

Manuscript: Quantum Graph Kernels, Symmetries, and Speedups

Jue Xu*

June 25, 2022

Abstract

We discuss the quantum analogue of graph kernels based on quantum random walks. Moreover, we prove the quantum advantages in machine learning from structures (symmetries) of problems.

Contents

1	Introduction	2
1.1	Preliminary and Notations	2
1.2	Terminology: SVM and Kernel trick	2
2	Graph Kernels and Quantum Random Walks	4
2.1	Diffusion kernel of a pair of vertices	4
2.2	Continuous-time quantum random walk	5
2.3	Graph kernels of a pair of graphs	5
2.4	Discrete-time quantum random walk	6
2.5	Relations, difference, and examples	6
3	Quantum Advantages and Speedups	7
3.1	Related works	7
3.2	Provable quantum speedups	9
3.3	Heuristic quantum advantages for learning physics systems	10
4	Experiments	11
4.1	Datasets and benchmark	11
5	Discussion and Conclusion	11
	References	11
A	Machine Learning and Group Theory	14
A.1	Machine learning	14
A.2	Group theory and symmetries	14
B	Symmetries in physics	14
B.1	Lagrangian formalism	14
B.2	Symmetries with Lagrangian	15

*juexu@cs.umd.edu

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]

1.1 Preliminary and Notations

a datum $\mathbf{x} := (x_1, x_2, \dots, x_d) \in \mathbb{R}^d$ is a vector where d is the number of *features*; dataset $\{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^m$ where the *label* $y \in \Sigma$ with some (discrete set) alphabet/category Σ . for binary classification, we have $\Sigma = \{-1, 1\}$, Ω ; computational basis $|z\rangle$ with $z \in \{1, 2, \dots, 2^n - 1, 2^n\}$ where n is the number of qubits, the binary representation $|\mathbf{x}\rangle = |x_1, x_2, \dots, x_n\rangle, x_j \in \{0, 1\}$. $|0\rangle^n, |\pm\rangle$. graph G , group \mathbb{G}

Definition 1 (inner product). *inner product* is a map

$$\langle \cdot, \cdot \rangle : V \times V \rightarrow \mathbb{F} \quad (1)$$

that $\forall \mathbf{x}, \mathbf{y}, \mathbf{z} \in V, a, b \in \mathbb{F}$ satisfies the following three properties

- **Conjugate symmetry:** $\langle \mathbf{x}, \mathbf{y} \rangle = \overline{\langle \mathbf{y}, \mathbf{x} \rangle}$
- **Linearity** in the first argument: $\langle a\mathbf{x} + b\mathbf{y}, \mathbf{z} \rangle = a\langle \mathbf{x}, \mathbf{z} \rangle + b\langle \mathbf{y}, \mathbf{z} \rangle$
- **Positive-definiteness:** $\langle \mathbf{x}, \mathbf{x} \rangle \geq 0$ with equality only when $\mathbf{x} = \mathbf{0}$.

In classical machine learning, we assume the base field is \mathbb{R} . The inner product gives rise to the *norm* $\|\mathbf{x}\| = \sqrt{\langle \mathbf{x}, \mathbf{x} \rangle}$, and a distance metric $d(\mathbf{x}, \mathbf{x}') = \|\mathbf{x} - \mathbf{x}'\|$.

Euclidean vector space \mathbb{R}^n with dot product is an inner product space,. While in the context of quantum mechanics, the inner product is replaced by Dirac notation $\langle \mathbf{x} | \mathbf{x}' \rangle$ with complex field \mathbb{C} . inner product can be understood as a ‘similarity’ metric between two vectors ?

Definition 2 (Hilbert space). A *Hilbert space* is a vector space \mathcal{H} induced by an *inner product* such that the inner product yields a complete metric space?.

1.2 Terminology: SVM and Kernel trick

supervised learning

1.2.1 Support Vector Machine (SVM)

training stage, classification stage. exponentially large space; *hyperplane* (\mathbf{w}, b) parametrized by a normal vector $\mathbf{w} \in \mathbb{R}^n$ and a *bias* term $b \in \mathbb{R}$. in the (high-dimensional) *feature space*. maximize the *margin* [ref]

$$f^* = \arg \max_f L(y, \tilde{y} = f(x)) + ||| \quad (2)$$

where the loss function L , slackness. called *support vector*.

1.2.2 Kernel trick (method)

kernel trick: feature map the input data to higher dimension such that the data are linearly separatable in this feature space. only depend on the inner product to avoid the expensive (exponential) calculation. [ref]

Definition 3 (Kernel function). a *kernel function* (mapping) $\mathcal{K} : \Omega \times \Omega \rightarrow \mathbb{R}$, is defined as [inner product](#)

$$\mathcal{K}(\mathbf{x}, \mathbf{x}') = \langle \Phi(\mathbf{x}), \Phi(\mathbf{x}') \rangle_{\mathcal{H}} \quad (3)$$

w.r.t a [feature map](#) $\Phi(\mathbf{x})$.

Definition 4 (Positive semi-definite). *positive semi-definite* (PSD/p.s.d).

$$\sum_{i=1}^m \sum_{j=1}^m \alpha_i \alpha_j \mathcal{K}(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) \geq 0 \quad (4)$$

Remark 1. A function \mathcal{K} (k) is a valid kernel if and only if? the (Gram) matrix $\mathcal{K}(x, x')$ is symmetric and PSD.

Definition 5 (feature map). The *feature map* is a function (mapping)

$$\Phi(\mathbf{x}) : \mathcal{X} \rightarrow \mathcal{H}_{\mathcal{K}} \quad (5)$$

from a low dimensional space non-linearly in to a high dimensional [Hilbert space](#) \mathcal{H} which is commonly referred to as the *feature space*. For example, $\Phi(\mathbf{x}) : \mathbb{R}^d \rightarrow \mathbb{R}^n$ with $n \gg d$.

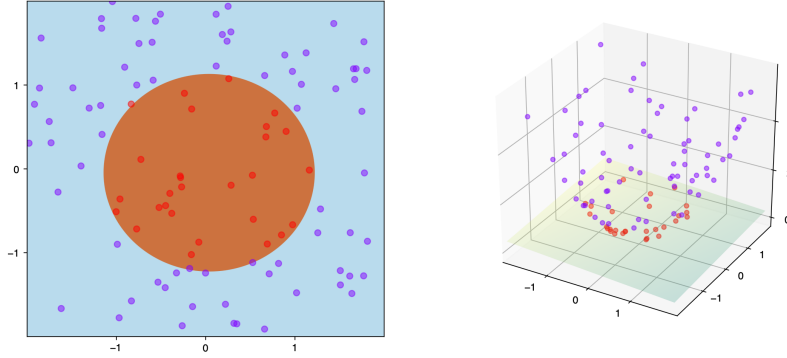


Figure 1: kernel trick idea: SVM with kernel given by $\phi(\mathbf{x} := (a, b)) = (a, b, a^2 + b^2)$ and thus $\mathcal{K}(\mathbf{x}, \mathbf{y}) = \mathbf{x} \cdot \mathbf{y} + \|\mathbf{x}\|^2 \|\mathbf{y}\|^2$. The training points are mapped from a 2-dimensional to a 3-dimensional space where a separating hyperplane can be easily found. (from Wikipedia: Kernel method)

Some common kernels:

- polynomial kernel: see Fig. 1
- *Gaussian (radial basis) kernel*:

$$\mathcal{K}(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{2\sigma^2}\right) = ? \quad (6)$$

with the feature map

graph kernels discuss in the remainder of this paper.

Definition 6 (Reproducing Kernel Hilbert Space). It is well known that any continuous, symmetric, positive definite [Kernel function](#) has corresponding Hilbert space \mathcal{H} , called the *Reproducing Kernel Hilbert Space* (RKHS),

$$f(x) = \langle f, \mathcal{K}_x \rangle \quad (7)$$

which induces a [feature map](#) satisfying Eq. (3).

Theorem 1 (Representer theorem). ?

2 Graph Kernels and Quantum Random Walks

We commence by reviewing the classical graphs kernels and quantum random walks. Largely, this development was driven by the empirical success of supervised learning of vector-valued data or image data. However, in many domains, such as chemo- and bioinformatics, social network analysis or computer vision, observations describe relations between objects or individuals and cannot be interpreted as vectors or fixed grids; instead, they are naturally represented by graphs. [KJM20] graph-structured data is to make use of graph kernels—functions which measure the similarity between graphs. **How similar are two graphs? How similar are two nodes of a graph?**

2.1 Diffusion kernel of a pair of vertices

[KL02]. generalize to regularization: We propose a family of regularization operators (equivalently, kernels) on graphs that include Diffusion Kernels as a special case, and show that this family encompasses all possible regularization operators invariant under permutations of the vertices in a particular sense. [SK03] with Euclidean space $\Omega = \mathbb{R}^m$

Definition 7 (Adjacency matrix). Given a (undirected, unweighted) graph $G(V, E)$, its *adjacency matrix* \hat{A} is defined as

$$\hat{A}_{v,v'} := \begin{cases} 1, & (v, v') \in E \\ 0, & \text{otherwise} \end{cases} \quad (8)$$

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

Definition 8 (Graph Laplacian). With the adjacency matrix \hat{A} , the graph Laplacian is obtained by

$$\hat{\mathcal{L}} := \hat{A} - \hat{D} \quad (9)$$

where $\hat{D}_{v,v} := \deg(v)$ is the diagonal degree matrix.

Analogously, the adjacency matrix and graph Laplacian of weighted graphs can be defined. Graph Laplacian $\hat{\mathcal{L}}$ is the discrete version of (continuous) Laplacian operator ∇^2 [Chu97].

Observation 1. The matrix exponential of any \hat{H} i.e., $e^{\beta\hat{H}}$, is a valid kernel (PSD). [to verify for $e^{-it\hat{H}}$]

Definition 9 (Diffusion kernel). The *diffusion kernel* of a graph w.r.t a pair of vertices (v, v') is

$$\mathcal{K}(v, v') := \left[\sum_k \frac{\beta^k}{k!} \hat{\mathcal{L}}^k \right]_{v,v'} = \left[e^{\beta\hat{\mathcal{L}}} \right]_{v,v'} \quad (10)$$

where the input space \mathcal{X} is the set of vertices V of graph G .

2.1.1 Diffusion, heat equation, and random walk

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

$$\frac{d}{dt} p_j(t) = \sum_{k \in V} \hat{\mathcal{L}}_{jk} p_k(t), \quad (11)$$

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 $\hat{\mathcal{L}}$ sum to 0, an initially normalized distribution remains normalized: the evolution of

the continuous-time random walk for any time t is a *stochastic process. random walk* (discrete-space, discrete-time), discretize the time derivative in Eq. (11)

$$p_j(t+1) = \frac{p_{j+1}(t) + p_{j-1}(t)}{2} \quad (12)$$

which is the finite difference equation of *heat equation*

$$\frac{\partial p(t, z)}{\partial t} = \frac{\partial^2 p(t, z)}{\partial z^2} \quad (13)$$

continuous-space (continuous-time) case. The solution to Eq. (13) is called *heat kernel* $\mathcal{K}(t; x, y) = \frac{1}{4\pi t} e^{-|x-y|^2/4t}$ (Gaussian).

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. (11) is very similar to the time-dependent (evolution) schrodinger equation governed by a Hamiltonian operator \hat{H}

$$i\hbar \frac{d}{dt} |\psi\rangle = \hat{H} |\psi\rangle \quad (14)$$

except that the factor of $i\hbar$.

Definition 10 (Quantum propagator). *Quantum propagator, transition amplitude.* Interestingly, this quantity is also called *quantum kernel* (much earlier than the concept of kernel tricks in machine learning),

$$\langle I | e^{-it\hat{H}} | F \rangle = \langle I | \hat{U} | F \rangle \quad (15)$$

The quantum propagator can be evaluated by *path integral (Lagrangian) formalism* (see Appendix B.1).

2.3 Graph kernels of a pair of graphs

R-convolution kernel proposed by Haussler [ref]. graphs kernels are designed to compare the similarity of each of the decompositions of a pair of graphs. Different kernels are defined, depending on how the graphs are decomposed. Most R-convolution kernels count the number of isomorphic substructures in the two graphs. random walk kernel (shortest paths) [Vis+10]. quantum kernel [Bai+15] survey [KJM20]

Definition 11 (Graph kernel). Given a pair of graphs (G, G') , a *graph kernel* is a function (mapping) $\mathcal{K}(G, G') : \{G\} \rightarrow \mathbb{R}$

$$\mathcal{K}(G, G') = \frac{1}{|G||G'|} \sum_k \frac{\lambda^k}{k!} \mathbf{e}^\top A_\times \mathbf{e} = \frac{1}{|G||G'|} \mathbf{e}^\top \exp(\beta \hat{A}_\times) \mathbf{e} \quad (16)$$

random walk kernel ?

Fact 1. the adjacency matrix of the product graph $A_\times = A \otimes A'$ ($\exp(A_\times) = \exp(A) \otimes \exp(A')$). In general, the Laplacian of the direct product graph $\hat{\mathcal{L}}_\times \neq \hat{\mathcal{L}}_1 \otimes \hat{\mathcal{L}}_2$.

[Chu97]

Definition 12 (Product of graphs). *direct product of graphs;*

$$G_\times := G(V, E) \times G'(V', E') := \{(v, v') \in V \times V', ((v, v'), (w, w')) : (v, w) \in E, (v', w') \in E'\} \quad (17)$$

tensor product of graphs;

$$G \otimes G' := \{\vee\} \quad (18)$$

Cartisan product of graphs;

$$G \times G' = \{\} \quad (19)$$

Kronecker sum (produca; factor graph; Hadamard product;

Remark 2. Random Walk on Product Graph is equivalent to simultaneous random walk on input graphs [?]

Remark 3. A natural question to ask is the following: Since diffusion can be viewed as a **continuous time** limit of random walks, can the ideas behind the random walk kernel be extended to diffusion? Unfortunately, the Laplacian of the product graph does not decompose into the Kronecker product of the Laplacian matrices of the constituent graphs; this rules out a straightforward extension. discrete-time quantum random walk (need coin space) [AKR05] [Chi04]; Szegedy's walk formalism. [Sze04]

Remark 4. for diffusion processes on factor graphs the kernel on the factor graph is given by the product of kernels on the constituents, that is

$$k((i, i'), (j, j')) = k(i, j)k'(i', j'). \quad (20)$$

2.4 Discrete-time quantum random walk

Discrete-time quantum random walk is the quantum analogy of random walk

2.5 Relations, difference, and examples

2.5.1 Line

(classical) diffusion kernel of a 1-dimensional lattice (line)

$$\mathcal{K}(v, v') = \quad (21)$$

Quantum propagator (quantum kernel)

$$\begin{aligned} \tilde{\mathcal{K}}(z_F, z_I) &= \langle z_F | e^{-it\hat{H}_0} | z_I \rangle = \sum_{p=1}^N e^{-it2 \cos(\frac{2\pi}{N}p) + i\frac{2\pi}{N}p(z_I - z_F)} \\ &\approx e^{2it} (-i)^d J_d(2t) \end{aligned} \quad (22) \quad (\text{large } N \text{ approx})$$

where the distance between .

Remark 5. 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 spreads as a wave packet with speed 2.

2.5.2 Hyercube

the unitary evolution operator of quantum diffusion on hypercube

$$e^{-it\hat{A}} = \prod_{j=1}^n e^{-it\hat{X}^{(j)}} = \bigotimes_{j=1}^n \begin{pmatrix} \cos t & -i \sin t \\ -i \sin t & \cos t \end{pmatrix} \quad (23)$$

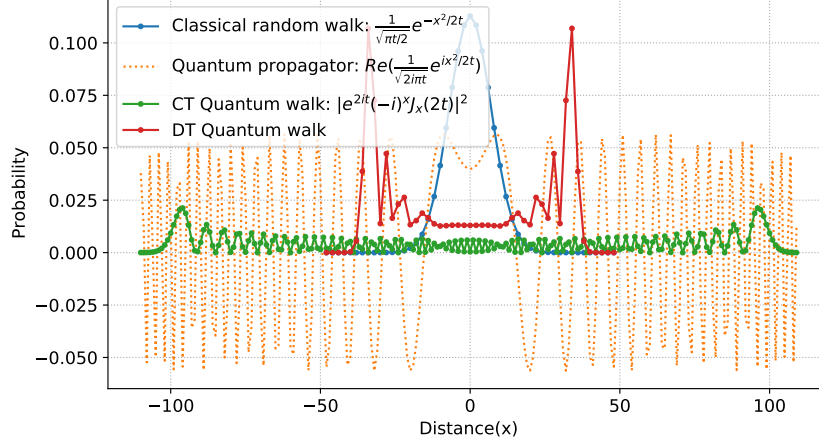


Figure 2: Different kinds of walks in 1d space

2.5.3 Tree

2.5.4 Cayley graphs

Definition 13 (Cayley graph). Cayley graph is a graph that encodes the abstract structure of a group.

3 Quantum Advantages and Speedups

A quantum version of this approach has already been proposed in [RML14], where an exponential improvement can be achieved if data is provided in a coherent superposition.

Remark 6. However, when data is provided in the conventional way, i.e. from a classical computer, then the methods of [15] cannot be applied.

input model, quantum RAM; quantum-inspired [Tan19]

3.1 Related works

3.1.1 Quantum SVM and kernel tricks

Quantum version of SVM was proposed [RML14] to exploit the power of quantum computer. Naturally, the *quantum kernel estimation* [SK19] [Hav+19] is studied to enhance the performance of quantum SVM.

Definition 14 (Quantum feature map). the quantum state space (Hilbert space) as the feature space to still obtain a quantum advantage mapping the input data non-linearly to a quantum state (density matrix)

$$\Phi(\mathbf{x}) : \Omega \rightarrow |\Phi(\mathbf{x})\rangle\langle\Phi(\mathbf{x})|, \quad (24)$$

the direct quantum analogy of classical [feature map](#). On quantum computers, the quantum feature map $\Phi(\mathbf{x})$ is realized by applying a unitary quantum circuit $\hat{U}_{\Phi(\mathbf{x})}$ to a reference state $|0^n\rangle$.

Explicit method (Quantum Variational Classification)

variational quantum circuit: generates a separating hyperplane in the quantum feature space

1. $\mathbf{x} \in \Omega$ (feature) mapped to a quantum state by applying a unitary circuit $U_{\Phi(\mathbf{x})}$ to a reference (initial) state $|0\rangle^n$

2. a short depth quantum circuit $W(\theta)$
3. for binary classification, apply a binary measurement $\{M_y\} = 2^{-1}(\mathbb{1} + y\mathbf{f})$?
4. to obtain the empirical distribution $p_y(\mathbf{x})$, perform repeated measurement shots. then assign the label according to p_y ?

Implicit method (Quantum kernel estimation)

estimate the kernel function quantumly and implement a conventional SVM. Rather than using a variational quantum circuit to generate the separating hyperplane, we use a classical SVM for classification.

1. the kernel $\mathcal{K}(\mathbf{x}, \mathbf{x}')$ is estimated on a quantum computer
2. the quantum computer is used a second time to estimate the kernel for a new datum (test) $\mathbf{s} \in S$ with all the support vectors.

The kernel entries are the fidelities between different feature vectors. The overlap can be estimated directly from the transition amplitude

Definition 15 (Quantum kernel estimation). The *quantum kernel estimation* is the *Hilbert-Schmidt inner product* between density matrices

$$\mathcal{K}(\mathbf{x}, \mathbf{x}') = \text{Tr}(|\Phi(\mathbf{x})\rangle\langle\Phi(\mathbf{x})| \cdot |\Phi(\mathbf{x}')\rangle\langle\Phi(\mathbf{x}')|) = |\langle\Phi(\mathbf{x})|\Phi(\mathbf{x}')\rangle|^2 = \left| \langle 0^n | \hat{U}_{\Phi(\mathbf{x})}^\dagger \hat{U}_{\Phi(\mathbf{x}')} | 0^n \rangle \right|^2. \quad (25)$$

exactly the [Quantum propagator](#).

measure the final state in the Z-basis R -times and record the number of $|0^n\rangle$. The frequency of this string is the estimate of the transition probability. The kernel entry is obtained to an additive sampling error of $\tilde{\epsilon}$ when $\mathcal{O}(\tilde{\epsilon}^{-2})$ shots are used.

Theorem 2 ([[Chi+03](#)]). *There exists exponential (classical-quantum) separation with respect to query complexity under the adjacency matrix (graph) model. (glued tree)*

[[Zhe+22](#)]; robust, provable speedup [[LAT21](#)]

3.1.2 Quantum graph kernels

quantum graph kernel defined in terms of quantum Jensen Shannon as a metric of dissimilarity of graphs density matrices associated with (representing) the evolution of continuous-time quantum random walks on graphs [[Bai+15](#)]. In (classical information theory), the Jensen-Shannon divergence is a dissimilarity measure between probability distributions.

$$D(p, p') \quad (26)$$

[[Bai+17](#)]

Remark 7. Unfortunately, the required composite entropy for the Jensen-Shannon kernel is computed from a product graph formed by a pair of graphs, and reflects no correspondence information between pairs of vertices. As a result, the Jensen-Shannon graph kernel lacks correspondence information between the probability distributions over the graphs, and thus cannot precisely reflect the similarity between graphs.

The quantum version of Jensen-Shannon divergence is defined as the distance measure between mixed quantum states (density matrices).

Definition 16. Given a graph $\mathbb{G}(V, E)$, The von Neumann entropy of \mathbb{G} is defined as

$$H_N(\rho_{\mathbb{G}}) = -\text{Tr}(\rho_{\mathbb{G}} \log \rho_{\mathbb{G}}) = -\sum_j^{|V|} \lambda_j \log \lambda_j \quad (27)$$

Given two density operators ρ and ρ' , the *quantum Jensen-Shannon divergence* is defined as

$$D_{QJS}(\rho, \rho') = H_N\left(\frac{\rho + \rho'}{2}\right) - \frac{1}{2}H_N(\rho) - \frac{1}{2}H_N(\rho') \quad (28)$$

D_{QJS} is always well defined, symmetric, negative definite and bounded, i.e., $0 \leq D_{QJS} \leq 1$?

evaluate the performance on the standard graph datasets from both bioinformatics and computer vision. Instead, we could exploit the structures inherent in physics systems and make use of quantum advantages.

3.1.3 Quantum diffusion map

Inspired by random walk on graphs, *diffusion map* (DM) is a class of **unsupervised** machine learning that offers automatic identification of **low-dimensional data structure hidden in a high dimensional dataset**. Given the normalized (similarity) matrix M , compute the k largest eigenvalues(vectors) of M^t . Use the diffusion map to get the embedding Ψ_t .

$$P, L \quad (29)$$

Though both of SVM and DM are machine learning techniques that utilize kernel tricks, DM is designed for dimension reduction, the ‘reverse direction’ of the kernel trick in SVM.

The quantum DM proposed by [Sor+21] takes as an input N classical data vectors, performs (quantumly) an eigen-decomposition of the Markov transition matrix in time $\mathcal{O}(\log^3 N)$, and classically constructs the diffusion map via the readout (tomography) of the eigenvectors, giving a total expected runtime proportional to $N^2 \text{poly log } N$.

3.2 Provable quantum speedups

structure is required for quantum speedup [AA14]. only polynomial speedup for total problem [ref]. only quadratic speedup for unstructured search [Gro97]

3.2.1 Quantum Fourier Transform (QFT)

hidden subgroup problem solved by quantum Fourier transformation[CvD10]; rigorous and robust quantum speedup with Discret Logarithm (DLOG) problem [LAT21]

Definition 17 (Hidden subgroup problem). Given a group \mathbb{G} and a black-box function $f : \mathbb{G} \rightarrow S$, f is promised to satisfy

$$f(x) = f(y) \text{ iff } x^{-1}y \in \mathbb{H} \quad (30)$$

for some unknow subgroup $\leq \mathbb{G}$. We say such a function f hides a subgroup \mathbb{H} . The goal of *hidden subgroup problem* (HSP) is to learn \mathbb{H} (specified in terms of a generating set) using queries to f .

Remark 8. For Simon’s problem (Abelian subgroup problem), the HSP with $\mathbb{G} = \mathbb{Z}_2^n$ and $\mathbb{H} = \{0, s\}$ for some $s \in \mathbb{Z}_2^n$.

Definition 18 (Discrete Logarithm problem). *discrete logarithm problem* is a special case of **Hidden subgroup problem** with

- **Input:** generator g , $y = g^x$ with some unknow x , black-box function f
- **Output:** $x = \log_g y$

3.2.2 Permutation, symmetry, and graph properties

symmetric functions rule out exponential speedup [Ben+20]. We have seen that the behavior of a quantum walk can be dramatically different from that of its classical counterpart. Next we will see an even stronger example of the power of quantum walk: a black-box problem that can be solved exponentially faster by a quantum walk than by any classical algorithm [Chi+03].

Consider a graph obtained by starting from two balanced binary trees of height n , and joining them by a random cycle of length $2 \cdot 2^n$ that alternates between the leaves of the two trees. For example, such a graph for $n = 4$ could look like Fig. 3

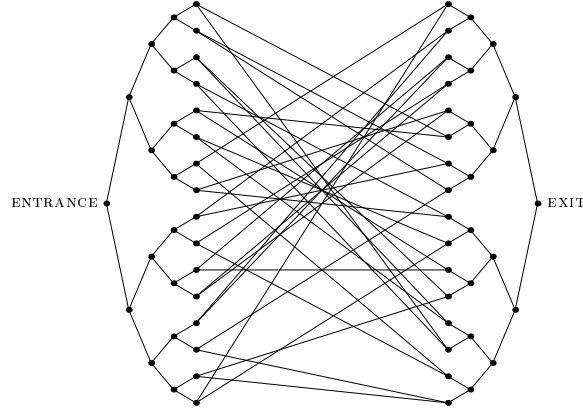


Figure 3: A typical graph exhibits rigorous exponential speedup over classical model in graph matrix representation. [Chi+03]

3.2.3 Quantum linear algebra

FFT [KSB09]; quantum linear algebra (qMAT) [Zha+19]:

- HHL [HHL09],
- matrices multiplication, matrix inversion, matrix exponentiation,
- quantum simulation techniques (evolution)
- FFT by quantum algorithms: $\mathcal{O}(n \log n)$

[Sor+21]

3.3 Heuristic quantum advantages for learning physics systems

problems of practical interest, not guaranteed

3.3.1 Groups and symmetries in physics and machine learning

[Kon08]; symmetries in physics [Bog+20] [Bog+22]; equivariant CNN [Zhe+22]. (classical) machine learning (neural network) for quantum many-body physics: determining the phase (transition) a standard feed-forward neural network can be trained to detect multiple types of order parameter directly from raw state configurations sampled with Monte Carlo. what if one was presented with a data set of Ising configurations from an unknown Hamiltonian, where the lattice structure (and therefore its T c) is not

known? We turn to the application of such techniques to problems of greater interest in modern condensed matter, such as disordered or topological phases, where no conventional order parameter exists. Ising lattice gauge theory, one of the most prototypical examples of a topological phase of matter. A straightforward implementation of supervised training fails to classify a test set containing samples of the two states to an accuracy over 50% – equivalent to simply guessing. Such failures typically occur because the neural network overfits to the training set. To overcome this difficulty we consider a convolutional neural network (CNN) [4, 22] which readily takes advantage of the two-dimensional structure of the input configurations, as well as the translational invariance of the model. [CM17] [CT17]

covariant quantum kernels for the data with group structures [Gli+21]

Definition 19 (Covariant). *covariant*

Definition 20 (Equivariance). Given a group \mathbb{G} and the actions $\rho : \mathbb{G} \times X \rightarrow X$ and $\rho' : \mathbb{G} \times Y \rightarrow Y$, a map $f : X \rightarrow Y$ is said to be *equivariant* if

$$\forall x \in X, g \in \mathbb{G}, f(\rho(g, x)) = \rho'(g, f(x)) \quad (31)$$

4 Experiments

4.1 Datasets and benchmark

preliminary experiment

4.1.1 Artificial data

we generate artificial data that can be fully separated by our feature map.

4.1.2 Real-world dataset

UCI [KL02], protein, JET? [Bog+20]; The MUTAG dataset consists of graphs representing 188 chemical compounds labeled ..; quantum many-body physics (phase transition) [CM17]

5 Discussion and Conclusion

to do

- quantum graph kernel with group structures
- quantum machine learning for physics problem with symmetries
- NISQ?

References

- [AA14] Scott Aaronson and Andris Ambainis. “The Need for Structure in Quantum Speedups”. Feb. 6, 2014. arXiv: [0911.0996 \[quant-ph\]](#) (cit. on p. 9).
- [AKR05] Andris Ambainis, Julia Kempe, and Alexander Rivosh. [Coins Make Quantum Walks Faster](#). Proceedings of the Sixteenth Annual ACM-SIAM Symposium on Discrete Algorithms. SODA ’05. USA: Society for Industrial and Applied Mathematics, Jan. 23, 2005, pp. 1099–1108. arXiv: [quant-ph/0402107](#) (cit. on p. 6).

- [Bai+15] Lu Bai et al. [A Quantum Jensen–Shannon Graph Kernel for Unattributed Graphs](#). *Pattern Recognition* 48.2 (Feb. 2015), pp. 344–355 (cit. on pp. 5, 8).
- [Bai+17] Lu Bai et al. [Quantum Kernels for Unattributed Graphs Using Discrete-Time Quantum Walks](#). *Pattern Recognition Letters* 87 (Feb. 2017), pp. 96–103 (cit. on p. 8).
- [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. 10).
- [Bia+17] Jacob Biamonte et al. [Quantum Machine Learning](#). *Nature* 549.7671 (Sept. 2017), pp. 195–202. arXiv: [1611.09347](#) (cit. on p. 14).
- [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 pp. 10, 11).
- [Bog+22] Alexander Bogatskiy et al. [Symmetry Group Equivariant Architectures for Physics](#). Mar. 11, 2022. arXiv: [2203.06153](#) [[astro-ph](#), [physics:hep-ex](#), [physics:hep-ph](#)] (cit. on p. 10).
- [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. 5).
- [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 pp. 8, 10).
- [Chi04] Andrew MacGregor Childs. “Quantum Information Processing in Continuous Time”. Thesis. Massachusetts Institute of Technology, 2004 (cit. on pp. 2, 6).
- [Chu97] Fan R. K. Chung. [Spectral Graph Theory](#). Regional Conference Series in Mathematics no. 92. Providence, R.I: Published for the Conference Board of the mathematical sciences by the American Mathematical Society, 1997. 207 pp. (cit. on pp. 4, 5).
- [CM17] Juan Carrasquilla and Roger G. Melko. [Machine Learning Phases of Matter](#). *Nature Phys* 13.5 (5 May 2017), pp. 431–434. arXiv: [1605.01735](#) (cit. on p. 11).
- [CT17] Giuseppe Carleo and Matthias Troyer. [Solving the Quantum Many-Body Problem with Artificial Neural Networks](#). *Science* 355.6325 (Feb. 10, 2017), pp. 602–606. arXiv: [1606.02318](#) (cit. on p. 11).
- [CvD10] Andrew M. Childs and Wim van Dam. [Quantum Algorithms for Algebraic Problems](#). *Rev. Mod. Phys.* 82.1 (Jan. 15, 2010), pp. 1–52. arXiv: [0812.0380](#) (cit. on p. 9).
- [Dir45] P. A. M. Dirac. [On the Analogy Between Classical and Quantum Mechanics](#). *Rev. Mod. Phys.* 17.2-3 (Apr. 1, 1945), pp. 195–199 (cit. on p. 15).
- [Far+00] Edward Farhi et al. “Quantum Computation by Adiabatic Evolution”. Jan. 28, 2000. arXiv: [quant-ph/0001106](#) (cit. on p. 2).
- [FHS10] Richard P. Feynman, Albert R. Hibbs, and Daniel F. Styer. [Quantum Mechanics and Path Integrals](#). Emended ed. Mineola, N.Y: Dover Publications, 2010. 371 pp. (cit. on p. 15).
- [Gli+21] Jennifer R. Glick et al. “Covariant Quantum Kernels for Data with Group Structure”. May 7, 2021. arXiv: [2105.03406](#) [[quant-ph](#)] (cit. on p. 11).
- [Gro97] Lov K. Grover. [Quantum Mechanics Helps in Searching for a Needle in a Haystack](#). *Phys. Rev. Lett.* 79.2 (July 14, 1997), pp. 325–328 (cit. on p. 9).
- [Hav+19] Vojtech Havlicek et al. [Supervised Learning with Quantum Enhanced Feature Spaces](#). *Nature* 567.7747 (Mar. 2019), pp. 209–212. arXiv: [1804.11326](#) (cit. on p. 7).

- [HHL09] Aram W. Harrow, Avinatan Hassidim, and Seth Lloyd. [Quantum Algorithm for Solving Linear Systems of Equations](#). *Phys. Rev. Lett.* 103.15 (Oct. 7, 2009), p. 150502. arXiv: [0811.3171 \[quant-ph\]](#) (cit. on p. 10).
- [KJM20] Nils M. Kriege, Fredrik D. Johansson, and Christopher Morris. [A Survey on Graph Kernels](#). *Appl Netw Sci* 5.1 (Dec. 2020), p. 6. arXiv: [1903.11835 \[cs, stat\]](#) (cit. on pp. 4, 5).
- [KL02] Risi Imre Kondor and John Lafferty. [Diffusion Kernels on Graphs and Other Discrete Structures](#) (2002), p. 8 (cit. on pp. 2, 4, 11).
- [Kon08] Risi Kondor. “Group Theoretical Methods in Machine Learning”. Thesis. Columbia University, 2008 (cit. on pp. 2, 10).
- [KSB09] Risi Kondor, Nino Shervashidze, and Karsten M. Borgwardt. [The Graphlet Spectrum](#). Proceedings of the 26th Annual International Conference on Machine Learning - ICML '09. The 26th Annual International Conference. Montreal, Quebec, Canada: ACM Press, 2009, pp. 1–8 (cit. on p. 10).
- [LAT21] Yunchao Liu, Srinivasan Arunachalam, and Kristan Temme. [A Rigorous and Robust Quantum Speed-up in Supervised Machine Learning](#). *Nat. Phys.* 17.9 (Sept. 2021), pp. 1013–1017. arXiv: [2010.02174 \[quant-ph\]](#) (cit. on pp. 8, 9).
- [RML14] Patrick Rebentrost, Masoud Mohseni, and Seth Lloyd. [Quantum Support Vector Machine for Big Data Classification](#). *Phys. Rev. Lett.* 113.13 (Sept. 25, 2014), p. 130503. arXiv: [1307.0471 \[quant-ph\]](#) (cit. on p. 7).
- [SK03] Alexander J. Smola and Risi Kondor. [Kernels and Regularization on Graphs](#). Learning Theory and Kernel Machines. Ed. by Bernhard Schölkopf and Manfred K. Warmuth. Red. by Gerhard Goos, Juris Hartmanis, and Jan van Leeuwen. Vol. 2777. Lecture Notes in Computer Science. Berlin, Heidelberg: Springer Berlin Heidelberg, 2003, pp. 144–158 (cit. on p. 4).
- [SK19] Maria Schuld and Nathan Killoran. [Quantum Machine Learning in Feature Hilbert Spaces](#). *Phys. Rev. Lett.* 122.4 (Feb. 1, 2019), p. 040504. arXiv: [1803.07128 \[quant-ph\]](#) (cit. on p. 7).
- [Sor+21] Apimuk Sornsaeng et al. [Quantum Diffusion Map for Nonlinear Dimensionality Reduction](#). *Phys. Rev. A* 104.5 (Nov. 10, 2021), p. 052410. arXiv: [2106.07302 \[quant-ph\]](#) (cit. on pp. 9, 10).
- [Sze04] Mario Szegedy. “Spectra of Quantized Walks and a $\sqrt{\delta\epsilon}$ Rule”. Jan. 9, 2004. arXiv: [quant-ph/0401053](#) (cit. on p. 6).
- [Tan19] Ewin Tang. [A Quantum-Inspired Classical Algorithm for Recommendation Systems](#). *Proc. 51st Annu. ACM SIGACT Symp. Theory Comput.* (June 23, 2019), pp. 217–228. arXiv: [1807.04271](#) (cit. on p. 7).
- [Vis+10] S.V.N. Vishwanathan et al. [Graph Kernels](#). *J. Mach. Learn. Res.* 11.40 (2010), pp. 1201–1242. arXiv: [0807.0093](#) (cit. on p. 5).
- [Xu21] Jue Xu. “On Lagrangian Formalism of Quantum Computation”. Dec. 7, 2021. arXiv: [2112.04892 \[quant-ph\]](#) (cit. on p. 14).
- [Zha+19] Liming Zhao et al. [Compiling Basic Linear Algebra Subroutines for Quantum Computers](#). Feb. 27, 2019. arXiv: [1902.10394 \[quant-ph\]](#) (cit. on p. 10).
- [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 pp. 8, 10).

A Machine Learning and Group Theory

supervised learning: classification, regression (SVM, neural network; gradient descent); unsupervised learning: clustering, dimension reduction; reinforced learning not discussed in this paper.

A.1 Machine learning

training set, test set.

A.1.1 SVM and kernel tricks

objective (cost function): *empirical risk* (error rate, loss function)

$$R_{emp}(\theta) = \frac{1}{|T|} \sum_{\mathbf{x} \in T} \mathbb{P}(\tilde{y} \neq y) \quad (32)$$

the dual quadratic program that (only uses access to the kernel) we maximize

$$L_D(\alpha) = \sum_{i=1}^t \alpha_i - \frac{1}{2} \sum_{i,j=1}^t y_i y_j \alpha_i \alpha_j \mathcal{K}(\mathbf{x}_i, \mathbf{x}_j) \quad (33)$$

subject to $\sum_{i=1}^t \alpha_i y_i = 0$ and $\alpha_i \geq 0$ for each i ?. construct the classifier

$$\tilde{m}(\mathbf{s}) := \text{sign} \left(\sum_{i=1}^t y_i \alpha_i^* \mathcal{K}(\mathbf{x}_i, \mathbf{s}) + b \right) \quad (34)$$

A.1.2 Quantum machine learning

[Bia+17]; neural network

A.2 Group theory and symmetries

group \mathbb{G}

A.2.1 Representation theory

B Symmetries in physics

B.1 Lagrangian formalism

B.1.1 Path integral and quantum computing

[Xu21] In optics, Fermat's principle states that the path taken by a ray between two given points is the path that can be traveled in the least (extremum) time. A similar argument, *principle of least action*, was developed in classical mechanics:

Axiom 1 (Principle of least action). *The actual path $q(t)$ taken by a classical system is the path that yields an extremum of its action \mathcal{S} . So, this principle is also called principle of stationary action. The action of the dynamics is the integral of Lagrangian over time*

$$\mathcal{S}[q(t)] := \int_{t_I}^{t_F} \mathcal{L}(q(t), \dot{q}(t); t) dt \quad (35)$$

where $\mathcal{L}(q, \dot{q})$ is the Lagrangian in terms of generalized coordinate q and velocity \dot{q} at certain time t .

The notion $\mathcal{S}[\cdot]$ reminds that action is a functional that takes a function (path) $q(t)$ as input. By varying the action, one have the equation of motion called *Euler-Lagrange equation*. This Lagrangian formalism was extended by Dirac [Dir45] and Feynman [FHS10] to explain quantum mechanics.

Axiom 2 (Path integral). *The amplitude (probability) of a quantum system evolving from $|q_I\rangle$ to $|q_F\rangle$ in a time interval can be evaluated by (functional) integrating over all possible paths with fixed initial and final position*

$$\langle q_F | e^{-it\hat{H}/\hbar} | q_I \rangle = \int_{q(t_I)=q_I}^{q(t_F)=q_F} \mathcal{D}q e^{i\mathcal{S}[q]/\hbar} \quad (36)$$

where the action defined in classical mechanics as Eq. (35).

The Larangian (path integral) formalism of quantum mechanics is proved to be equivalent to the well-known Schrödinger equation Eq. (14) [FHS10, Chp4] which is a differential equation determining the evolution of quantum state. In the classical limit (Planck's constant $\hbar \rightarrow 0$), [Path integral](#) reduces to [Principle of least action](#) because only the paths around the stationary point of the action contribute (the other paths' contributions frequently oscillate and cancel out).

B.2 Symmetries with Lagrangian

B.2.1 \mathbb{Z}

Ising

B.2.2 $\mathbb{U}(1)$

local, gauge symmetry

B.2.3 $\mathbb{SU}(2)$

non-abelian

B.2.4 $\mathbb{SO}(1,3)$

Lorentz invariance