

Quantum Algorithms lecture

Quantum algorithm for Topological data analysis



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What is topological data analysis?

The topological data analysis pipeline

- Going from a dataset to a topological object

- Studying topological object using homology

What can quantum computers bring to the table?

The Lloyd, Garnerone & Zanardi algorithm

What is topological data analysis?

studying the shape of a dataset

Topological data analysis studies the *topology* of your dataset.



- I.e., features that are invariant under *continuous* deformations.

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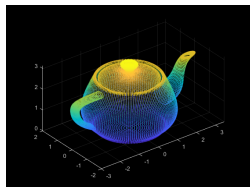
studying the shape of a dataset

Topological data analysis studies the *topology* of your dataset.



- I.e., features that are invariant under *continuous* deformations.

Typically, the dataset is a point cloud in a d -dimensional space such as \mathbb{R}^d .

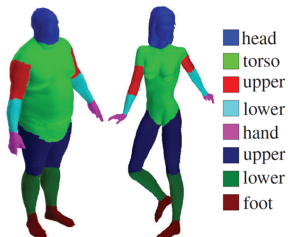


- E.g, a point cloud sampled from a 3d object.

What can topological data analysis be used for?

an example of an application of topological data analysis

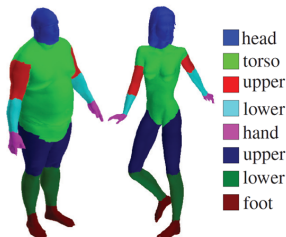
Suppose we would like to classify parts of the human body.



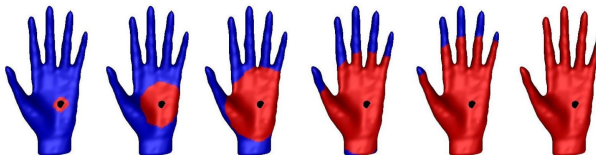
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an example of an application of topological data analysis

Suppose we would like to classify parts of the human body.



TDA does this by studying *persistent topological* features.



► I.e., features of neighbourhoods around points at different scales.

What topological features do we study? How do we study them?

an example of an important topological feature

Important topological feature to study: *the number of holes*.



(a) One hole



(b) Two holes

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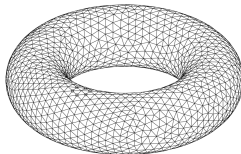


(a) One hole



(b) Two holes

Algebraic topology: use algebra to compute topological features.



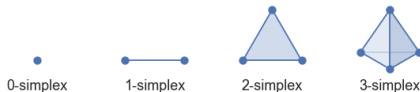
- Triangulate object and study connections between triangles using algebra.

Going from a dataset to a simplicial complex

The Vietoris-Rips complex

1st step TDA pipeline: converting point-cloud to a *simplicial complex*.

- A collection of points, lines, triangles and their k -dimensional counterparts.

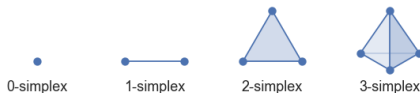


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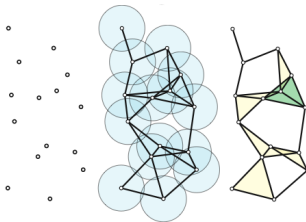
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- A collection of points, lines, triangles and their k -dimensional counterparts.



Vietoris-Rips complex: draw circles with radius $\epsilon > 0$ around data-points and connect data-points if their circles overlap.



- *Persistent topology*: how does topology change if we vary ϵ ?

Studying topology of simplicial complex using homology

turning simplicial complex into a complex vector space

2nd step TDA pipeline: study topology of Vietoris-Rips complex using *homology*.

- ▶ A tool from algebraic topology to extract topological features.

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First, for a point cloud $\mathcal{D} = \{v_i\}_{i=1}^n$ encode the k -simplices of the Vietoris-Rips complex as n -bit strings.

$$\text{VR}(\mathcal{D}, \epsilon)_k := \{j \in \{0, 1\}^n \mid j \text{ has } k \text{ ones and } \forall j_i, j_l = 1 \text{ we have } \|v_i - v_l\| < \epsilon\}.$$

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Next, we turn this into a complex vector space

$$\mathcal{H}_k^\epsilon := \text{span}_{\mathbb{C}}\{|j\rangle \mid j \in \text{VR}(\mathcal{D}, \epsilon)_k\} \subset (\mathbb{C}^2)^{\otimes n}.$$

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We now have an algebraic object to study!

Studying topology of simplicial complex using homology

the boundary operator

In order to study \mathcal{H}_k^ϵ we consider the so-called *k-th boundary map*

$$\partial_k^\epsilon : \mathcal{H}_k^\epsilon \rightarrow \mathcal{H}_{k-1}^\epsilon$$

$$|j\rangle \mapsto \sum_{i=1}^k (-1)^i |j(\hat{i})\rangle,$$

where $j(\hat{i})$ is obtained from j by setting i -th 1 to 0.

Studying topology of simplicial complex using homology

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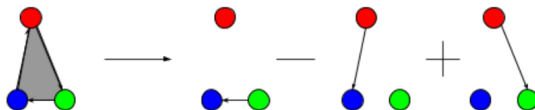
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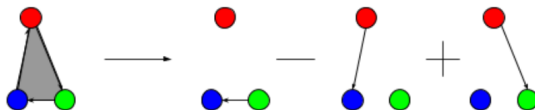
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Maps triangle to alternating sum of its edges and tetrahedron to sum of its faces.



Using this map we can study how simplices are connected to each other!

Studying topology of simplicial complex using homology

the homology group

Important object to study is the so-called *k-th homology group* defined as

$$H_k^\epsilon = (\ker \partial_k^\epsilon) / (\operatorname{im} \partial_{k+1}^\epsilon) .$$

- Quotient of vector spaces \leftrightarrow subtracting bases of vector spaces.

Studying topology of simplicial complex using homology

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- ▶ Quotient of vector spaces \leftrightarrow subtracting bases of vector spaces.

Its dimension, called the *k-th betti-number*, is an important topological feature.

$$\beta_k^\epsilon = \dim H_k^\epsilon.$$

- ▶ Turns out: β_k^ϵ is equal to number of *k*-dimensional holes at scale ϵ .

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Goal in TDA: compute β_k^ϵ to extract topological features of your point cloud.

Studying topology of simplicial complex using homology

Combinatorial Laplacian and Hodge theory

To compute β_k^ϵ we consider the so-called *k-th combinatorial Laplacian*

$$\Delta_k^\epsilon := \partial_k^T \partial_k + \partial_{k+1} \partial_{k+1}^T : \mathcal{H}_k^\epsilon \rightarrow \mathcal{H}_k^\epsilon.$$

► Hermitian matrix!

Studying topology of simplicial complex using homology

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We do so because it can be shown that the following holds

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Question: can we use quantum computers to efficiently compute this dimension?

What can quantum computers bring to the table?

Quantum linear algebra: Hamiltonian simulation and quantum phase estimation

Quantum computers are generally very good at doing linear algebra.

- ▶ Δ_k^ϵ is Hermitian \implies Hamiltonian simulation can implement $U = e^{i\Delta_k^\epsilon}$!
- ▶ Also, can use quantum phase estimation to investigate eigenvalues of U .

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We are interested in the number of eigenvalues that are equal to 0 since

$$\beta_k^\epsilon = \dim(\ker \Delta_k^\epsilon) = \#\{j : \lambda_j(\Delta_k^\epsilon) = 0\},$$

where $\lambda_1(\Delta_k^\epsilon), \dots, \lambda_N(\Delta_k^\epsilon)$ denote the eigenvalues of Δ_k^ϵ .

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LGZ algorithm: combine Hamiltonian simulation and QPE to estimate number of eigenvalues that are equal to 0.

The Lloyd, Garnerone & Zanardi algorithm

an overview of the algorithm

Goal: estimate $\beta_k^\epsilon = \dim(\ker \Delta_k^\epsilon) = \#\{j : \lambda_j(\Delta_k^\epsilon) = 0\}$.

To do so, the LGZ algorithm takes the following steps:

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1. Use Grover's algorithm to prepare the *simplex-state* given by

$$|\psi_k\rangle := \frac{1}{\sqrt{\dim \mathcal{H}_k^\epsilon}} \sum_{j \in \text{VR}(\mathcal{D}, \epsilon)_k} |j\rangle.$$

- I.e., the uniform superposition over the complex vector space \mathcal{H}_k^ϵ .

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 - ▶ Actually, since Δ_k^ϵ is not sparse we implement e^{iB_k} , for $B_k \approx \sqrt{\Delta_k^\epsilon}$.

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4. Estimate the number of eigenvalues $\lambda_j(\Delta_k^\epsilon) = 0$.
 - ▶ Either using quantum counting or Monte-Carlo estimation.

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a Grover-step to prepare simplex state

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- First, check whether j contains exactly k ones.
- Afterwards, check pairwise distance between all v_i for which $j_i = 1$.
 - Requires a total of $O(k^2)$ computations of pairwise distances $\|v_i - v_j\|$.

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Allows us to efficiently implement a quantum oracle to the membership function

$$f : \{0, 1\}^n \rightarrow \{0, 1\}$$

$$f(j) = \begin{cases} 1 & \text{if } j \in \text{VR}(\mathcal{D}, \epsilon)_k, \\ 0 & \text{else.} \end{cases}$$

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Therefore, Grover's algorithm allows us to implement the mapping

$$\frac{1}{\sqrt{2^n}} \sum_{j \in \{0, 1\}^n} |j\rangle \mapsto |\psi_k\rangle = \frac{1}{\sqrt{\dim \mathcal{H}_k^\epsilon}} \sum_{j \in \text{VR}(\mathcal{D}, \epsilon)_k} |j\rangle.$$

The Lloyd, Garnerone & Zanardi algorithm

using Hamiltonian simulation and QPE to uniformly sample from the eigenvalues of Δ_k^ϵ

We would like to use HS and QPE to sample from the eigenvalues of $e^{i\Delta_k^\epsilon}$.

- ▶ Similar to Problem 3 of last tutorial, this gives us the eigenvalues of Δ_k^ϵ .
- ▶ We don't know eigenvectors of Δ_k^ϵ . What input quantum state do we use?

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From the simplex-state $|\psi_k\rangle$ we can efficiently prepare the mixed state

$$P_{\mathcal{H}_k^\epsilon} = \frac{1}{\dim \mathcal{H}_k^\epsilon} \sum_{j \in \text{VR}(\mathcal{D}, \epsilon)_k} |j\rangle \langle j| = \text{"Projector onto } \mathcal{H}_k^\epsilon \text{"}.$$

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We can rewrite this mixed state in terms of the eigenvectors of Δ_k^ϵ

$$P_{\mathcal{H}_k^\epsilon} = \frac{1}{\dim \mathcal{H}_k^\epsilon} \sum_{j=1}^{\dim \mathcal{H}_k^\epsilon} |\psi_j\rangle \langle \psi_j|.$$

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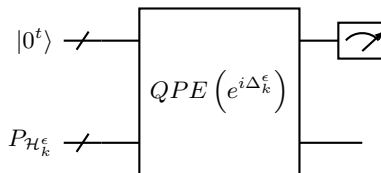
So, the mixed state $P_{\mathcal{H}_k^\epsilon}$ is the j -th eigenstate $|\psi_j\rangle$ with probability $\frac{1}{\dim \mathcal{H}_k^\epsilon}$.

Let's use this state as input to the HS + QPE routine!

The Lloyd, Garnerone & Zanardi algorithm

the circuit and the output distribution

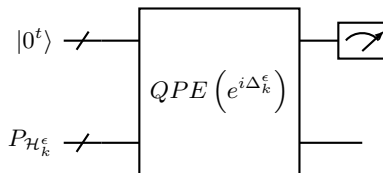
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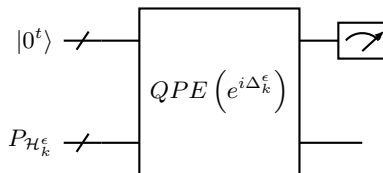
$P_{\mathcal{H}_k^\epsilon}$ is in an eigenstate $|\psi_j\rangle$ with uniform probability, thus the probability of measuring an eigenvalue λ is

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$$\Pr(\lambda) = \frac{\#\{j \mid \lambda_j = \lambda\}}{\dim \mathcal{H}_k^\epsilon}.$$

In particular, the probability of measuring $\lambda = 0$ is given by

$$\Pr(0) = \frac{\#\{j \mid \lambda_j = 0\}}{\dim \mathcal{H}_k^\epsilon} = \frac{\beta_k^\epsilon}{\dim \mathcal{H}_k^\epsilon}.$$

Using quantum counting or Monte-Carlo estimation, we can now estimate β_k^ϵ .

References

where to find the papers

- ▶ Nature: <https://www.nature.com/articles/ncomms10138>
- ▶ Arxiv: <https://arxiv.org/pdf/1408.3106.pdf>
- ▶ Nice review paper: <https://arxiv.org/pdf/1906.07673.pdf>

My research

why am I looking at this algorithm? what are the interesting questions?

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- ▶ **Question:** can we use samples from the eigenvalues of Δ_k^ϵ for something else than computing Betti numbers?
 - So-called applications of “simplicial spectral theory”.