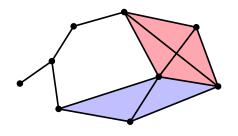
A (SIMPLE) CLASSICAL ALGORITHM FOR ESTIMATING BETTI NUMBERS



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with Sander Gribling, Dániel Szabó (IRIF, Paris) and Sayantan Sen (ISI Kolkata)

Phasecraft, February '23

BETTI NUMBERS

A QUANTUM ALGORITHM

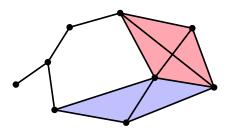
A CLASSICAL ALGORITHM

(abstract) simplicial complex

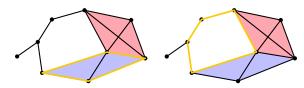
= downward closed set system $K \subseteq 2^{[n]}$

(abstract) simplicial complex

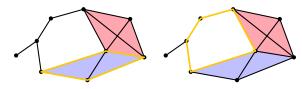
= downward closed set system $K \subseteq 2^{[n]}$ e.g., clique complex



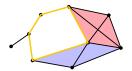
a *k*-dimensional hole **has** no boundary



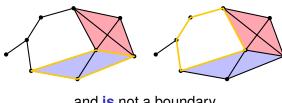
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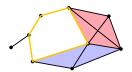
and is not a boundary



a k-dimensional hole has no boundary

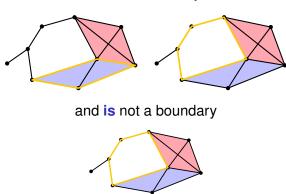


and is not a boundary



k-th Betti number $\beta_k = \# k$ -dimensional holes

a *k*-dimensional hole **has** no boundary

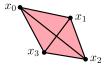


k-th Betti number β_k = # k-dimensional holes relevant notion in topological data analysis

algebraically:

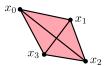
algebraically:

$$k$$
-face $|S\rangle = |[x_0, x_1, \dots, x_k]\rangle$

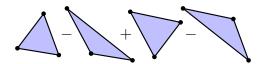


algebraically:

$$k$$
-face $|S\rangle = |[x_0, x_1, \dots, x_k]\rangle$



boundary operator $\partial_k |S\rangle = \sum_{\ell=0}^k (-1)^\ell |S\setminus \{x_\ell\}\rangle$



$$|\psi\rangle = \sum \alpha_{S} |S\rangle$$

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has no boundary

$$\partial_k |\psi\rangle = 0$$

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has no boundary

$$\partial_k \ket{\psi} = 0$$

and is not a boundary

$$|\psi\rangle \neq \partial_{k+1} |\phi\rangle, \ \forall |\phi\rangle$$

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$$|\psi\rangle \neq \partial_{k+1} |\phi\rangle, \ \forall |\phi\rangle$$



$$|\psi\rangle \in \ker(\partial_k) \backslash \operatorname{im}(\partial_{k+1})$$

$$|\psi\rangle = \sum \alpha_S |S\rangle$$

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Betti number $\beta_k = \dim (\ker(\partial_k) \setminus \operatorname{im}(\partial_{k+1}))$

$$\Delta_k = \partial_k^{\dagger} \partial_k + \partial_{k+1} \partial_{k+1}^{\dagger}$$

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 we have

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

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computable in time $poly(n^k)$

$$\Delta_k = \partial_k^{\dagger} \partial_k + \partial_{k+1} \partial_{k+1}^{\dagger}$$

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

1

computable in time $poly(n^k)$

clique complexes: exponential in input size!

faster algorithms?

faster algorithms?

QMA1-hard to multiplicatively approximate

Betti number of clique complex

[Crichigno-Kohler '22]

faster algorithms?

QMA1-hard to multiplicatively approximate

Betti number of clique complex

[Crichigno-Kohler '22]

additive approximation $\beta_k/d_k \pm \varepsilon$ in time poly(n)?

Hermitian matrix A dimension $d \le n!$ $\operatorname{poly}(n)$ -sparse nonzero eigenvalues in $[\gamma, 1]$

 $\begin{array}{c} \text{Hermitian matrix } A \\ \text{dimension } d \leq n! \\ \text{poly}(n)\text{-sparse} \\ \text{nonzero eigenvalues in } [\gamma, 1] \end{array}$

?
$$\frac{\dim(\ker(A))}{d} \pm \varepsilon$$
 ?

 $\begin{array}{c} \text{Hermitian matrix } A \\ \text{dimension } d \leq n! \\ \text{poly}(n) \text{-sparse} \\ \text{nonzero eigenvalues in } [\gamma, 1] \end{array}$

?
$$\frac{\dim(\ker(A))}{d} \pm \varepsilon$$
 ?

sampling access to *A*: random element from domain, query neighbors

BETTI NUMBERS

A QUANTUM ALGORITHM

in $poly(n, 1/\gamma, 1/\varepsilon)$

A CLASSICAL ALGORITHM

• Hamiltonian simulation

Hamiltonian simulation

given sparse access to Hamiltonian H, maps

$$|\psi\rangle \stackrel{\mathsf{HS}}{\longrightarrow} e^{iH} \, |\psi
angle$$

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quantum phase estimation

Hamiltonian simulation

given sparse access to Hamiltonian H, maps

$$|\psi\rangle \stackrel{\mathrm{HS}}{\longrightarrow} e^{iH} |\psi\rangle$$

quantum phase estimation

for a unitary $U = \sum_{\ell} e^{i\theta_{\ell}} \ket{v_{\ell}} \bra{v_{\ell}}$, maps

$$\sum_{\ell} \alpha_{\ell} \left| v_{\ell} \right\rangle \left| 0 \right\rangle \stackrel{\mathsf{QPE}}{\longrightarrow} \sum_{\ell} \alpha_{\ell} \left| v_{\ell} \right\rangle \left| \tilde{\theta}_{\ell} \right\rangle$$

with $|\tilde{\theta}_{\ell} - \theta_{\ell}| \leq \varepsilon$ using $1/\varepsilon$ calls to U

quantum algorithm:

[Lloyd-Garnerone-Zanardi '14]

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let
$$H = \Delta_k$$
 and $U = e^{iH}$

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1. pick random k-face

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angle = \sum_{\ell} lpha_{\ell}^{S} |v_{\ell}
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2. apply quantum phase estimation on $|S\rangle$ and U with precision γ

$$\sum_{\ell} \alpha_{\ell}^{S} \left| v_{\ell} \right\rangle \left| 0 \right\rangle \longrightarrow \sum_{\ell} \alpha_{\ell}^{S} \left| v_{\ell} \right\rangle \left| \tilde{\theta}_{\ell} \right\rangle$$

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3. measure phase register: "0" with probability

$$\mathbb{E}\|\Pi_0|S\rangle\|^2 = \mathbb{E}\sum_{\ell:\tilde{\theta}_s=0}|\alpha_\ell^S|^2 = \beta_k/d_k$$

[Lloyd-Garnerone-Zanardi '14]

- **1.** pick random *k*-face $|S\rangle = \sum_{\ell} \alpha_{\ell}^{S} |v_{\ell}\rangle$
- **2.** apply quantum phase estimation on $|S\rangle$ and U with precision γ

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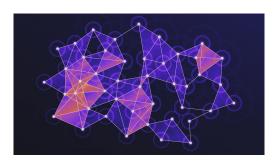
3. measure phase register: "0" with probability $\|\Pi_0 |S\rangle\|^2 = \beta_k/d_k$



estimate
$$\frac{\beta_k}{d_k} \pm \varepsilon$$
 in time $poly(n, 1/\gamma, 1/\varepsilon)$

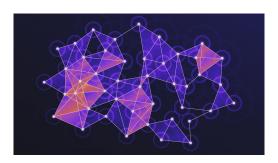


After a Quantum Clobbering, One Approach Survives Unscathed





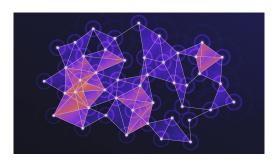
After a Quantum Clobbering, One Approach Survives Unscathed



? interesting regimes ? (clique complex with large gap and many holes)



After a Quantum Clobbering, One Approach Survives Unscathed



? interesting regimes ? (clique complex with large gap and many holes)

? classical algorithm?

BETTI NUMBERS

A QUANTUM ALGORITHM

in $poly(n, 1/\gamma, 1/\varepsilon)$

A CLASSICAL ALGORITHM

in $\operatorname{poly}(n^{\frac{1}{\gamma}\log\frac{1}{\varepsilon}})$

main classical technique:

• path integral Monte Carlo

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for 2^n -dimensional matrix H, return estimate

$$\langle y|H^r|x\rangle \pm \varepsilon$$

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path integral Monte Carlo

for 2^n -dimensional matrix H, return estimate

$$\langle y|H^r|x\rangle \pm \varepsilon$$

in time $poly(n, r, ||H||_1^r, 1/\varepsilon)$

$$\langle y|H^r|x_0\rangle = \sum_{x_1,\dots,x_r} \langle y|x_r\rangle \langle x_r|H|x_{r-1}\rangle \dots \langle x_2|H|x_1\rangle \langle x_1|H|x_0\rangle$$

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= $\mathbb{E}_{(x_0,\dots,x_r)}[\langle y|x_r\rangle],$

$$\langle y|H^r|x_0\rangle = \sum_{x_1,\dots,x_r} \langle y|x_r\rangle \langle x_r|H|x_{r-1}\rangle \dots \langle x_2|H|x_1\rangle \langle x_1|H|x_0\rangle$$

= $\mathbb{E}_{(x_0,\dots,x_r)}[\langle y|x_r\rangle],$

with (x_0, \ldots, x_r) path sampled from Markov chain P with

$$P(x, x') = \langle x' | H | x \rangle$$

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 \rightarrow unbiased estimator, variance ≤ 1

$$\langle y|H^r|x_0\rangle = \sum_{r=1}^{\infty} \langle y|x_r\rangle \langle x_r|H|x_{r-1}\rangle \dots \langle x_2|H|x_1\rangle \langle x_1|H|x_0\rangle$$

$$\langle y|H^r|x_0\rangle = \sum_{x_1,\dots,x_r} \langle y|x_r\rangle \langle x_r|H|x_{r-1}\rangle \dots \langle x_2|H|x_1\rangle \langle x_1|H|x_0\rangle$$
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with

$$Y(x_0,\ldots,x_r) = \langle y|x_r\rangle \prod_{\ell=0}^{r-1} \operatorname{sign}(\langle x_{\ell+1}|H|x_{\ell}\rangle) \cdot ||H|x_{\ell}\rangle ||_1$$

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and (x_0, \ldots, x_r) path sampled from Markov chain P with

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and (x_0, \ldots, x_r) path sampled from Markov chain P with

$$P(x, x') = \frac{|\langle x'|H|x\rangle|}{\|H|x\rangle\|_1}$$

 \rightarrow unbiased estimator, variance $\leq \|H\|_1^{2r}$

Betti numbers via PIMC:

$$H = I - \Delta_k / \lambda_{\text{max}}$$

$$\sigma(H) \xrightarrow[0]{\quad \text{$\mathbf{x} \ \mathbf{x} \times \mathbf{x} \times$$

Betti numbers via PIMC:

$$H = I - \Delta_k/\lambda_{\max}$$

$$\sigma(H) \underset{0}{\vdash \times \times \times \times \times \times \times \times + \dots \times } \beta_k$$

so that

$$\operatorname{Tr}(H^r) = \beta_k \pm \varepsilon d_k$$
if $r \ge \frac{1}{\gamma} \log \frac{1}{\varepsilon}$

$$\frac{1}{d_k}\operatorname{Tr}(H^r)$$

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$$= \mathbb{E}_{(x_0, \dots, x_r)} \left[Y(x_0, \dots, x_r) \right]$$

estimate $\beta_k/d_k \pm \varepsilon$ in time

$$\operatorname{poly}(n, r, ||H||_1^r, 1/\varepsilon) \in \operatorname{poly}\left(n^{\frac{1}{\gamma}\log\frac{1}{\varepsilon}}\right)$$

Improvements:

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• approximate H^r by degree- $\widetilde{O}(\sqrt{r})$ polynomials

$$n^{rac{1}{\gamma}\lograc{1}{arepsilon}} \longrightarrow n^{rac{1}{\sqrt{\gamma}}\lograc{1}{arepsilon}}$$

Improvements:

• approximate H^r by degree- $\widetilde{O}(\sqrt{r})$ polynomials

$$n^{\frac{1}{\gamma}\log\frac{1}{\varepsilon}}\quad\longrightarrow\quad n^{\frac{1}{\sqrt{\gamma}}\log\frac{1}{\varepsilon}}$$

• better bound on $||H||_1 \in O(n/k)$ for clique complexes

$$n^{\frac{1}{\sqrt{\gamma}}\log\frac{1}{\varepsilon}} \longrightarrow \left(\frac{n}{\lambda_{\max}}\right)^{\frac{1}{\sqrt{\gamma}}\log\frac{1}{\varepsilon}} \leq \left(\frac{n}{k}\right)^{\frac{1}{\sqrt{\gamma}}\log\frac{1}{\varepsilon}}$$

Betti number estimation in $\operatorname{poly}(n,1/\gamma,1/\varepsilon) \quad \text{(quantum)} \\ \operatorname{poly}(n^{\frac{1}{\sqrt{\gamma}}\log\frac{1}{\varepsilon}}) \quad \text{or} \quad \operatorname{poly}(2^{\frac{1}{\sqrt{\gamma}}\log\frac{1}{\varepsilon}}) \quad \text{(classical)}$

Betti number estimation in $\operatorname{poly}(n,1/\gamma,1/\varepsilon) \quad \text{(quantum)}$ $\operatorname{poly}(n^{\frac{1}{\sqrt{\gamma}}\log\frac{1}{\varepsilon}}) \quad \text{or} \quad \operatorname{poly}(2^{\frac{1}{\sqrt{\gamma}}\log\frac{1}{\varepsilon}}) \quad \text{(classical)}$

close gap?

$$_{\rm (slightly\ more)}$$
 general case is DQC1-hard for $\varepsilon, \gamma = 1/\operatorname{poly}(n)$ [Cade-Crichigno '21]

Betti number estimation in
$$\underset{\text{poly}(n, 1/\gamma, 1/\varepsilon)}{\operatorname{poly}(n, 1/\gamma, 1/\varepsilon)} \ \ \text{(quantum)}$$

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close gap?

(slightly more) general case is DQC1-hard for
$$\varepsilon, \gamma = 1/\operatorname{poly}(n)$$
 [Cade-Crichigno '21]

• query complexity?

"Betti numbers are testable" [Elek '10]

Betti number estimation in
$$\operatorname{poly}(n,1/\gamma,1/\varepsilon) \quad \text{(quantum)}$$

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$$arepsilon, \gamma = 1/\operatorname{poly}(n)$$
 [Cade-Crichigno '21]

query complexity?

"Betti numbers are testable"
[Elek '10]

run classical algorithm?

find interesting regimes?

RELATED WORKS

"Dequantizing the Quantum Singular Value Transformation"

by S. Gharibian and F. Le Gall, '21

related ideas

exact path calculation:

space
$$\operatorname{poly}(n) \to n^{\frac{1}{\gamma}\log\frac{1}{\varepsilon}}$$

our PIMC can exploit small $||H||_1$:

$$n^{rac{1}{\gamma}\lograc{1}{arepsilon}} o 2^{rac{1}{\gamma}\lograc{1}{arepsilon}}$$
 for clique complexes

RELATED WORKS

"Quantifying Quantum Advantage in Topological Data Analysis" by D. Berry, Y. Su, C. Gyurik, R. King, J. Basso, A. Del Toro Barba, A. Rajput, N. Wiebe, V. Dunjko and R. Babbush, '22

similar PIMC approach based on (Trotterized) imaginary time evolution

more complex distribution over paths to minimize variance

runtime exponential in k and $1/\varepsilon$

RELATED WORKS

"Betti Numbers are Testable"

by G. Elek, '10

for bounded degree complexes (so $k \in O(1)$)

additive ε -approximation of β_k/d_k with $f(\varepsilon)$ queries

no gap assumptions