

Spatial search on Johnson graphs by continuous-time quantum walk

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(joint work with Mohamed Sabri and Renato Portugal)

Research **C**enter for **P**ure and **A**ppplied **M**athematics

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How I started this work

- I am a mathematician specializing in **distance-regular graphs** and **association schemes**, in particular their **Terwilliger algebras**.
 - Etsuo Segawa (a specialist in quantum walks) invited Portugal to Tohoku U in Jan–Feb 2018, and Portugal gave a series of lectures on search algorithms based on quantum walks.
 - Sabri was a student of Segawa, and became my Ph.D. student in Sep 2019.
- ⇒ I started studying quantum walks.

General set-up

- $G = (V, E)$: a finite simple graph, where $|V| = N$
- $\mathcal{H} = \text{span}\{ |v\rangle : v \in V \}$, where $\langle v | v' \rangle = \delta_{v,v'}$
- A : the **adjacency matrix** of G :

$$A_{v,v'} = \begin{cases} 1 & \text{if } v \sim v' \\ 0 & \text{otherwise} \end{cases} \quad (v, v' \in V)$$

- $w \in V$: the marked vertex
- Consider a Hamiltonian of the form (Childs–Goldstone, 2004)

$$H = -\gamma A - |w\rangle\langle w|$$

where $\gamma \in \mathbb{R}$.

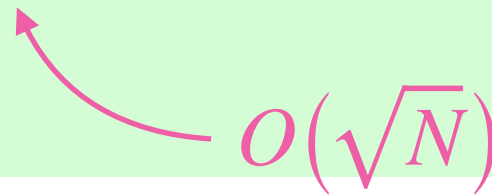
General set-up

$$H = -\gamma A - |w\rangle\langle w|$$

- $|\psi(0)\rangle \in \mathcal{H}$: the initial state
- $|\psi(t)\rangle = e^{-iHt} |\psi(0)\rangle$: the state at time t
- $|\langle w | \psi(t) \rangle|^2$: the finding probability at time t

Problem.

Choose $|\psi(0)\rangle \in \mathcal{H}$, $\gamma \in \mathbb{R}$, $t \in \mathbb{R}$ which maximize the finding probability !!



Remark.

- $A \in$ the adjacency algebra
- $H, e^{-iHt} \in$ the Terwilliger algebra w.r.t. w

Some previous work

- complete graphs (Childs–Goldstone, 2004) ← DRGs
- hypercubes (Childs–Goldstone, 2004) ← DRGs
- Cartesian powers of cycles (Childs–Goldstone, 2004)
- strongly regular graphs (Janmark–Meyer–Wong, 2014) ← DRGs
- Johnson graphs with diameter 3 (Wong, 2016) ← DRGs
- Erdős–Renyi graphs (Chakraborty–Novo–Ambainis–Omar, 2016)

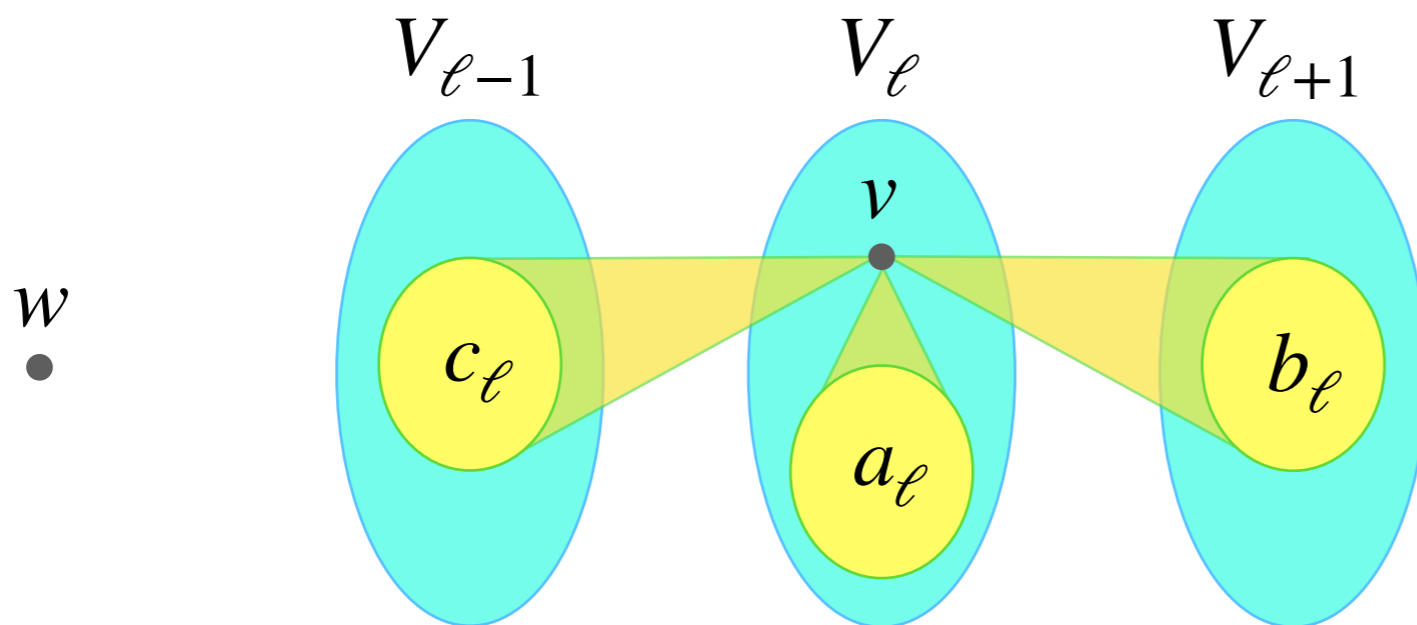
Today's topic

- Johnson graphs with any fixed diameter

[arXiv:2108.01992](https://arxiv.org/abs/2108.01992)

Johnson graphs

- $n, k \in \mathbb{N}$ ($1 \leq k \leq n/2$)
- V : the set of k -subsets of $\{1, 2, \dots, n\}$ $\implies N = \binom{n}{k}$
- $v \sim v' \stackrel{\text{def}}{\iff} |v \cap v'| = k - 1$ ($v, v' \in V$)
- $G = J(n, k)$
- $V_\ell = \{v \in V : |v \cap w| = k - \ell\}$ ($0 \leq \ell \leq k$)



$$a_\ell = \ell(n - 2\ell)$$

$$b_\ell = (k - \ell)(n - k - \ell)$$

$$c_\ell = \ell^2$$

$$V_\ell = \{v : |v \cap w| = k - \ell\}$$

- $|V_\ell\rangle = \frac{1}{\sqrt{|V_\ell|}} \sum_{v \in V_\ell} |v\rangle \quad (0 \leq \ell \leq k)$
- $|V_0\rangle = |w\rangle$
- $\mathcal{H}_{\text{inv}} = \text{span}\{|V_\ell\rangle : 0 \leq \ell \leq k\}$
- \mathcal{H}_{inv} : invariant under $A, |w\rangle\langle w|, H, e^{-iHt}$

We will work with \mathcal{H}_{inv} !!

Remark.

- \mathcal{H}_{inv} : the **primary module** for the Terwilliger algebra

General strategy

$$H = -\gamma A - |w\rangle\langle w|$$

- $|\psi(0)\rangle := |s\rangle = \frac{1}{\sqrt{N}} \sum_{v \in V} |v\rangle \in \mathcal{H}_{\text{inv}}$
- Find eigenvalues ρ_1, ρ_2 and eigenvectors $|\xi_1\rangle, |\xi_2\rangle$ of H
s.t. $|s\rangle \approx \frac{1}{2} |\xi_1\rangle - \frac{1}{2} |\xi_2\rangle, \quad |w\rangle \approx \frac{1}{2} |\xi_1\rangle + \frac{1}{2} |\xi_2\rangle.$
- Take the smallest $t > 0$ s.t. $(\rho_1 - \rho_2)t \equiv \pi \pmod{2\pi}.$

$$\begin{aligned} \implies |\psi(t)\rangle &= e^{-iHt} |s\rangle \approx \frac{e^{i\rho_1 t}}{2} |\xi_1\rangle - \frac{e^{i\rho_2 t}}{2} |\xi_2\rangle \\ &= e^{i\rho_1 t} \left(\frac{1}{2} |\xi_1\rangle - \frac{e^{i\pi}}{2} |\xi_2\rangle \right) \approx e^{i\rho_1 t} |w\rangle \end{aligned}$$

$$\therefore |\langle w | \psi(t) \rangle|^2 \approx 1 !!$$

Johnson graphs with fixed diameter

Fix k and let $n \rightarrow \infty$!!

- The matrix expression of A w.r.t. $|V_0\rangle, |V_1\rangle, \dots, |V_k\rangle$ is

$$D \cdot \begin{pmatrix} a_0 & b_0 & & & & \\ c_1 & a_1 & b_1 & & & \\ & c_2 & \cdot & \cdot & & \\ & & \cdot & a_{k-1} & b_{k-1} & \\ & & & c_k & a_k & \end{pmatrix} \cdot D^{-1}$$

where $D = \text{diag}(|V_0|, \dots, |V_k|)$.

difficult to handle !!

Johnson graphs with fixed diameter

- A has $k + 1$ distinct eigenvalues 

$$\theta_\ell = (k - \ell)(n - k - \ell) - \ell \quad (0 \leq \ell \leq k).$$

- E_ℓ : the projection onto the eigenspace in \mathcal{H} w.r.t. θ_ℓ

- $|\theta_\ell\rangle = \frac{1}{\|E_\ell |w\rangle\|} E_\ell |w\rangle \in \mathcal{H}_{\text{inv}} \quad (0 \leq \ell \leq k)$

- $\mathcal{H}_{\text{inv}} = \text{span}\{ |\theta_\ell\rangle : 0 \leq \ell \leq k \}$

- $\|E_\ell |w\rangle\|^2 = \frac{\binom{n}{\ell} - \binom{n}{\ell-1}}{\binom{n}{k}} = \frac{k!(n-k)!(n-2\ell+1)}{\ell!(n-\ell+1)!}$

$$\mathcal{H}_{\text{inv}} = \text{span}\{|\theta_\ell\rangle : 0 \leq \ell \leq k\}$$

- ~~The matrix expression of A w.r.t. $|\theta_0\rangle, |\theta_1\rangle, \dots, |\theta_k\rangle$ is~~

$$A = \text{diag}(\theta_0, \dots, \theta_k).$$

- ~~Easy to see that the matrix expression of $|w\rangle\langle w|$ is~~

$$|w\rangle\langle w| = \left(\|E_\ell |w\rangle\| \|E_{\ell'} |w\rangle\| \right)_{\ell, \ell'=0}^k.$$

- $H = -\gamma \text{diag}(\theta_0, \dots, \theta_k) - \left(\|E_\ell |w\rangle\| \|E_{\ell'} |w\rangle\| \right)_{\ell, \ell'=0}^k.$

- For convergence, however, we will work with

$$-\eta H, \quad \text{where } \eta := \frac{1}{\gamma n}.$$

$$-\eta H, \eta = 1/\gamma n$$

● $\epsilon := \frac{1}{\sqrt{n}}$ ← viewed as a variable

viewed as a variable

● $-\eta H = \eta(\gamma A + |w\rangle\langle w|)$
 $= \epsilon^2 A + \eta |w\rangle\langle w|$

$$= \text{diag}(r_0(\epsilon), r_1(\epsilon), \dots, r_k(\epsilon)) + \eta (p_\ell(\epsilon) p_{\ell'}(\epsilon))_{\ell, \ell'=0}^k$$

where

$$r_\ell(\epsilon) := \epsilon^2 \theta_\ell = (k - \ell)(1 - (k + \ell)\epsilon^2) - \ell \epsilon^2$$

$$p_\ell(\epsilon) := \|E_\ell |w\rangle\|$$

$$= \epsilon^{k-\ell} \sqrt{\frac{k!(1 - (2\ell - 1)\epsilon^2)}{\ell!(1 - (\ell - 1)\epsilon^2) \cdots (1 - (k - 1)\epsilon^2)}}$$

- We are now concerned with eigenvalues and eigenvectors of

$$-\eta H = \text{diag}(r_0(\epsilon), r_1(\epsilon), \dots, r_k(\epsilon)) + \eta \left(p_\ell(\epsilon) p_{\ell'}(\epsilon) \right)_{\ell, \ell'=0}^k$$

that “connect”

variables

$$|s\rangle = |\theta_0\rangle = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad |w\rangle = \begin{pmatrix} p_0(\epsilon) \\ p_1(\epsilon) \\ \vdots \\ p_k(\epsilon) \end{pmatrix} \longrightarrow \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix} \quad (\epsilon \rightarrow 0).$$

- For $(\epsilon, \eta) = (0, k)$, we have

$$-\eta H = \text{diag}(k, k-1, \dots, 2, 1, k).$$

Proposition.

- For every $a \in \mathbb{R} \setminus \{0\}$, there exist analytic functions

$$\eta(\epsilon), \lambda(\epsilon), \xi_\ell(\epsilon) \quad (0 \leq \ell \leq k)$$

s.t. $\eta(0) = k$, $\xi_0(\epsilon) \equiv a$, and

$$-\eta(\epsilon)H|\xi(\epsilon)\rangle = \lambda(\epsilon)|\xi(\epsilon)\rangle,$$

where

$$|\xi(\epsilon)\rangle = \begin{pmatrix} \xi_0(\epsilon) \\ \vdots \\ \xi_k(\epsilon) \end{pmatrix} \longrightarrow \begin{pmatrix} a \\ 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix} \quad (\epsilon \rightarrow 0).$$

Proposition (continued).

- Moreover,

$$\lambda(\epsilon) = r_0(\epsilon) + \frac{\sqrt{k!} k}{a} \epsilon^k + O(\epsilon^{k+1}),$$

$$\eta(\epsilon) = \left(\sum_{\ell=1}^k \frac{p_\ell(\epsilon)^2}{r_0(\epsilon) - r_\ell(\epsilon)} \right)^{-1} + \sqrt{k!} k \left(\frac{1}{a} - a \right) \epsilon^k + O(\epsilon^{k+1}).$$

Perturbation theory

- $X(\epsilon) = (X_{i,j}(\epsilon))_{i,j=1}^d$: an analytic $d \times d$ matrix function

Example : $X(\epsilon) = X_0 + \epsilon X_1$

- Assume that eigenvalues and eigenvectors are analytic functions of ϵ :

$$X(\epsilon) |\xi(\epsilon)\rangle = \lambda(\epsilon) |\xi(\epsilon)\rangle$$

- Then we can derive many identities by equating coefficients of ϵ^m ($m = 0, 1, 2, \dots$) on both sides.

Theorem (Implicit Function Theorem).

- $\varphi_i(\mathbf{x}, \mathbf{y})$ ($1 \leq i \leq q$) : analytic functions ($\mathbf{x} \in \mathbb{C}^p, \mathbf{y} \in \mathbb{C}^q$)
- $\varphi_i(\mathbf{x}^0, \mathbf{y}^0) = 0$ ($1 \leq i \leq q$)
- $\det \left(\frac{\partial \varphi_j}{\partial y_i} \right)_{i,j=1}^q \Big|_{(\mathbf{x}^0, \mathbf{y}^0)} \neq 0$

\implies ① $\exists U$: a neighborhood of $(\mathbf{x}^0, \mathbf{y}^0)$

② $g_1(\mathbf{x}), \dots, g_q(\mathbf{x})$: analytic functions

s.t., on U ,

$$\varphi_i(\mathbf{x}, \mathbf{y}) = 0 \quad (1 \leq i \leq q) \iff \mathbf{y} = (g_1(\mathbf{x}), \dots, g_q(\mathbf{x}))$$

determined by $a \in \mathbb{R} \setminus \{0\}$

- Recall

$$\eta(\epsilon) = \left(\sum_{\ell=1}^k \frac{p_{\ell}(\epsilon)^2}{r_0(\epsilon) - r_{\ell}(\epsilon)} \right)^{-1} + \sqrt{k!} k \left(\frac{1}{a} - a \right) \epsilon^k + O(\epsilon^{k+1}).$$

- For the search algorithm, we choose $\eta(\epsilon) = \eta^{\circ}(\epsilon)$, where

$$\eta^{\circ}(\epsilon) = \left(\sum_{\ell=1}^k \frac{p_{\ell}(\epsilon)^2}{r_0(\epsilon) - r_{\ell}(\epsilon)} \right)^{-1}.$$

- Then we have two “approximate” eigenvectors

$$|\xi^{+}(\epsilon)\rangle \longrightarrow \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}, \quad |\xi^{-}(\epsilon)\rangle \longrightarrow \begin{pmatrix} -1 \\ 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix} \quad (\epsilon \rightarrow 0).$$

$a = 1$ $a = -1$

$$|s\rangle = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad |w\rangle \approx \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}, \quad |\xi^+\rangle \approx \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}, \quad |\xi^-\rangle \approx \begin{pmatrix} -1 \\ 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}$$

$$\therefore |s\rangle \approx \frac{1}{2} |\xi_1\rangle - \frac{1}{2} |\xi_2\rangle, \quad |w\rangle \approx \frac{1}{2} |\xi_1\rangle + \frac{1}{2} |\xi_2\rangle$$

- From the formula for the “approximate” eigenvalues $\lambda^\pm(\epsilon)$, we can compute the running time:

$$t = \frac{\pi}{2\sqrt{k!} \epsilon^k} = \frac{\pi n^{k/2}}{2\sqrt{k!}} \approx \frac{\pi\sqrt{N}}{2}$$

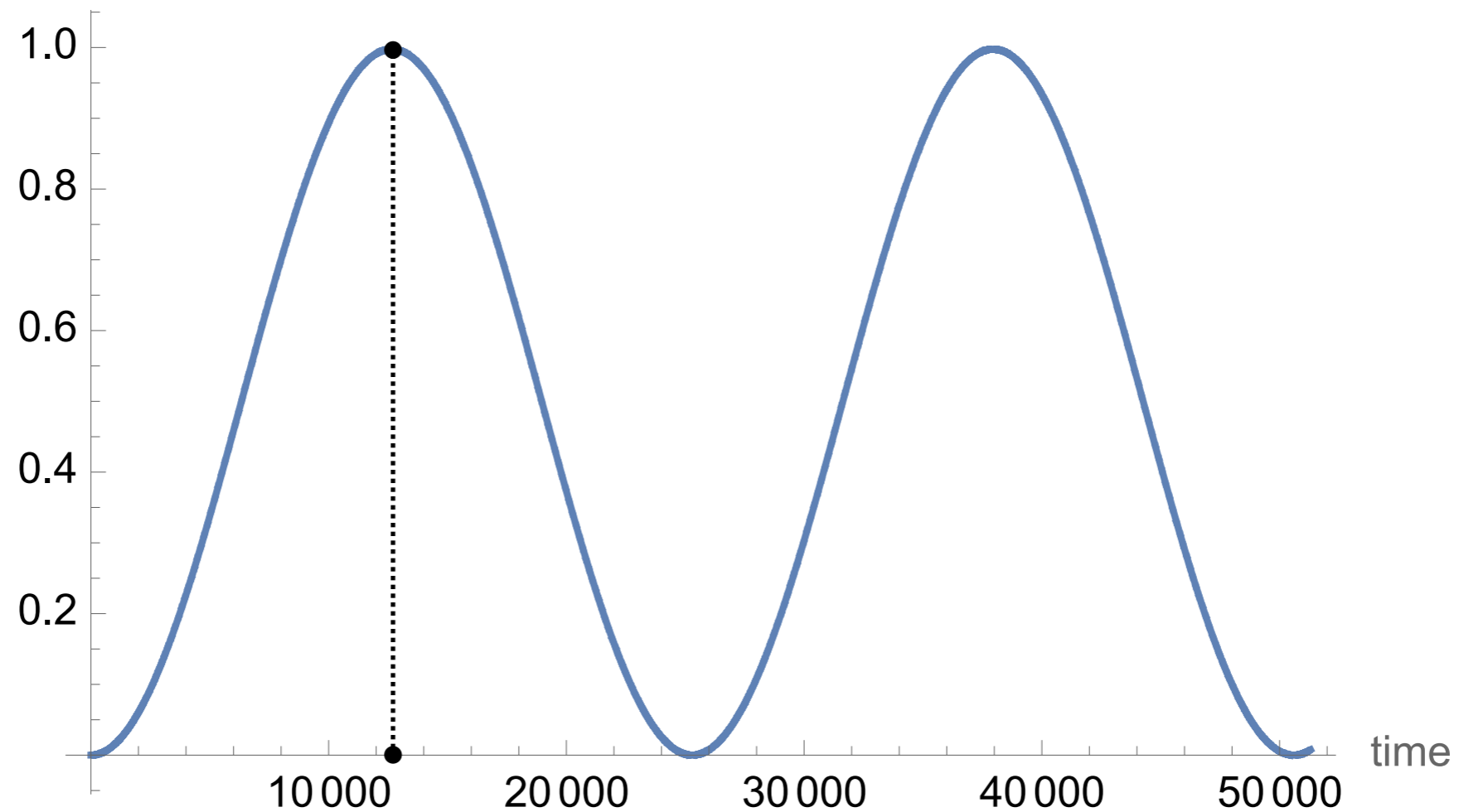
$N = \binom{n}{k}$

$\epsilon = 1/\sqrt{n}$

Example ($k = 4, n = 200$).

● $t = \frac{\pi n^{k/2}}{2\sqrt{k!}} \approx 12,825.5$

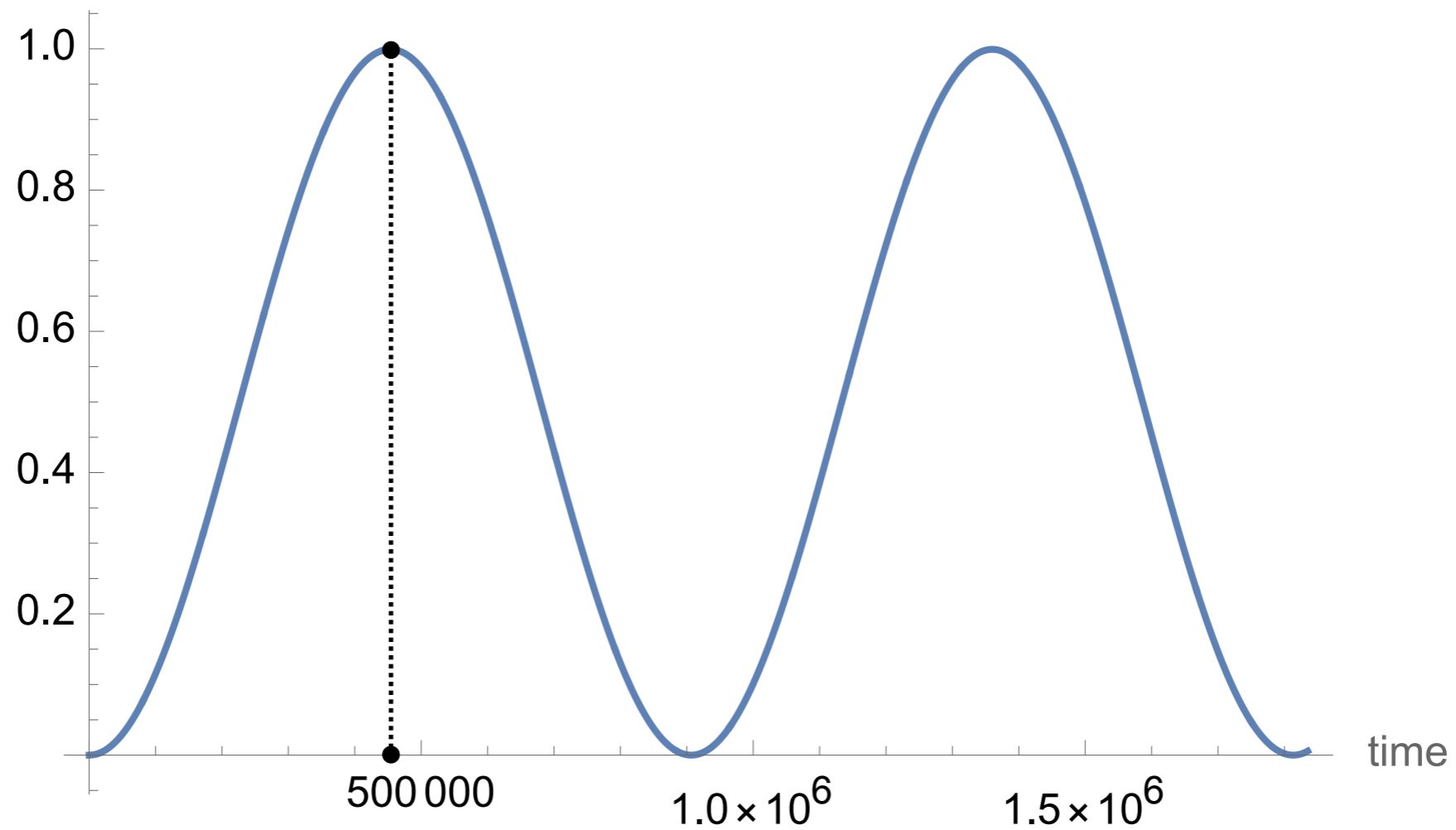
success probability



Example ($k = 5, n = 400$).

● $t = \frac{\pi n^{k/2}}{2\sqrt{k!}} \approx 458,859$

success probability



$$H = -\gamma A - |w\rangle\langle w|$$

$$\bullet \gamma = \frac{\epsilon^2}{\eta} = \epsilon^2 \sum_{\ell=1}^k \frac{p_{\ell}(\epsilon)^2}{r_0(\epsilon) - r_{\ell}(\epsilon)}$$

$$\frac{\epsilon^2}{3} + \frac{7\epsilon^4}{6} + O(\epsilon^6)$$

$$k = 3 : \frac{\epsilon^2(1 - 3\epsilon^2)(2 + \epsilon^2 + 16\epsilon^4 - 52\epsilon^6 + 24\epsilon^8)}{6(1 - \epsilon^2)^2(1 - 2\epsilon^2)^2}$$

$$k = 4 : \frac{\epsilon^2(1 - 4\epsilon^2)(3 - 11\epsilon^2 + 33\epsilon^4 + 47\epsilon^6 - 660\epsilon^8 + 1116\epsilon^{10} - 432\epsilon^{12})}{12(1 - \epsilon^2)^2(1 - 2\epsilon^2)^2(1 - 3\epsilon^2)^2}$$

$$k = 5 : \frac{\epsilon^2(1 - 5\epsilon^2)(12 - 117\epsilon^2 + 532\epsilon^4 - 1107\epsilon^6 + 2508\epsilon^8 - 22588\epsilon^{10} + 80448\epsilon^{12} - 99648\epsilon^{14} + 34560\epsilon^{16})}{60(1 - \epsilon^2)^2(1 - 2\epsilon^2)^2(1 - 3\epsilon^2)^2(1 - 4\epsilon^2)^2}$$

- In the notation of Bannai–Ito, describing γ above amounts to describing

$$\sum_{\ell=1}^d \frac{m_{\ell}}{\theta_0 - \theta_{\ell}}$$

k multiplicity

Future work

- other families of DRGs, or more general graphs
- discrete-time case (see Xue–Ruan–Liu (2019) for $J(n,3)$)
- More than one marked vertex