Reducing Overhead for Quantum Advantage in Topological Data Analysis

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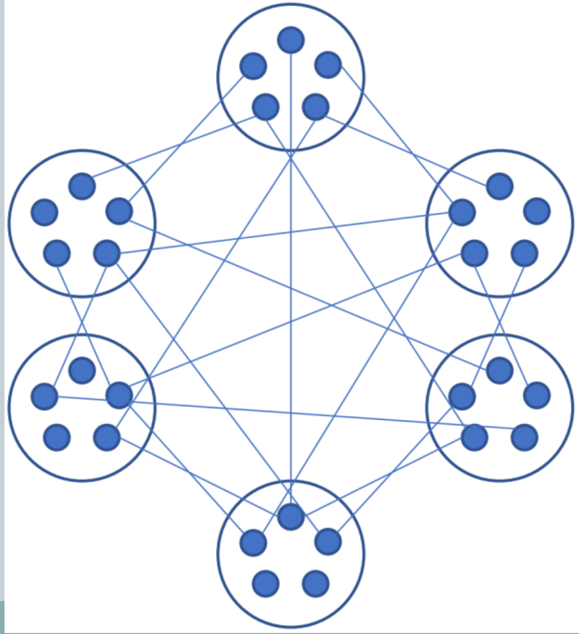
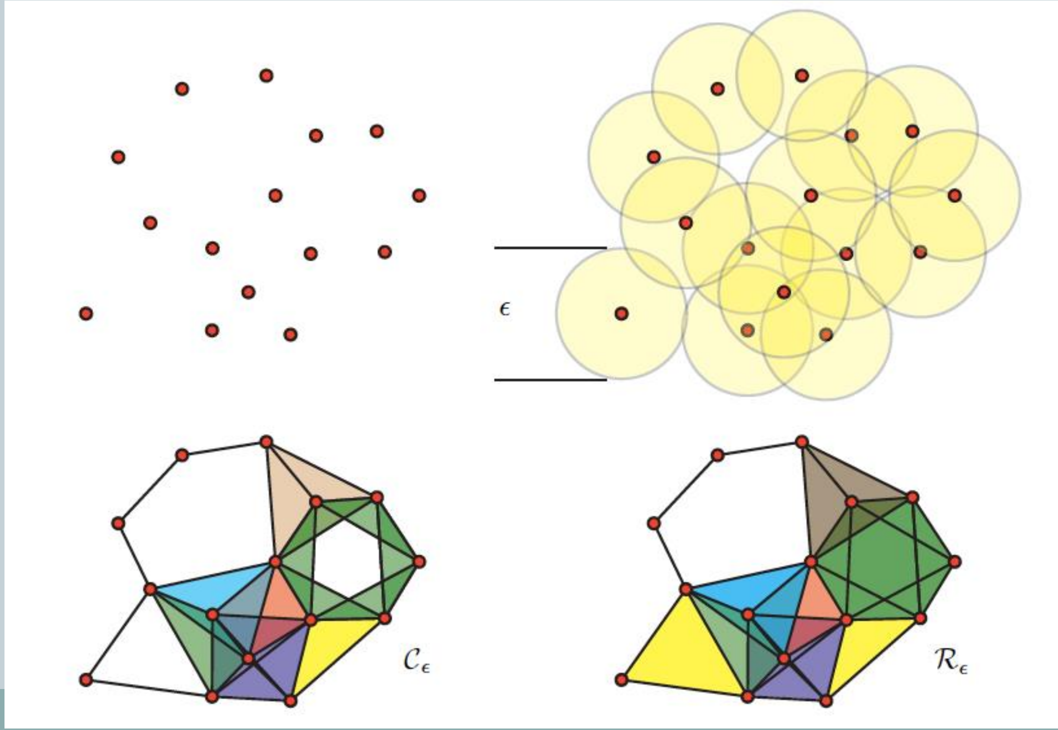


Čech or Vietoris-Rips complex

- Construct a graph based on distances between points.

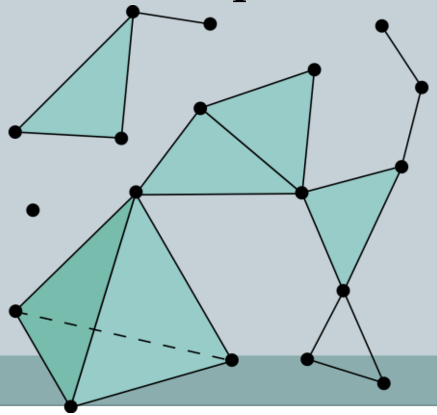


https://mathtuition88.com/2017/01/20/introduction-to-persistent-homolgy-cech-and-vietoris-rips-complex/

Topology

- k-simplex is generalisation of triangles and tetrahedra.

- Simplicial complex is collection of simplices.



Representation on quantum computer

- Vertices of graph represented as ones; 3-clique is $|1\rangle|1\rangle|1\rangle|0\rangle|0\rangle|0\rangle$.
- Boundary map flips 1 to 0 in superposition

$$\partial_k|x\rangle = \sum_{j=0}^{k}(-1)^j|x\backslash(j)\rangle$$

- Hamiltonian is

$$\begin{bmatrix} 0 & \partial_{k-1}^G & 0 \\ {\partial_{k-1}^G}^\dagger & 0 & \partial_k^G \\ 0 & {\partial_k^G}^\dagger & 0 \end{bmatrix}$$

- Dimension of kernel is Betti number β_{k-1}^G.

Recipe for quantum algorithm

- Prepare superposition over states with k ones.
    -
    -
- Simulate the Hamiltonian and estimate the eigenvalue.
    -
    -
- Repeat to find the proportion of zero eigenvalues (dimension of kernel).
    -
    -

S. Lloyd, S. Garnerone, P. Zanardi, Nature Communications 7, 10138 (2016).

Improvements in quantum algorithm

- Prepare superposition over states with k ones.
  - Dicke state preparation problem.
  - Need to check we have a clique.
- Simulate the Hamiltonian and estimate the eigenvalue.
  - Block encode the Hamiltonian rather than simulating time evolution.
  - Use filtering of the zero eigenvalue rather than phase estimation.
- Repeat to find the proportion of zero eigenvalues (dimension of kernel).
  - An amplitude estimation problem.
  - Improve amplitude estimation using Kaiser windows.

Dicke state preparation

$$|111000\rangle \quad + |110100\rangle \quad + |110010\rangle \quad + |110001\rangle \quad + \cdots$$

Dicke state preparation

- Entanglement with ancilla state is allowed:

$$|111000\rangle|\psi_0\rangle + |110100\rangle|\psi_1\rangle + |110010\rangle|\psi_2\rangle + |110001\rangle|\psi_3\rangle + \cdots$$

- Methods to give $O(n \log^2 n)$ complexity:

1. Prepare $|111000\rangle$ then apply our symmetrisation procedure via inverse sort.
2. Inequality test with threshold. Prepare n registers in equal superposition, and produce 1 and 0 via inequality test. Threshold is adjusted until there are k ones.

Detecting the cliques

- Graph given by classical database of edges (pairs of vertices).

- Procedure is:
  1. Run through classical list of edges.
  2. For each pair of nodes, perform Toffoli with qubits corresponding to nodes as control.
  3. Add target into accumulator register.
  4. At the end, check value in accumulator register is $k(k-1)/2$.

- Total complexity (Dicke preparation and clique checking) is

$$6|E| + n\log^2 n$$

Detecting the cliques & amplification

- Graph given by classical database of edges (pairs of vertices).

- Procedure is:
  1. Run through classical list of edges.
  2. For each pair of nodes, perform Toffoli with qubits corresponding to nodes as control.
  3. Add target into accumulator register.
  4. At the end, check value in accumulator register is $k(k-1)/2$.

- Total complexity (Dicke preparation and clique checking) with amplification is

$$\frac{\pi}{4}\sqrt{\frac{\binom{n}{k}}{|\mathrm{Cl}_k(G)|}}\left(6|E| + n\log^2 n\right)$$

Simulating the Hamiltonian

- Hamiltonian

$$\begin{bmatrix} 0 & \partial_{k-1}^{G} & 0 \\ {\partial_{k-1}^{G}}^{\dagger} & 0 & \partial_{k}^{G} \\ 0 & {\partial_{k}^{G}}^{\dagger} & 0 \end{bmatrix}$$

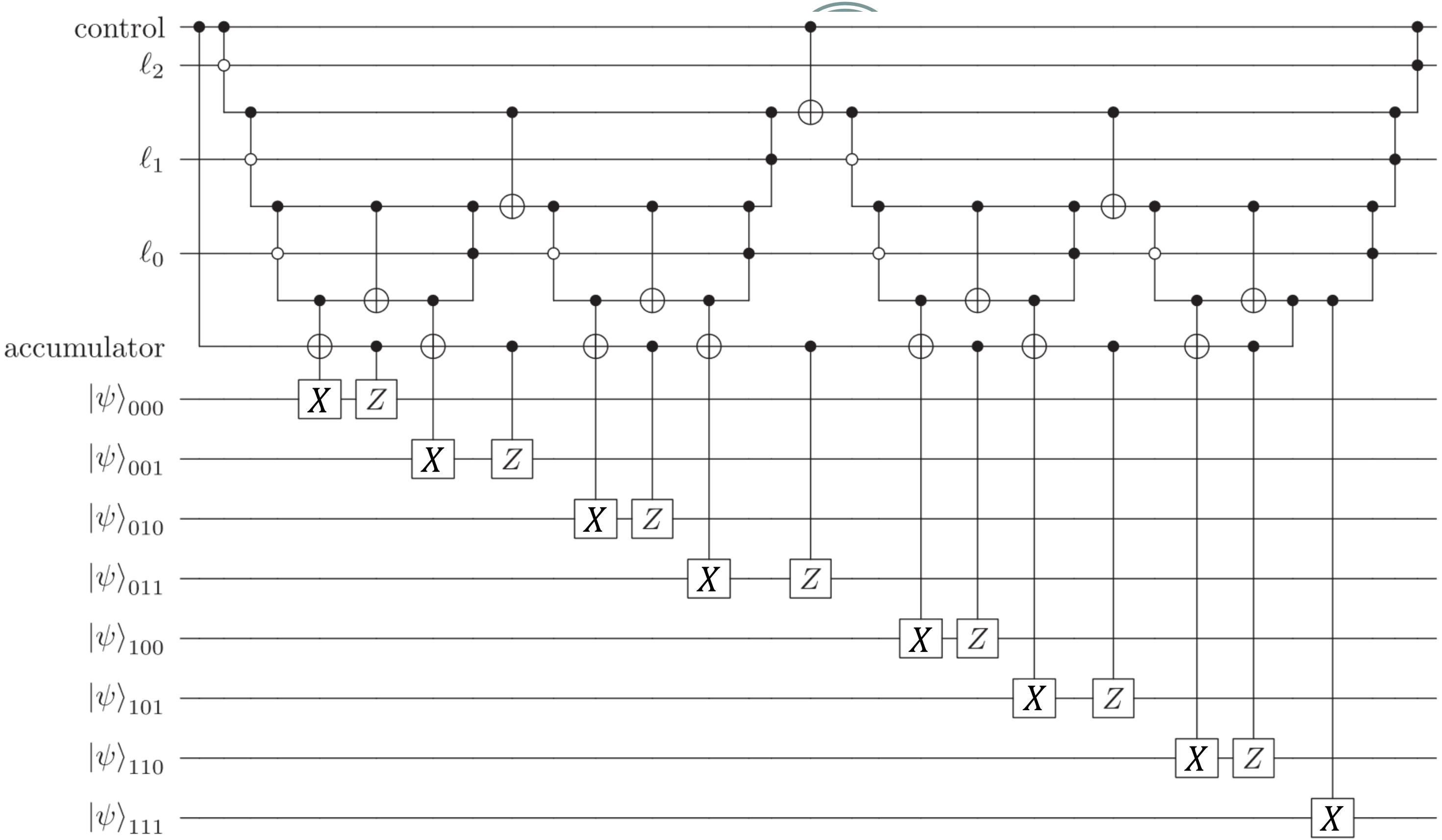
- Equivalent to

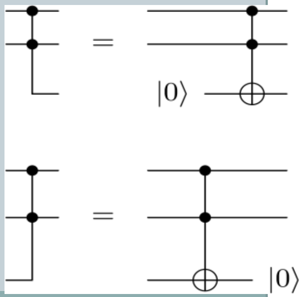
$$H = \sum_{p=1}^{n} Z_1 \otimes Z_2 \otimes \cdots \otimes Z_{p-1} \otimes X_p$$

- Linear combination of unitaries:

1. first prepare equal superposition of p,
2. then apply $Z_1 \otimes Z_2 \otimes \cdots \otimes Z_{p-1} \otimes X_p$ controlled by p register.

Controlled Pauli strings



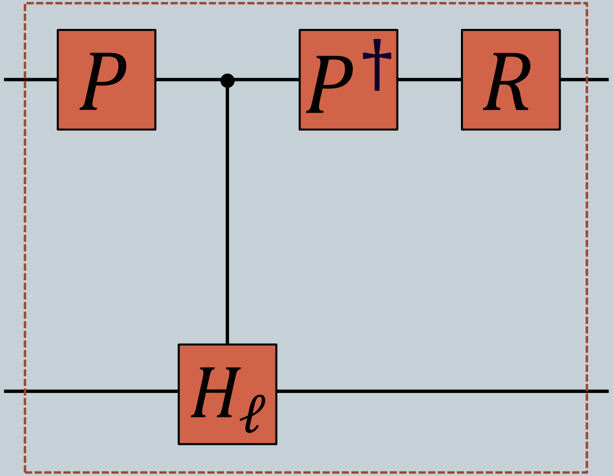


R. Babbush, C. Gidney, D. W. Berry, N. Wiebe, J. McClean, A. Paler, A. Fowler, H. Neven, Physical Review X **8**, 041015 (2018).

Qubitisation

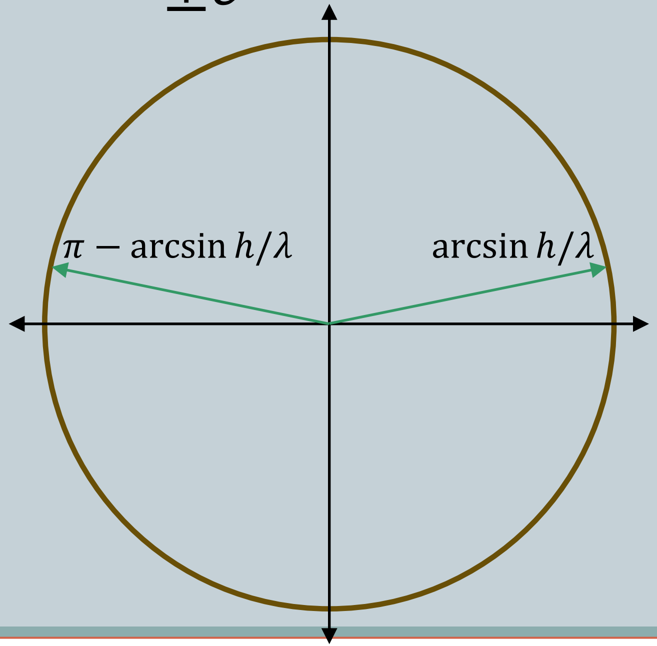
$$H = \sum_{\ell} w_\ell H_\ell$$

$$W =$$



eigenvalues

$$\pm e^{\pm i \arcsin(H/\lambda)}$$



D. W. Berry, M. Kieferová, A. Scherer, Y. R. Sanders, G. H. Low, N. Wiebe, C. Gidney, R. Babbush, npj QI **4**, 22 (2018).

Optimal filtering of eigenvalues

- Linear combination of powers

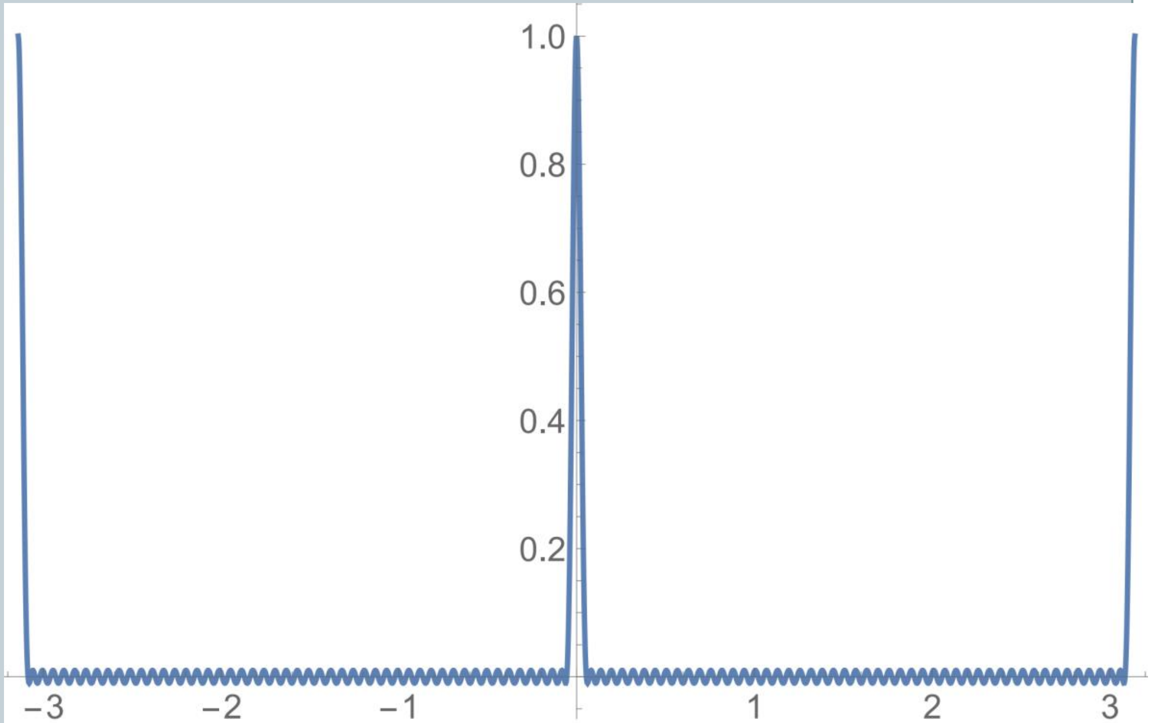
$$\sum_{j=-\ell}^{\ell} w_j U^j$$

- Choose w_j for Chebyshev filter:

$$\epsilon T_\ell(\beta \cos(\phi))$$

- To filter out values beyond gap by ϵ

$$\ell = \frac{n}{\lambda_{\min}} \ln(2/\epsilon)$$

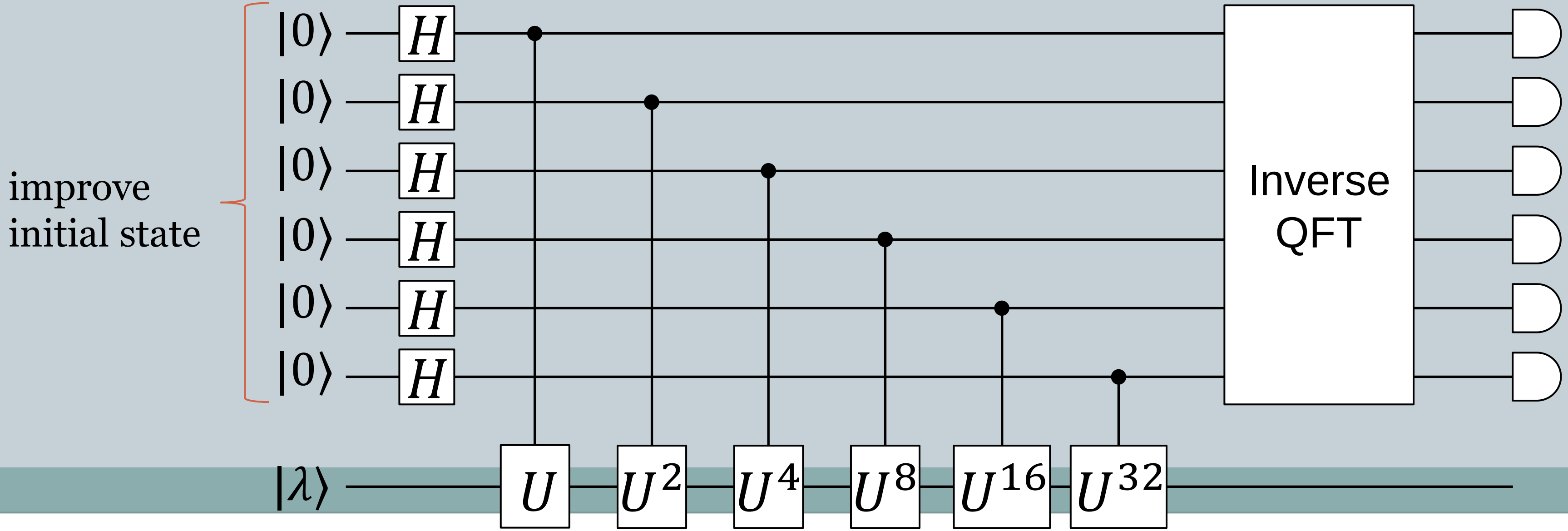


Amplitude estimation via Kaiser window

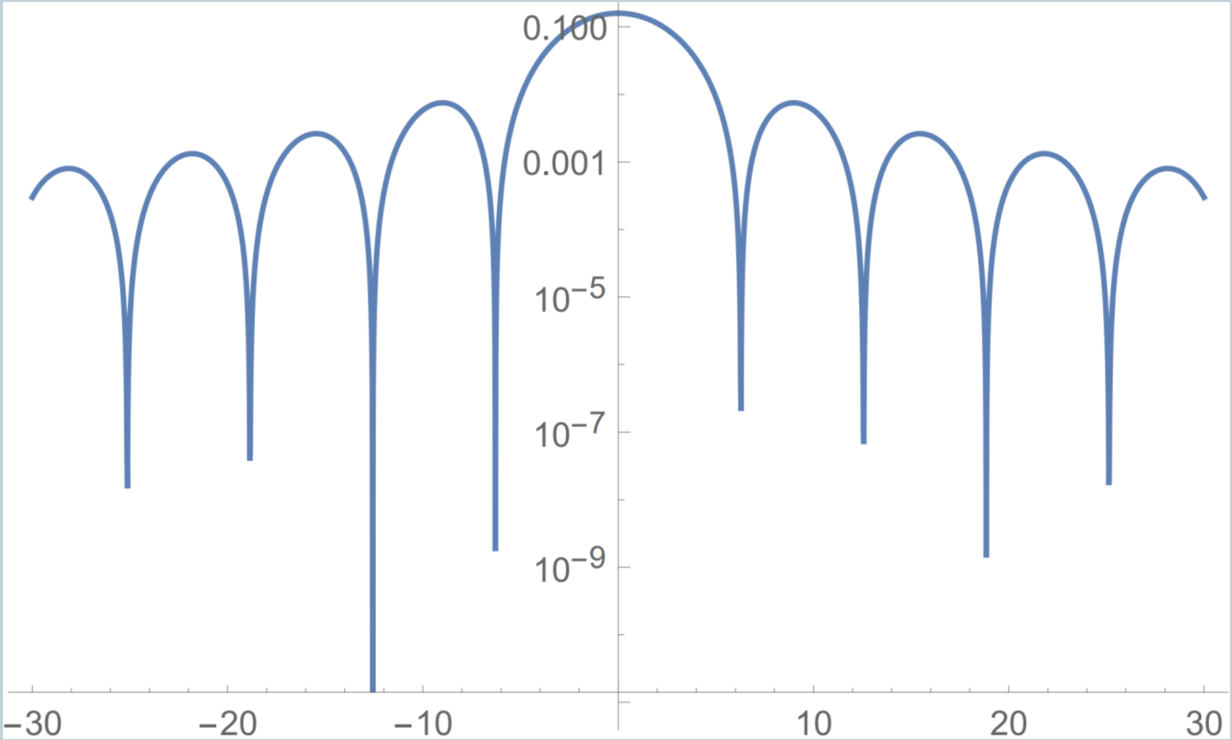
- Amplitude estimation is via phase estimation on step of amplitude amplification.
- For confidence interval width 2ϵ and confidence level $1-\delta$, complexity

$$\frac{1}{2\epsilon}\ln(1/\delta)+O(\epsilon^{-1}\ln\ln(1/\delta))$$

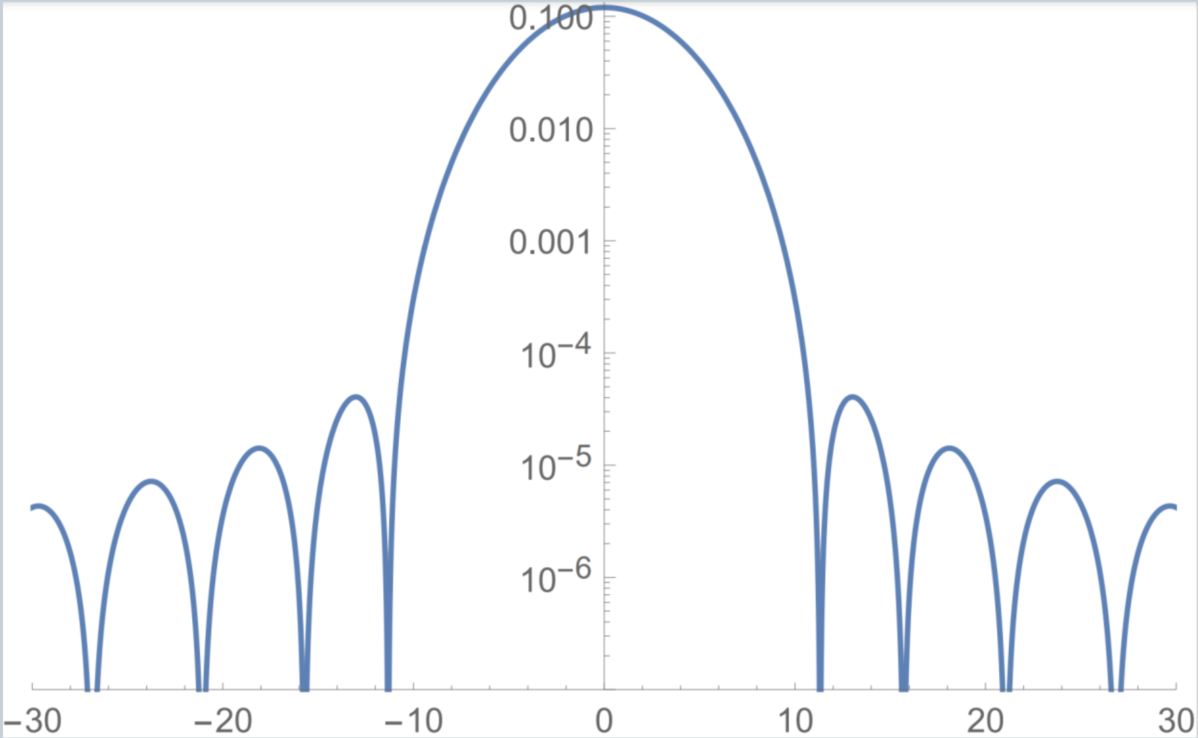
- Standard method gives $1/\delta$.



Window functions - standard



Window functions - Kaiser



Amplitude estimation

- Amplitude estimation gives factor

$$\frac{\ln(1/\delta)}{\epsilon}$$

- ϵ is error in ratio $\sqrt{\beta_{k-1}^G / |\mathrm{Cl}_k(G)|}$.

- For *relative* error of r in β_{k-1}^G, factor is

$$2\,\frac{\ln(1/\delta)}{r}\sqrt{\frac{|\mathrm{Cl}_k(G)|}{\beta_{k-1}^G}}$$

Total costing

- Scaling of complexity

$$2\frac{\ln(1/\delta)}{r}\sqrt{\frac{|\mathrm{Cl}_k(G)|}{\beta_{k-1}^G}} \times \frac{\pi}{4}\sqrt{\frac{\binom{n}{k}}{|\mathrm{Cl}_k(G)|}} \times (6|E| + n\log^2 n)$$

- Simplifies to factor

$$\sqrt{\frac{\binom{n}{k}}{\beta_{k-1}^G}}$$

Large Betti numbers

- Betti number

$$(m-1)^k$$

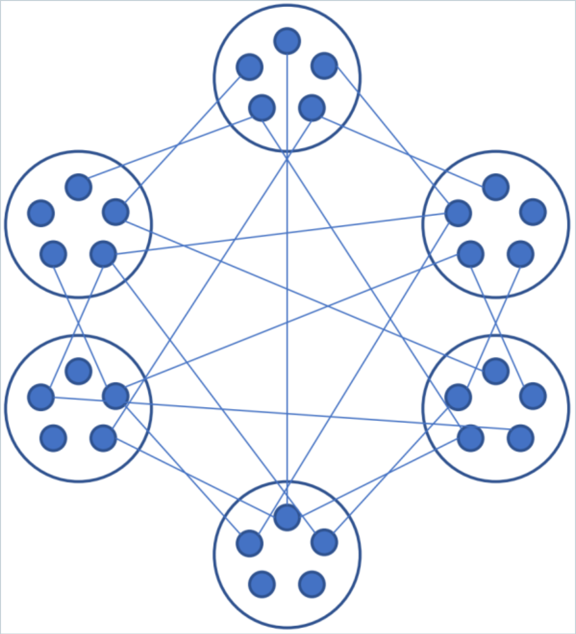
- Classical complexity with $k = n/m$

$$\binom{n}{k} \sim \left(\frac{m^{1+1/m}}{m-1}\right)^n \sim e^{k(1+\ln m)}$$

- Quantum complexity has factor

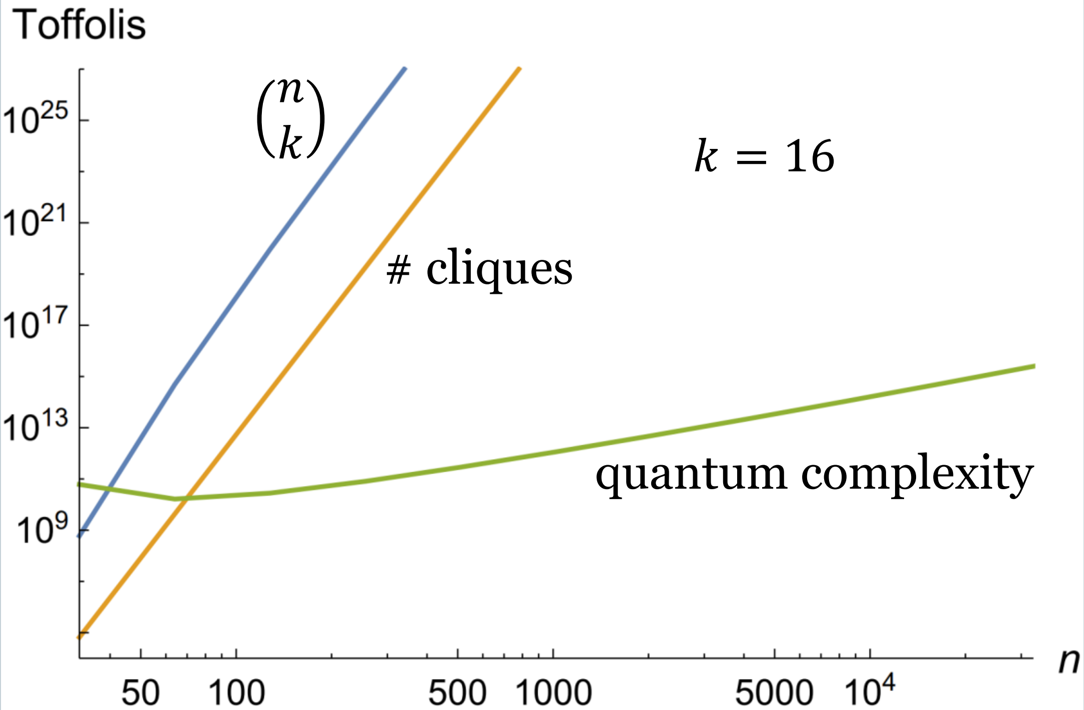
$$\left(\frac{m}{m-1}\right)^{(n/2)(1+1/m)} \sim e^{(k/2)(1+1/m)}$$

- Speedup is roughly $2(1+\ln m)$ root.



Large Betti numbers

- $k = m = 16, \quad n = 256$
- ~80 billion Toffolis
- $2(1 + \ln m) \sim 7.5$
- Dimension $\binom{n}{k} \sim 10^{25}$



Conclusions

- Betti numbers give topological properties of data.
- It can be encoded in Hamiltonian simulation problem.
- Our improved techniques:
  - Dicke state preparation via thresholding.
  - Amplitude estimation with Kaiser windows.
  - Filtering via Chebyshev polynomials.
- Speedup better than square root for large Betti numbers.
- Classically intractable example would take 80 billion Toffolis.

D. W. Berry, Y. Su, C. Gyurik, R. King, J. Basso, A. D. T. Barba, A. Rajput, N. Wiebe, V. Dunjko, R. Babbush, arXiv:2209.13581.