Mauscript: Quantum Diffusion Kernels on Graphs, Symmetries, Groups, and Speedups

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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

1.2 SVM and Kernel trick

Hilbert space

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 *(feature) mapping* $\phi : \Omega \mapsto \mathcal{H}_{\mathcal{K}}$

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

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

Definition 1 (Feature map)**.** *feature map*; *feature space*;

Definition 2 (Kernel function)**.** 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 3 (Adjacency matrix)**.** Given a (undirected, unweighted) graph $G = (V, E)$, its *adjacency matrix* $\hat{A}$ is defined as

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

where the matrix entry is 1 if the two vertices (labels of the column and the row) are connected by an edge, otherwise 0.

Definition 4 (Graph Laplacian)**.** With the adjacency matrix $\hat{A}$, 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.

Remark 1. Graph Laplacian $\hat{\mathfrak{L}}$ is the discrete version of (continuous) Laplacian operator ∇^2.

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

2.1.1 Diffusion, heat equation, random walk,

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). By a direct observation, Eq. (4) is very similar to the time-dependent (evolution) schrodinger equation governed by a Hamiltonian operator $\hat{H}$

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

except that the factor of $i\hbar$.

Definition 5 (Quantum propagator, kernel, transition)**.**

2.3 Relation and examples

2.3.1 Ring (closed line)

classical kernel

$$\mathcal{K}() \tag{7}$$

quantum propagation (kernel)

$$\begin{aligned} \langle z_F|e^{-\mathrm{i}t\hat{H}_0}|z_I\rangle &= \sum_{p=1}^{N} e^{-\mathrm{i}t2\cos\left(\frac{2\pi}{N}p\right)+\mathrm{i}\frac{2\pi}{N}p(z_I-z_F)} && (8) \\ &\approx e^{2\mathrm{i}t}(-\mathrm{i})^d J_d(2t) && (9) \end{aligned}$$

Remark 2. 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 Tree

2.3.3 Hyercube

3 Quantum Speedups via QKE

3.1 Previous works: Quantum Kernel Estimation

quantum kernel estimation [SK19] [Hav+19]

3.1.1 Explicit method

variational quantum circuit

3.1.2 Implicit method

quantum feature map. quantum propagation, kernel in the path-integral formalism.

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

[Zhe+22]
[LAT21]

3.2 Provable: Symmetries, graph properties, and quantum speedups

symmetric functions rule out exponential speedup [Ben+20]

3.2.1 Permutation, symmetry, and speedup

3.3 Heuristic: Group, invariance, symmetries, physical systems

3.3.1 Group, symmetries in physics

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

3.3.2 Group theory and machine learning

[KL02]

4 Experiment

4.1 Datasets and benchmark

5 Discussion and Conclusion

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A Machine Learning, Group Theory, and Lagrangian

A.1 Machine learning

A.2 Group theory and symmetries

A.3 Lagrangian formalism

[Xu21]