Topological Data Analysis on Noisy Quantum Computers

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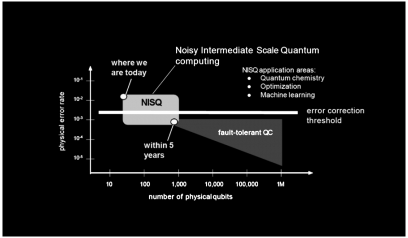
IBM Research, Wits University, and Royal Institute

International Conference on Learning Representations (ICLR), 2024

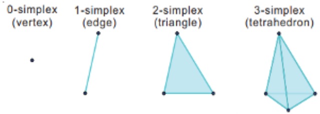
Quantum Advantage

- *Power of quantum computers* - ability to perform computations in very large computational (Hilbert) spaces, accessed via small physical systems.
- An arduous search for algorithms that achieve exponential computational speedups over classical algorithms.
- **Quantum advantage**: Quantum computers outperforming current classical supercomputers.
- *Not yet achieved* for problems of commercial value.
- Noisy Intermediate-Scale Quantum (NISQ).

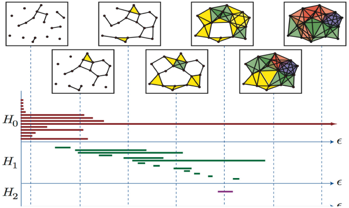


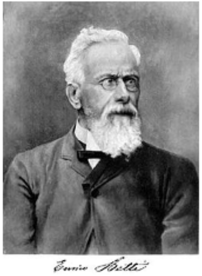
Topological Data Analysis

- *Topological Data Analysis* (TDA): “**Shape**” of data; Interpretable, High-dimensional.
- *Persistent Homology:* local and global features.
- k-**Simplex**: simplest possible polytope - points, lines, triangles, etc.

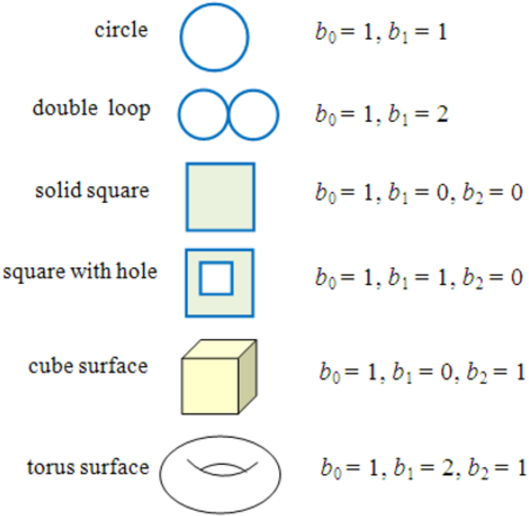


- **Simplicial Complex**: collection of simplices.
- Study shape of data – number of connected components, holes, voids and higher-dimensional counterparts.

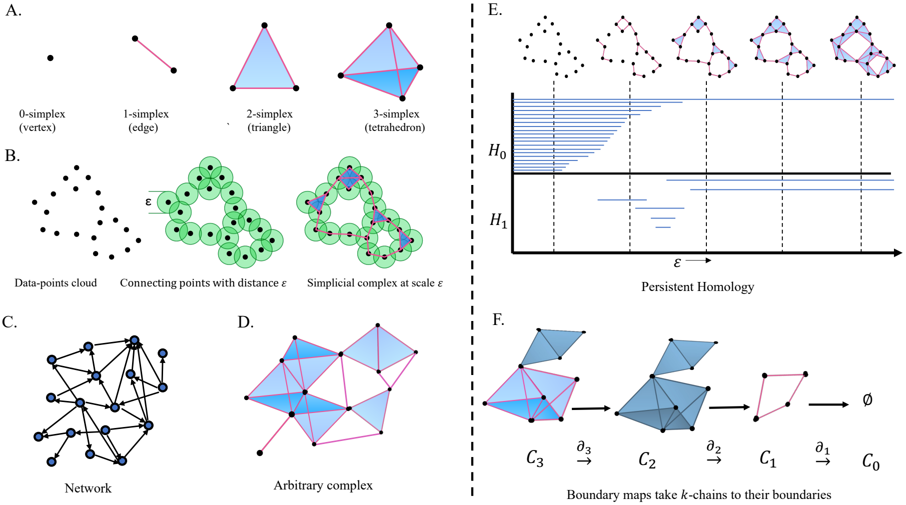


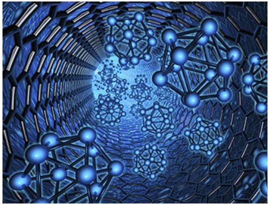


- b_0 # of connected component
- b_1 # of holes
- b_2 # voids

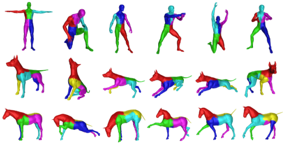


TDA

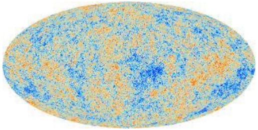

A.
0-simplex
(vertex)
1-simplex
(edge)
2-simplex
(triangle)
3-simplex
(tetrahedron)
B.
ε
Data-points cloud
Connecting points with distance ε
Simplicial complex at scale ε
C.
Network
D.
Arbitrary complex
E.
H_0
H_1
ε ⟶
Persistent Homology
F.
∅
$C_3 \xrightarrow{\partial_3} C_2 \xrightarrow{\partial_2} C_1 \xrightarrow{\partial_1} C_0$
Boundary maps take k-chains to their boundaries



Material Science

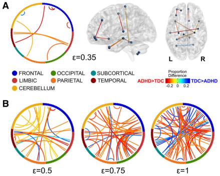


3D shape analysis

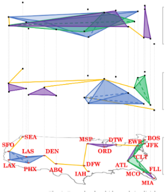


Cosmic Microwave Background analysis

Genomics



fMRI analysis

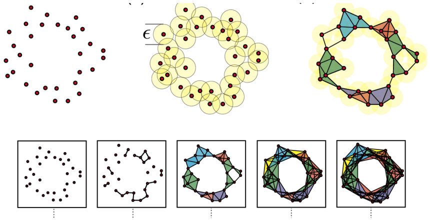


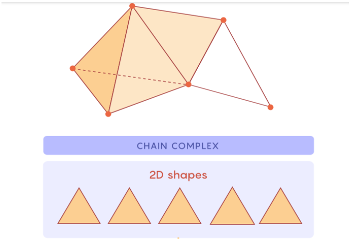
Transportation networks

TDA applications - many promising results in numerous fields.

Homology Definitions

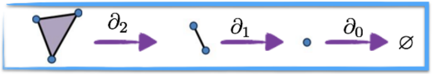
- *Given:* A set of n data-points $\{x_i\}_{i=1}^n$ in some ambient space, a distance metric $\mathcal{D}$, and a resolution scale ε.
- *Vietoris-Rips simplicial complex* kick-started by connecting points x_i and x_j : $\mathcal{D}(x_i, x_j) \leq \varepsilon$.
- k-simplex added for subset of $k+1$ data-points that are pair-wise connected.
- S_k - set of k-simplices in the Vietoris–Rips complex $\Gamma = \{S_k\}_{k=0}^{n-1}$,
  $s_k \in S_k$ written as $[j_0, \ldots, j_k]$ - j_i is the ith vertex of s_k.
- *Chain Group:* $|s_k\rangle$ a basis state, natural encoding of $s_k \in S_k$.
  $\mathcal{H}_k = \binom{n}{k+1}$-dim Hilbert space with basis vectors of all possible k- simplices. $\tilde{\mathcal{H}}_k$ subspace of $\mathcal{H}_k$ spanned by the basis vectors of simplices in $S_k \in \Gamma$.
- The n-qubit Hilbert space: $\mathbb{C}^{2^n} \cong \bigoplus_{k=0}^{n-1} \mathcal{H}_k$.





Homology and Betti Numbers

- Homology counts components, holes, voids, etc. Computable via linear algebra.
- *Boundary Map*: $\partial_k : \mathcal{H}_k \rightarrow \mathcal{H}_{k-1}$ Sends a simplex to a combination of its faces.



$$\partial_k |s_k\rangle = \sum_{l=0}^{k-1} (-1)^l |s_{k-1}(l)\rangle .$$

- Boundary map $\tilde{\partial}_k : \tilde{\mathcal{H}}_k \rightarrow \tilde{\mathcal{H}}_{k-1}$ restricted to a given Γ : $\tilde{\partial}_k = \partial_k \tilde{P}_k$, $\tilde{P}_k$ projector onto the space $S_k \in \Gamma$.
- *k-homology group* - the quotient space $\mathbb{H}_k := \ker(\tilde{\partial}_k)/\mathrm{img}(\tilde{\partial}_{k+1})$. Maximum amount of cuts made before separating a surface into two pieces.
- *k-th Betti Number*:

$$\beta_k := \dim \mathbb{H}_k .$$

- *Combinatorial Laplacians*: $\Delta_k := \tilde{\partial}_k^\dagger \tilde{\partial}_k + \tilde{\partial}_{k+1} \tilde{\partial}_{k+1}^\dagger$.

$$\beta_k := \dim \ker(\Delta_k).$$

NISQ-TDA

We present *NISQ-TDA*, a quantum topological data analysis algorithm that has an improved speedup and a short depth complexity.

Our algorithm involves *three* key ingredients:

- Efficient quantum representation of Δ_k using Fermionic operators;
- Quantum rejection sampling to project onto complex; and
- Stochastic rank estimation method to estimate the normalized Betti number.

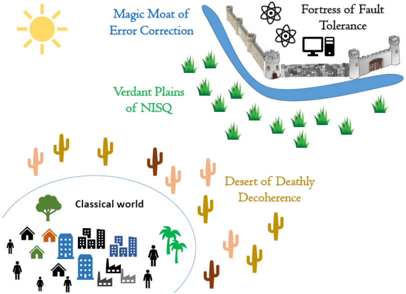


Figure by Daniel Gottesman.

Efficient Representation of Δ_k

- Full boundary map operator $\partial = \bigoplus_k \partial_k$ of all possible simplices:

$$\begin{aligned}
\partial &= a \otimes I \otimes I \otimes \dots I \\
&\quad + \sigma_z \otimes a \otimes I \otimes \dots I \\
&\quad + \sigma_z \otimes \sigma_z \otimes a \otimes \dots I \\
&\quad\quad \vdots \\
&\quad + \sigma_z \otimes \sigma_z \otimes \sigma_z \otimes \dots \otimes a \\
&= \sum_{i=0}^{n-1} a_i,
\end{aligned}$$

- a_i - Jordan-Wigner Pauli embeddings of n-spin fermionic annihilation operators, and

$$a = \frac{(\sigma_x + i\sigma_y)}{2} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}.$$

- Hermitian operator:

$$B = \partial^\dagger + \partial = \sum_{i=0}^{n-1} a_i + a_i^\dagger \quad .$$

- Quantum circuit with $O(n)$ depth and without any Trotterization or Taylor series approximation errors

Efficient Representation of Δ_k

- Boundary map $\partial_k : \mathcal{H}_k \to \mathcal{H}_{k-1}$ on (all) k-dim simplices,

$$\partial_k = P_{k-1} B P_k,$$

  where P_k is the projection onto all simplices of order k (i.e., $\mathcal{H}_k$).
- Combinatorial Laplacian of all simplices in a given Γ

$$\Delta = P_\Gamma B P_\Gamma B P_\Gamma,$$

  where P_Γ is the projector onto all simplices in Γ.
- Combinatorial Laplacian of k-simplices Δ_k is then

$$\Delta_k = P_k \Delta P_k.$$

- k-Betti number is given by $\beta_k = \dim\ker(\Delta_k)$.
- Next we discuss how to construct the projectors P_Γ and P_k in quantum.

Simplicial complex construction

- We propose a NISQ approach based on *all-pairs testing* and *rejection sampling*.
- Assume classical encoding of ε-close pairs (adjacency graph of Γ).
- Entangle the k-simplices with flag registers. $n/2$ qubits used to process $n/2$ pairs of vertices at a time in $n-1$ rounds, covering all $\binom{n}{2}$ potential ε-close pairs of vertices.
- Check $n/2$ pairs and for all simplices in superposition (quantum speedup). C-C-NOT (Toffoli gate), controlling chosen pair into the flag register.
- **Approach 1:** Mid-circuit measurements allows reuse. Need $n-1$ measure-and-reset operations and a $n/2$-qubit flag register.
- **Approach 2:** We can use $\binom{n}{2}$-qubit flag register. Block encoding of $\tilde{\Delta}_k$.
- The collapse succeeds with probability $\sim \zeta$ (repeat $\frac{1}{\zeta}$ times), ζ - fraction of simplices in the complex.
- Number of gates required is $O(n^2)$, whereas the depth is only $O(n)$ since $n/2$ of these gates are in parallel.

Projection onto k-simplices

- Restrict a superposition onto the k-simplex subspace.
- We use a circuit that conditionally implements a count increment.
- Condition on each qubit of the n-simplex register to increment a $\log(n)$-sized count register.
- Entangle the simplex register with the count register - each simplex entangled with the binary representation of its order.
- Measure the count register and obtain a specific simplex order, collapsing the simplex register into a superposition of all simplices of that order only.
- Addtional $\log n$ qubits and depth complexity of $O(n)$.

Stochastic rank estimation

- For β_k calculation, we need to compute the rank of Δ_k.
- Our rank estimation approach is inspired by classical *stochastic Chebyshev* method.
- Rank as trace of a step function of the matrix:

$$\text{rank}(A) \stackrel{def}{=} \text{trace}(h(A)), \text{ where } h(x) = \begin{cases} 1 & \text{if } x > \delta \\ 0 & \text{otherwise} \end{cases}.$$

  the smallest nonzero eigenvalue of $A \geq \delta$.

- **Stochastic trace estimator:** For a Hermitian matrix $A \in \mathbb{R}^{N\times N}$, and random vector states $|v_l\rangle$ with (i.i.d.) entries, $l = 1, .., \mathrm{n_v}$,

$$\text{trace}(A) \approx \frac{1}{\mathrm{n_v}} \sum_{l=1}^{\mathrm{n_v}} \langle v_l | A | v_l \rangle.$$

- We consider $|v_l\rangle = |h_{c(l)}\rangle$, random Hadamard column with $c(l)$ defining the random index. Columns are pairwise independent.

Stochastic rank estimation

$$\text{rank}(A) \stackrel{def}{=} \text{trace}(h(A)), \text{ where } h(x) = \begin{cases} 1 & \text{if } x > \delta \\ 0 & \text{otherwise} \end{cases}.$$

- **Chebyshev approximation:** Approximate the step function as:

$$h(A) \approx \sum_{j=0}^{m} c_j T_j(A),$$

where T_j - jth-degree Chebyshev polynomial of first kind and c_j - coefficients.

- Stochastic Chebyshev method for rank estimation:

$$\text{rank}(A) \approx \frac{1}{\mathrm{n_v}} \sum_{l=1}^{\mathrm{n_v}} \left[\sum_{j=0}^{m} c_j \langle v_l | T_j(A) | v_l \rangle \right]. \quad (1)$$

- The Chebyshev moments $\langle v_l | T_j(A) | v_l \rangle$ computed using qubitization.

Algorithm 1 NISQ-TDA Algorithm

Input: Adjacency graph (ε-close pairs) of n data points; ϵ, δ; and $\mathrm{n_v}$ n-bit random binary numbers.
Output: Betti number estimates χ_k, $k = 0, \ldots, n-1$.
for $l = 1, \ldots, \mathrm{n_v} = O(\epsilon^{-2})$ **do**
  for $j = 0, \ldots, m = O(\log(1/\epsilon))$ **do**
    1. Prepare a random Hadamard state vector $|v_l\rangle$ from $|0\rangle$ using the l-th random number.
    2. Use the circuits for P_k, P_Γ, and $\tilde{B} = B/\sqrt{n}$ to compute
    $|\phi_l\rangle = |0^q\rangle \tilde{\Delta}_k |v_l\rangle + \left|\tilde{\perp}\right\rangle$, where $q = \#$auxiliary qubits needed for projections.
    3. Use qubitization to form: $\left|\psi_l^{(j)}\right\rangle = \left|0^{q+1}\right\rangle T_j(\tilde{\Delta}_k)|v_l\rangle + |\perp\rangle$ from $|\phi_l\rangle$.
    4. Compute the Chebyshev moments $\theta_l^{(j)} = \langle v_l| T_j(\tilde{\Delta}_k) |v_l\rangle$ from $\left|\psi_l^{(j)}\right\rangle$.
  end for
  For $j = 0$, estimate $|S_k|$ using the average norm of the $P_\Gamma P_k |v_l\rangle$.
end for
Estimate $\chi_k = 1 - \frac{1}{\mathrm{n_v}} \sum_{l=1}^{\mathrm{n_v}} \left[\sum_{j=0}^{m} c_j \theta_l^{(j)}\right]$.
Repeat for $k = 0, \ldots, n-1$.

NISQ-TDA Analysis

Theorem

Given adjacency graph (ε-close pairs) of n data points, parameters $(\epsilon, \delta, \eta) \in (0,1)$; an integer $0 \le k \le n-1$. Further assume the eigenvalues of the scaled Laplacian $\tilde{\Delta}_k$ are in the interval $\{0\} \cup [\delta, 1]$, and choose $\mathrm{n_v}$ and m such that

$$\mathrm{n_v} = O\left(\frac{\log(1/\eta)}{\epsilon^2}\right) \qquad \text{and} \qquad m > \frac{\log(1/\epsilon)}{\sqrt{\delta}}.$$

Then, the Betti number estimation $\chi_k \in [0,1]$ by NISQ-TDA, with probability at least $1-\eta$, satisfies

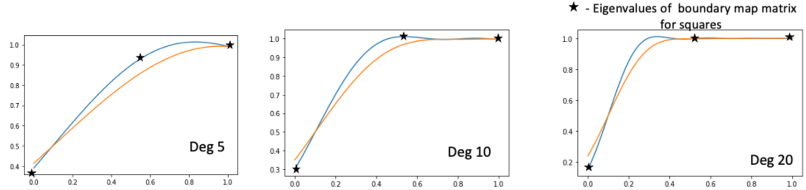
$$\left|\chi_k - \frac{\beta_k}{|S_k|}\right| \le \epsilon.$$

- *Random Hadamard columns* : multiplicative error guarantee with $\mathrm{n_v} \ge \frac{r_H^2(A)\log(2/\eta)}{\epsilon^2}$, $r_H(A) = \max_i A_{ii}$.
- Vectors with *4-wise independent* entries, $\mathrm{n_v} \ge \frac{2}{\epsilon^2 \eta}$. t-designs.

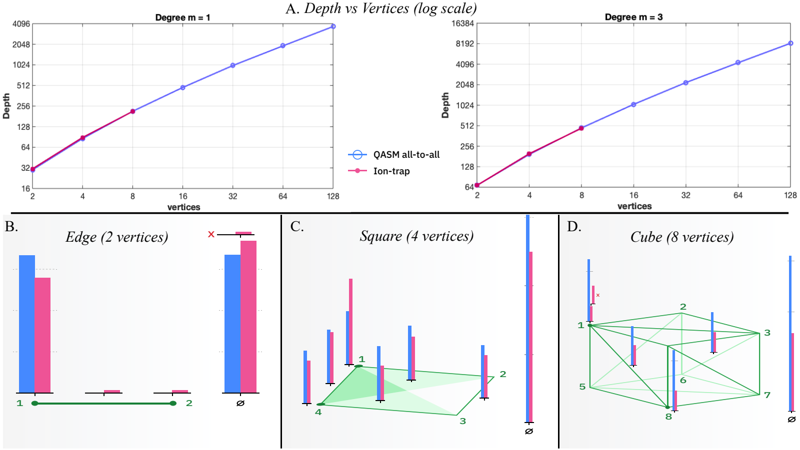
NISQ-TDA

Methods	# Qubits	# Gates	Depth	Time
Lloyd et al., 2016	$2n + \log n + \frac{1}{\delta}$	$O\left(\frac{n^2}{\delta\sqrt{\zeta}}\right)$	$O\left(\frac{n^2}{\delta\sqrt{\zeta}}\right)$	$O\left(\frac{n^4}{\epsilon^2\delta\sqrt{\zeta}}\right)$
Ours (NISQ-QTDA-1)	$3n/2$	$O(n^2\log(1/\epsilon)/\sqrt{\delta})$	$O(n\log(1/\epsilon)/\sqrt{\delta})$	$O\left(\frac{1}{\epsilon^2}\max\left\{\frac{n\log(1/\epsilon)}{\sqrt{\delta}}, \frac{n}{\zeta}\right\} \times \|c\|_2^2\right)$
Ours (NISQ-QTDA-2)	$\tilde{O}(n^2)$	$O(n^2\log(1/\epsilon)/\sqrt{\delta})$	$O(n\log(1/\epsilon)/\sqrt{\delta})$	$O\left(\frac{1}{\epsilon^2}\max\left\{\frac{n\log(1/\epsilon)}{\sqrt{\delta}}, \frac{n}{\zeta}\right\}\right)$

- Potentially the *first* QML algorithm with $O(n)$-depth and significant speedup!
- Quantum speedups for:
  - **Simplices/Clique dense complexes** - ζ is large or $|S_k| \in O(\text{poly}(n))$;
  - **Large spectral gap**- δ of $\tilde{\Delta}_k$ is not too small.
  - **Large Betti number** – β_k (and the ratio $\beta_k/|S_k|$) needs to be large.

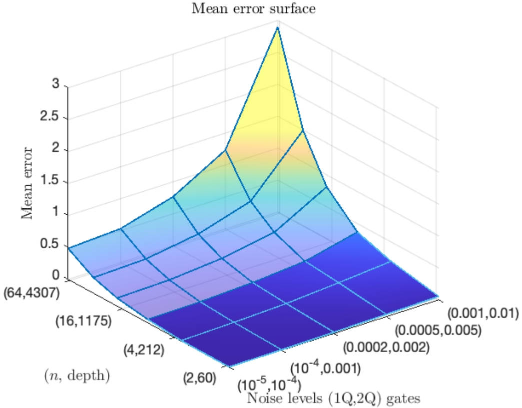


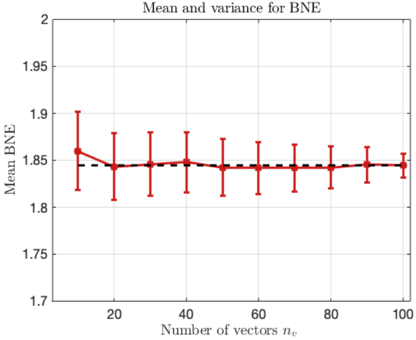
Results from real hardware



Circuit depth versus the number of vertices. Histograms of the probability measurements as obtained from the hardware and a simulator.

Noisy simulation results





Mean error surface as a function of the noise levels in (1-qubit, 2-qubits) gates and (n, circuit depth). Mean and the variance of the Betti number estimated as a function of n_v.

Summary

- *Fully* implemented QML algorithm with short-depth complexity (NISQ), and potential speedup on certain inputs.
- Small input, big compute, and small output.
- Our algorithm neither suffers from the data-loading problem nor does it require fault-tolerant coherence.
- Implementation and successful execution of the algorithm on real quantum hardware and noisy simulations was demonstrated.
- **Applications:** Analysis of neural networks, Non-Gaussianity in CMB data, Genomics, and others.
- Potential NISQ algorithms for other geometric AI problems, co-homology and others.

Questions?