Quantum sampling in Markov chains

DANTE BENCIVENGA, XINING CHEN, PETER HØYER

DEPARTMENT OF COMPUTER SCIENCE
UNIVERSITY OF CALGARY
AB, CANADA

Main Results

- First quantum algorithm with a quadratic speed-up for sampling from any probability distribution over states of a Markov chain
- Generalizes controlled quantum walk framework [DH17]
- Emulates a generalized version of the quantum interpolated walk [KMOR16]

DH17: Dohotaru and Høyer 2017
KMOR16: Krovi, Magniez, Ozols, Roland 2016

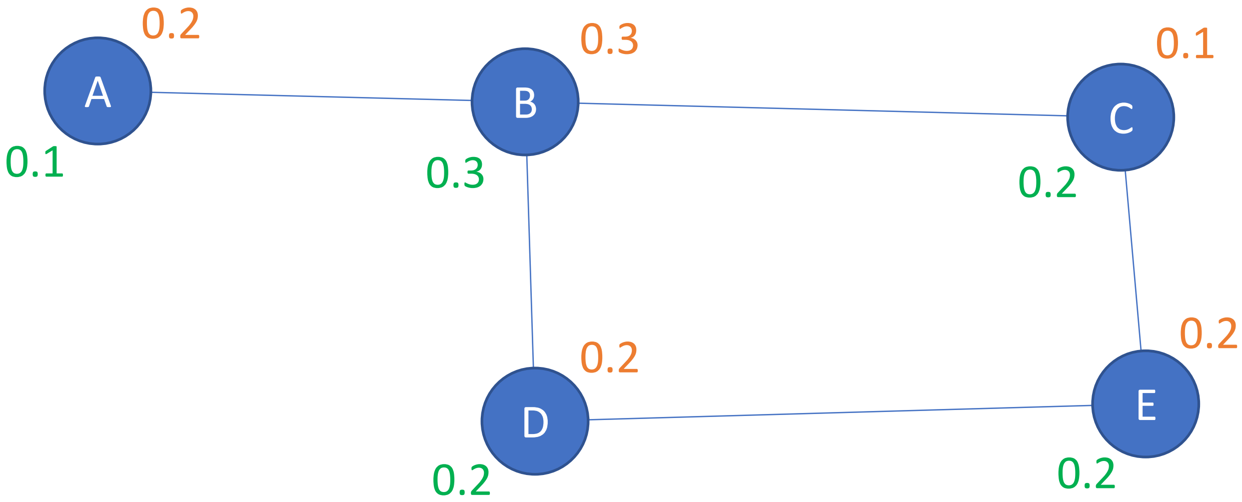
Classical Sampling Problem

Given:

- Reversible random walk represented by its transition matrix P
- A sample of its unique stationary distribution $\vec{\pi}$
- A desired target distribution $\vec{\tau}$

Goal:

- Generate a sample according to $\vec{\tau}$

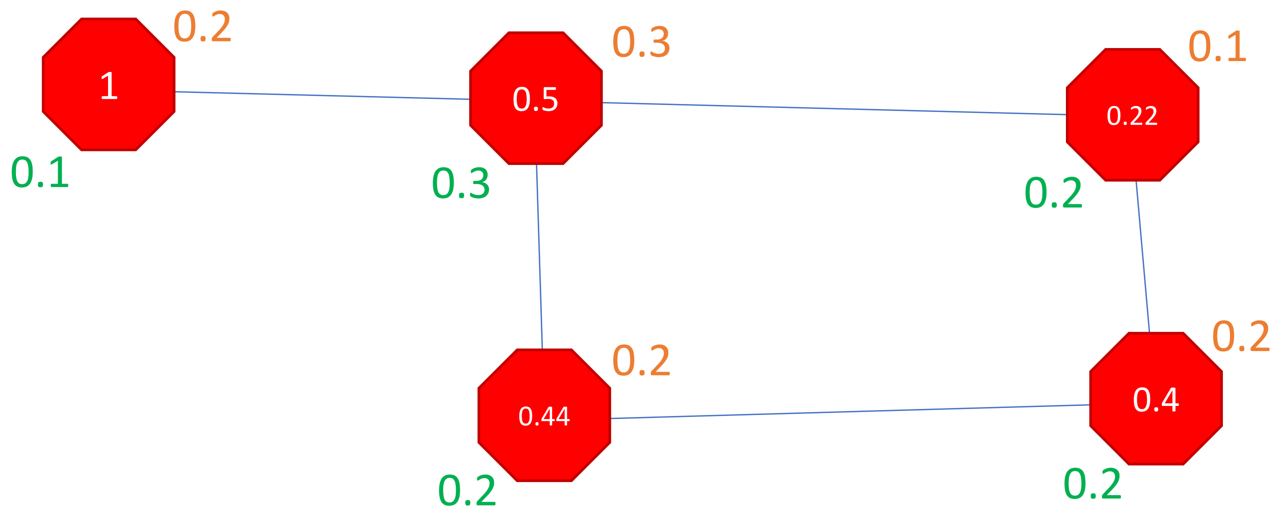


$$P = \begin{pmatrix} 0 & 1/3 & 0 & 0 & 0 \\ 1 & 0 & 1/2 & 1/2 & 0 \\ 0 & 1/3 & 0 & 0 & 1/2 \\ 0 & 1/3 & 0 & 0 & 1/2 \\ 0 & 0 & 1/2 & 1/2 & 0 \end{pmatrix}$$

Stopping Rules

Definition: A *stopping rule* consists of a function which maps finite paths on the graph to a stopping probability.

- Examples:
  - Stopping after 5 steps
  - Stopping upon hitting a set of marked vertices
  - Stopping with a specified probability for each vertex



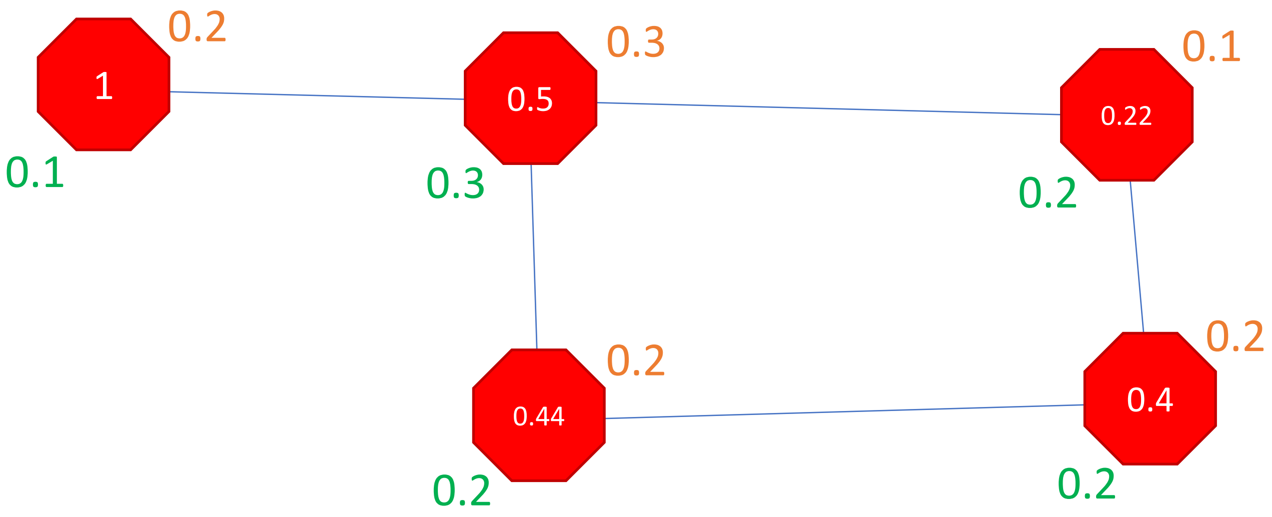
Pitman 1977
Lovász and Winkler 1995

Access Time

- An optimal stopping rule generates $\vec{\tau}$ from $\vec{\pi}$ using P in the smallest expected number of steps

Definition: The *access time* of a walk P from $\vec{\pi} \rightarrow \vec{\tau}$ equals the cost of this optimal stopping rule, and we denote it as

$$\mathrm{HT}(\mathrm{P}, \vec{\pi} \rightarrow \vec{\tau})$$



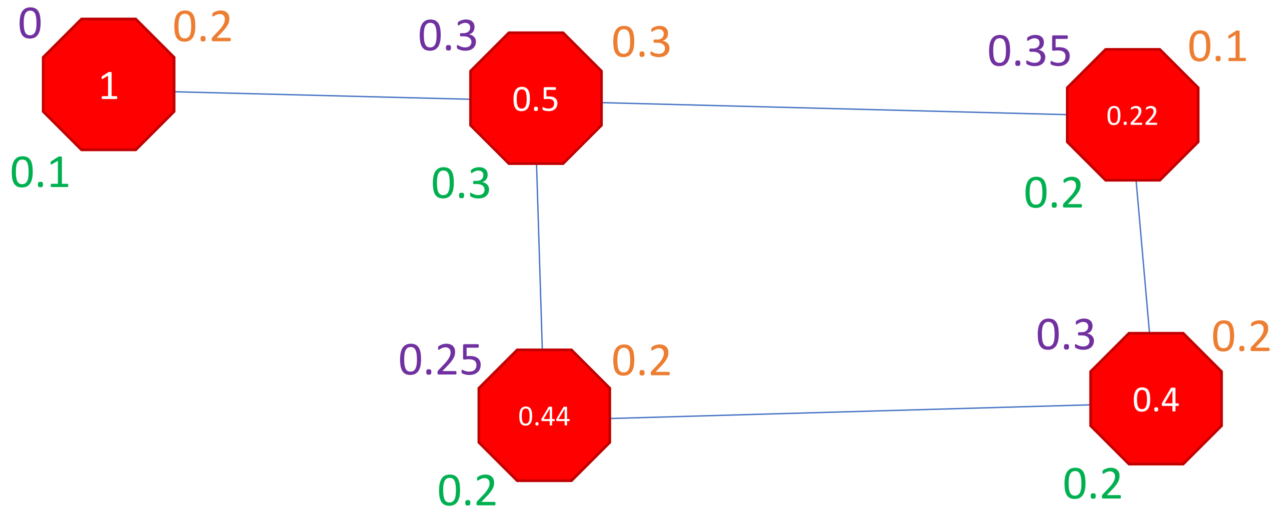
Pitman 1977
Lovász and Winkler 1995

Exit Frequencies

Definition: The *exit frequencies* of a walk P starting in $\vec{\pi}$ and ending in $\vec{\tau}$, denoted as the vector $\vec{x}$, give the expected number of times the random walk exits each vertex during execution of the stopping rule.

$$\|\vec{x}\|_1 = \mathrm{HT}(\mathrm{P}, \vec{\pi} \to \vec{\tau})$$

$$\vec{\tau} = \vec{\pi} + \mathrm{P}\vec{x} - \vec{x}$$



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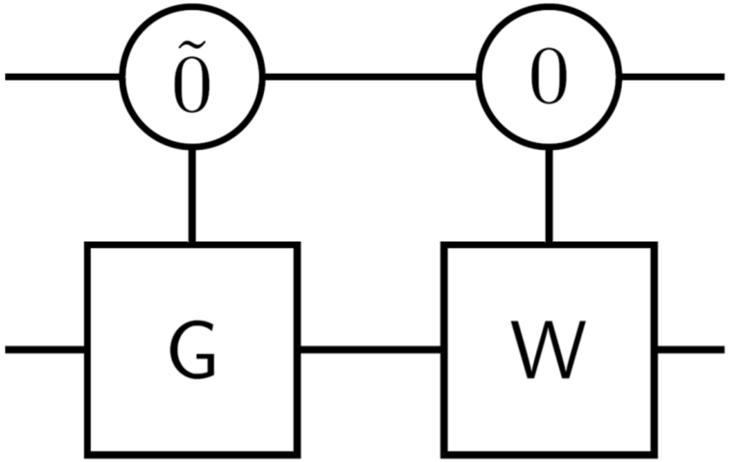
Controlled Quantum Walk

$$|\tilde{0}\rangle = \cos\theta\,|0\rangle + \sin\theta\,|1\rangle$$



$$= \mathrm{U}(\theta)$$

- Quantum walks [Amb04, Sze04] consist of G which reflects marked vertices and W which reflects superpositions of outgoing edges
- The controlled quantum walk [DH17] finds a marked vertex
  - Parametrized by angle θ
  - Finds a marked vertex quadratically faster than the extended hitting time
  - Vertex sampled according to $\vec{\pi}_{\mathcal{M}}$

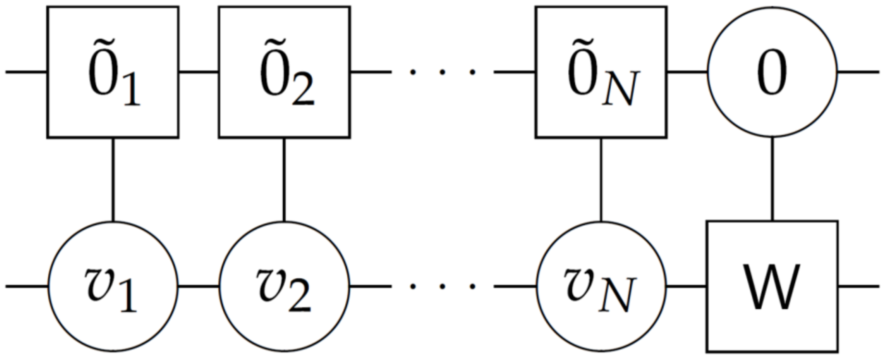
Amb04: Ambainis 2004

Sze04: Szegedy 2004

DH17: Dohotaru and Høyer 2017

Adding Multiple Angles

$U(\vec{\theta}) =$



$$|\tilde{0}_i\rangle = \cos\theta_i\,|0\rangle + \sin\theta_i\,|1\rangle$$

$$\cos\theta_i = \sqrt{\frac{\tau_i}{\pi_i + \tau_i}} = \left(\frac{\pi_i}{\tau_i} + 1\right)^{-1/2}$$

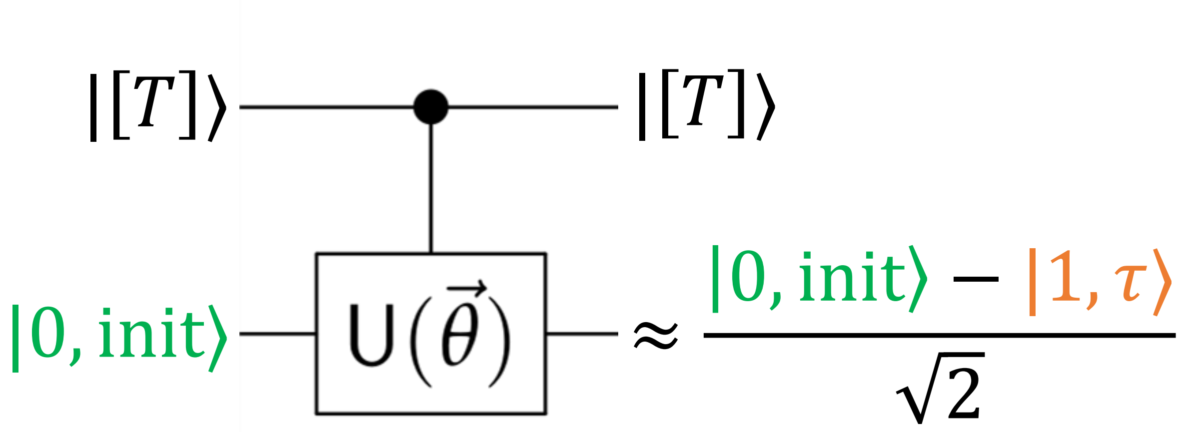
- Only need local computations for θ_i
- Sample from any distribution $\vec{\tau}$ over the vertices

Algorithm to generate target state

$$|\text{init}\rangle = \sum_i \sqrt{\pi_i}|v_i\rangle$$

$$|\tau\rangle = \sum_i \sqrt{\tau_i}|v_i\rangle$$

$$|[T]\rangle = \frac{1}{\sqrt{T}}\sum_{i=0}^{T-1}|i\rangle$$



1. Compute angles $0 \le \theta_i \le \pi/2$ such that $\cos\theta_i = \sqrt{\frac{\tau_i}{\pi_i+\tau_i}}$
2. Prepare the state $|[T]\rangle|0, \text{init}\rangle$
3. Apply $\sum_{i=0}^{T-1} |i\rangle\langle i| \otimes \text{U}(\vec{\theta})^i$
4. Apply the measurement $\{\Pi_0, 1 - \Pi_0\}$ where $\Pi_0 = |[T]\rangle\langle[T]| \otimes |1\rangle\langle 1| \otimes 1$
5. If we measure Π_0, output "success" and we have an approximation of the state $|\tau\rangle$ in the third register. Otherwise, output "failure"

Main Theorems

Theorem 1: The complexity of phase estimation to run $\mathrm{U}(\vec{\theta})$ starting from $|0,\mathrm{init}\rangle$, which we measure by the quantum hitting time, equals

$$\mathrm{QHT}\big(\mathrm{U}(\vec{\theta}), |0,\mathrm{init}\rangle\big) = \sqrt{\frac{1}{2}\left(\mathrm{HT}(\mathrm{P}, \vec{\pi} \to \vec{\tau}) - \left\|\frac{\vec{\tau}}{\vec{\pi}} \cdot \vec{x}\right\|_1\right)}$$

Theorem 2: The complexity of phase estimation to run $\mathrm{U}(\vec{\theta})$ starting from $|0,\overline{\mathrm{init}}\rangle$, which corresponds to $\vec{\pi}$ limited to a set of unmarked vertices and renormalized (denoted $\vec{\bar{\pi}}$) and where $\vec{\tau}$ has support only on marked vertices, equals

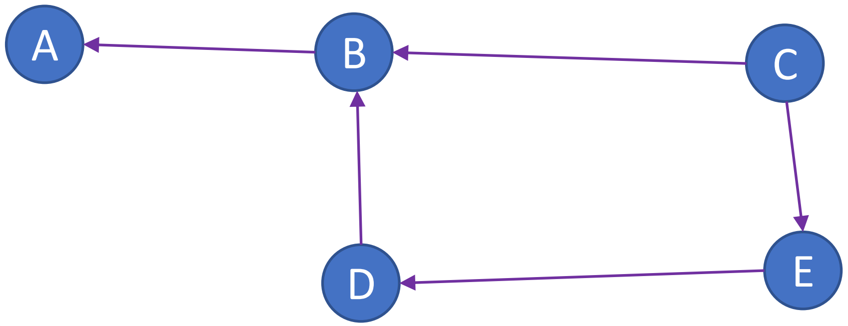
$$\mathrm{QHT}\big(\mathrm{U}(\vec{\theta}), |0,\overline{\mathrm{init}}\rangle\big) = \sqrt{\frac{1}{2}\left(\mathrm{HT}\big(\mathrm{P}, \vec{\bar{\pi}} \to \vec{\tilde{\tau}}\big) - \delta\right)}$$

where

$$\vec{\tilde{\tau}} = \frac{1}{1-\varepsilon}\big((1-2\varepsilon)\vec{\tau} + \vec{\pi}_{\mathcal{M}}\big), \qquad \delta = (1-\varepsilon)\left\|\frac{\vec{\tilde{\tau}}}{\vec{\bar{\pi}}} \cdot \vec{\tilde{x}}\right\|_1 + \left\|\vec{\tilde{x}}_{\mathcal{M}}\right\|_1 + 1, \qquad \varepsilon = \|\vec{\pi}_{\mathcal{M}}\|_1$$

Quantum Analogue of Exit Frequencies

- The key insight to our proof used a quantum analogue of the classical exit frequencies



Isometry $\mathrm{T} = \sum_i |v_i\rangle\langle i| = \sum_i \left(\sum_j \sqrt{P_{j\leftarrow i}}|i,j\rangle\right)\langle i|$

- Embeds from vertex to edge space

Swap $\mathrm{S} = \sum_{i,j} |j,i\rangle\langle i,j|$

- Swaps directions of edges

$$|x\rangle = (\mathrm{I} - \mathrm{S})\,\mathrm{T}\,\frac{\vec{x}}{\sqrt{\vec{\pi}}}$$

Projects to anti-symmetric subspace

Embeds from vertex space to edge space

Entry-wise division changes basis to discriminant matrix

Quantum Rejection Sampling

Problem Statement: Given access to sample of a distribution $\vec{\pi}$, produce a sample from a distribution $\vec{\tau}$ over the same space

- Optimal classical algorithm: rejection sampling [vN51]
  - Involves a global computation to find a parameter $\gamma = \min_i \frac{\pi_i}{\tau_i}$
- Embedding rejection sampling into amplitude amplification [ORR13] gives a quantum algorithm with a quadratic speed-up
  - Uses the parameter γ
- Our algorithm also samples quadratically faster than rejection sampling, without any global computation

vN51: von Neumann 1951

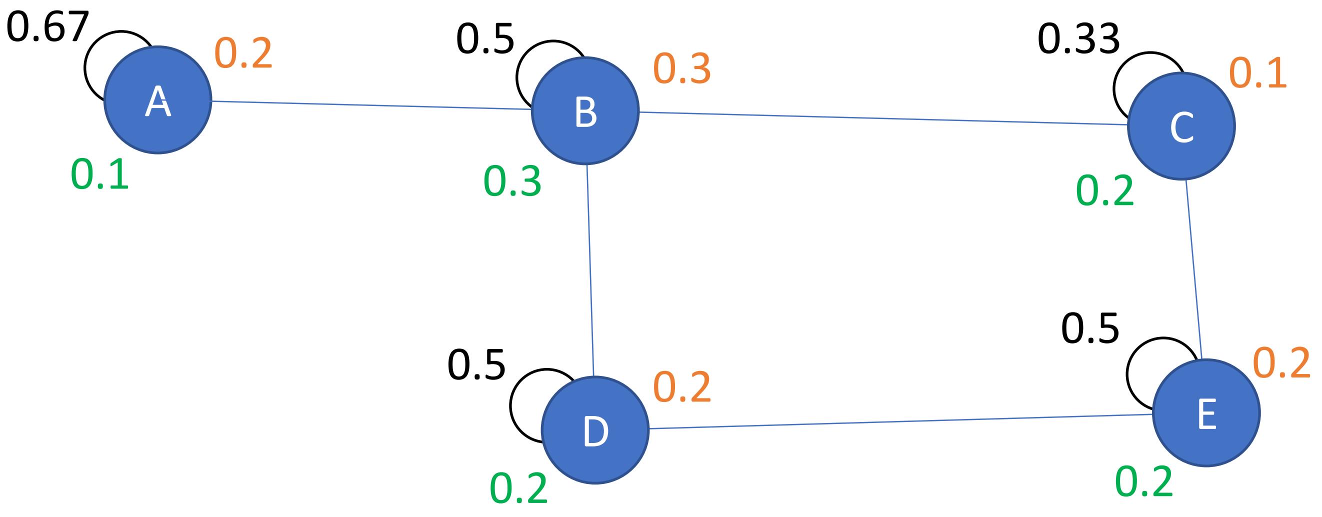
ORR13: Ozols, Roetteler, Roland 2013

Emulation of Quantum Interpolated Walk

- The [DH17] controlled quantum walk can emulate the quantum interpolated walk [KMOR16]
  - [KMOR16] use a single interpolation parameter *s*
- Our walk emulates a generalized quantum interpolated walk
  - Uses different self-loop s_i for each vertex

$$s_i = \frac{\tau_i}{\pi_i + \tau_i} = \cos^2 \theta_i$$

$$\vec{\pi}_s = \frac{\vec{\pi} + \vec{\tau}}{2}$$



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Comparison Table

Algorithm	Reference	Highlights	Complexity
Rejection sampling	vN51	Classical sampling, global pre-computation	γ^{-1}
Stopping rules	Pit77, LW95	Classical sampling from walk, global pre-computation	$\mathrm{HT}(\mathrm{P}, \vec{\pi} \rightarrow \vec{\tau})$
Quantum rejection sampling	ORR13	Quantum sampling, global pre-computation	$\Theta\left(\sqrt{\gamma^{-1}}\right)$
Quantum interpolated walk	KMOR16*	Quantum finding	$\mathrm{O}\left(\sqrt{\mathrm{HT}\left(\mathrm{P}, \vec{\vec{\pi}} \rightarrow \frac{1}{\varepsilon} \vec{\pi}_{\mathcal{M}}\right)}\right)$
Controlled quantum walk	DH17	Quantum finding	$\mathrm{O}\left(\sqrt{\mathrm{HT}\left(\mathrm{P}, \vec{\vec{\pi}} \rightarrow \frac{1}{\varepsilon} \vec{\pi}_{\mathcal{M}}\right)}\right)$
Generalized controlled quantum walk	This work	Quantum sampling from walk, local pre-computation	$\mathrm{O}\left(\sqrt{\mathrm{HT}(\mathrm{P}, \vec{\pi} \rightarrow \vec{\tau})}\right)$

* Newly generalized

Summary

- First quantum algorithm that gives a quadratic speed-up over the classical access time to sample from a desired distribution over states of a Markov chain after starting in the stationary distribution
  - Generalizes controlled quantum walks using multiple angles
- Quantum analogue of rejection sampling without global computations
- Emulation of generalized quantum interpolated walks

Thank you!