$, (bottom, right) $p = 0.1$.

End of the talk.

Thank you! :-)