Quantum Diffusion Kernels, Symmetries, Groups

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Abstract

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

Contents

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]

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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 $\phi : \Omega \mapsto \mathcal{H}_K$

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

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

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

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

$$\hat{\mathfrak{L}} := \hat{A} - \hat{D} \tag{3}$$

where $\hat{D}_{vv} := \mathsf{deg}(v)$ 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**

$$\frac{\mathrm{d}}{\mathrm{d}t} p_j(t) = \sum_{k \in V} \hat{\mathfrak{L}}_{jk}\ p_k(t), \tag{4}$$

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

Since the columns of L sum to 0

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

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 $\hat{H}$

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} |\psi\rangle = \hat{H} |\psi\rangle \tag{6}$$

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

2.3 Relation and examples

2.3.1 Ring (closed line)

kernel ? quantum propagation

$$\langle z_F | e^{-\mathrm{i}t\hat{H}_0} | z_I \rangle = \sum_{p=1}^{N} e^{-\mathrm{i}t 2\cos\left(\frac{2\pi}{N}p\right) + \mathrm{i}\frac{2\pi}{N}p(z_I - z_F)} \tag{7}$$

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

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

[Gli+21] group theory, [Kon08]; symmetries in physics [Bog+20]; equivariant CNN [Zhe+22]

4 Experiments

4.1 Datasets

5 Discussion and Conclusion

References

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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]