

Quantum Diffusion Kernels, Symmetries, Groups

Jue Xu*

June 11, 2022

Abstract

We discuss the quantum analogue of diffusion kernels on graphs. prove the quantum speedup in terms of groups and symmetries.

Contents

1	Introduction	1
1.1	Preliminary and Notations	2
2	Diffusion Kernels and Continuous-Time Quantum Random Walk	2
2.1	Classical diffusion kernels on graphs	2
2.2	Continuous-time quantum random walk	2
2.3	Relation and examples	3
2.4	Quantum Machine Learning	3
3	Provable Quantum Speedups	3
3.1	Symmetries, graph properties, and quantum speedups	3
3.2	Group, invariance, symmetries, physical systems	3
4	Experiments	3
4.1	Datasets	3
5	Discussion and Conclusion	3
	References	3
A	Machine Learning, Group Theory, and Lagrangian	4
A.1	Kernel trick in machine learning	4
A.2	Group theory and symmetries	4
A.3	Lagrangian formalism	4

1 Introduction

group theoretical methods in machine learning by Kondor [Kon08]. diffusion kernel on graphs [KL02]

Many insightful and powerful models, like adiabatic quantum computation [Far+00], quantum random walks [Chi04]

*juexu@cs.umd.edu

1.1 Preliminary and Notations

2 Diffusion Kernels and Continuous-Time Quantum Random Walk

2.1 Classical diffusion kernels on graphs

[KL02] a kernel function (mapping) $\mathcal{K} : \Omega \times \Omega \mapsto \mathbb{R}$, a mapping $\phi : \Omega \mapsto \mathcal{H}_K$

$$\mathcal{K}(x, x') = \langle \phi(x), \phi(x') \rangle \quad (1)$$

with Euclidean space $\Omega = \mathbb{R}^m$

Definition 1 (Kernel). A function \mathcal{K} is a valid kernel (in machine learning) if and only if the matrix $\mathcal{K}(x, x')$ is symmetric and positive semi-definite.

Definition 2 (Graph Laplacian). Given a graph $G = (V, E)$, its *adjacency matrix* \hat{A} is defined as

$$\hat{A}(v, v') := \begin{cases} 1, & (v, v') \in E \\ 0, & \text{otherwise} \end{cases} \quad (2)$$

With \hat{A} at hand, the graph Laplacian is defined as

$$\hat{\mathcal{L}} := \hat{A} - \hat{D} \quad (3)$$

where $\hat{D}_{vv} := \deg(v)$ is its diagonal degree of (vertex v) matrix. discrete version of (continuous) Laplacian operator

Lemma 1. *exponential of i.e., $e^{\beta \hat{H}}$ is a valid kernel*

The continuous-time random walk on G is defined as the **solution of the differential equation**

$$\frac{d}{dt} p_j(t) = \sum_{k \in V} \hat{\mathcal{L}}_{jk} p_k(t), \quad (4)$$

where $p_j(t)$ denotes the probability associated with vertex j at time t and $\hat{\mathcal{L}}$ is [Graph Laplacian](#).

Since the columns of L sum to 0

$$\frac{d}{dt} \sum_{j \in V} p_j(t) = \sum_{j, k \in V} \hat{\mathcal{L}}_{jk} p_k(t) = 0 \quad (5)$$

which shows that an initially normalized distribution remains normalized: the evolution of the continuous-time random walk for any time t is a *stochastic process. random walk, heat equation*

2.2 Continuous-time quantum random walk

The continuous-time quantum random walk [CFG02] is the quantum analogue of classical diffusion (continuous-time random walk). It is a direct observation that Eq. (4) is very similar to the time-dependent (evolution) schrodinger equation with a Hamiltonian \hat{H}

$$i\hbar \frac{d}{dt} |\psi\rangle = \hat{H} |\psi\rangle \quad (6)$$

except that it lacks the factor of $i\hbar$.

2.3 Relation and examples

2.3.1 Ring (closed line)

kernel ? quantum propagation

$$\langle z_F | e^{-it\hat{H}_0} | z_I \rangle = \sum_{p=1}^N e^{-it2\cos(\frac{2\pi}{N}p) + i\frac{2\pi}{N}p(z_I - z_F)} \quad (7)$$

$$\approx e^{2it}(-i)^d J_d(2t) \quad (8)$$

Remark 1. The random walk on this graph starting from the origin (in either continuous or discrete time) typically moves a distance proportional to \sqrt{t} in time t . In contrast, the quantum random walk evolves as a wave packet with speed 2.

2.3.2 Hyercube

2.4 Quantum Machine Learning

3 Provable Quantum Speedups

Theorem 1 ([Chi+03]). *There exists exponential separation with respect to query complexity in the adjacency matrix model*

[Zhe+22]

3.1 Symmetries, graph properties, and quantum speedups

symmetric functions rule out exponential speedup [Ben+20]

3.2 Group, invariance, symmetries, physical systems

group theory, [Kon08] symmetries in physics [Bog+20]

4 Experiments

4.1 Datasets

5 Discussion and Conclusion

References

- [Ben+20] Shalev Ben-David et al. [Symmetries, Graph Properties, and Quantum Speedups](#). *2020 IEEE 61st Annu. Symp. Found. Comput. Sci. FOCS* (Nov. 2020), pp. 649–660. arXiv: [2006.12760](#) (cit. on p. 3).
- [Bog+20] Alexander Bogatskiy et al. [Lorentz Group Equivariant Neural Network for Particle Physics](#). Proceedings of the 37th International Conference on Machine Learning. International Conference on Machine Learning. PMLR, Nov. 21, 2020, pp. 992–1002 (cit. on p. 3).
- [CFG02] Andrew M. Childs, Edward Farhi, and Sam Gutmann. [An Example of the Difference between Quantum and Classical Random Walks](#). *Quantum Inf. Process.* 1.1/2 (2002), pp. 35–43. arXiv: [quant-ph/0103020](#) (cit. on p. 2).

- [Chi+03] Andrew M. Childs et al. [Exponential Algorithmic Speedup by Quantum Walk](#). *Proc. Thirty-Fifth ACM Symp. Theory Comput. - STOC 03* (2003), p. 59. arXiv: [quant-ph/0209131](#) (cit. on p. 3).
- [Chi04] Andrew MacGregor Childs. “Quantum Information Processing in Continuous Time”. Thesis. Massachusetts Institute of Technology, 2004 (cit. on p. 1).
- [Far+00] Edward Farhi et al. “Quantum Computation by Adiabatic Evolution”. Jan. 28, 2000. arXiv: [quant-ph/0001106](#) (cit. on p. 1).
- [KL02] Risi Imre Kondor and John Lafferty. [Diffusion Kernels on Graphs and Other Discrete Structures](#) (2002), p. 8 (cit. on pp. 1, 2).
- [Kon08] Risi Kondor. “Group Theoretical Methods in Machine Learning”. Thesis. Columbia University, 2008 (cit. on pp. 1, 3).
- [Xu21] Jue Xu. “On Lagrangian Formalism of Quantum Computation”. Dec. 7, 2021. arXiv: [2112.04892 \[quant-ph\]](#) (cit. on p. 4).
- [Zhe+22] Han Zheng et al. “Speeding up Learning Quantum States through Group Equivariant Convolutional Quantum Ansatz”. Jan. 20, 2022. arXiv: [2112.07611 \[math-ph, physics:quant-ph, stat\]](#) (cit. on p. 3).

A Machine Learning, Group Theory, and Lagrangian

A.1 Kernel trick in machine learning

A.1.1 SVM and Kernel

A.1.2 Quantum machine learning

A.2 Group theory and symmetries

A.3 Lagrangian formalism

[Xu21]