



# Topics in Quantum Topological Data Analysis

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Quantum 6, 855 (2022), arXiv:2209.13581



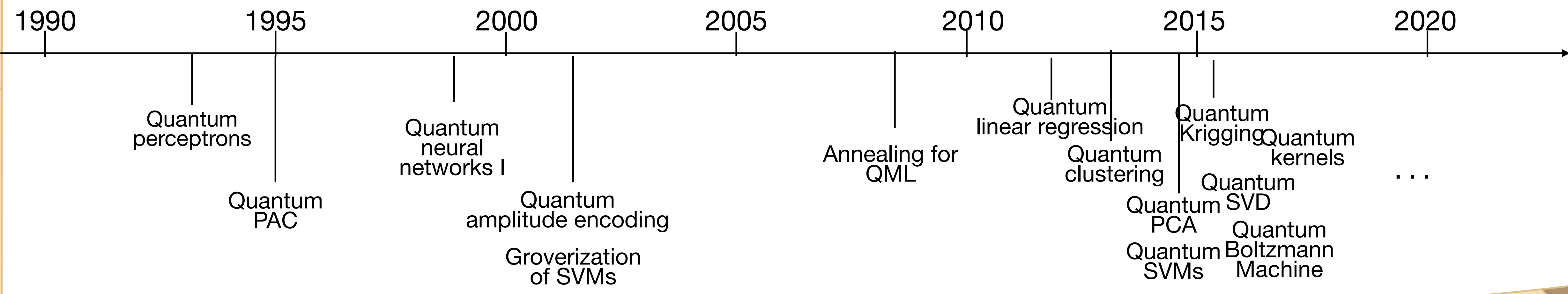
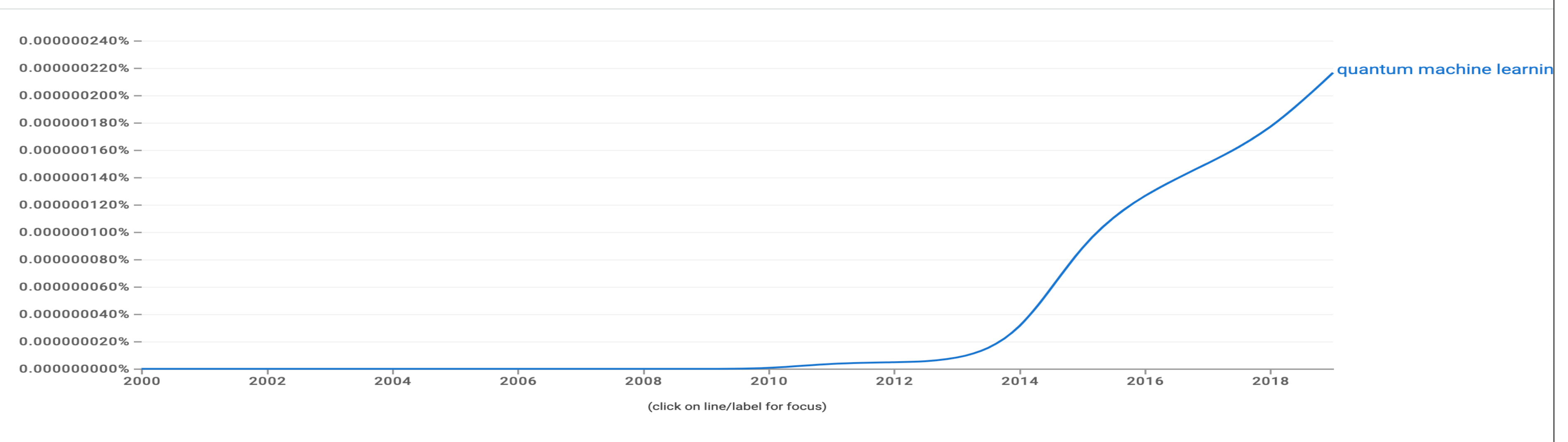
w/ Casper Gyurik

and: Cade, Crichigno, Berry, Su, King, Basso, Del Toro Barba, Rajput, Wiebe, Babbush

## Outline:

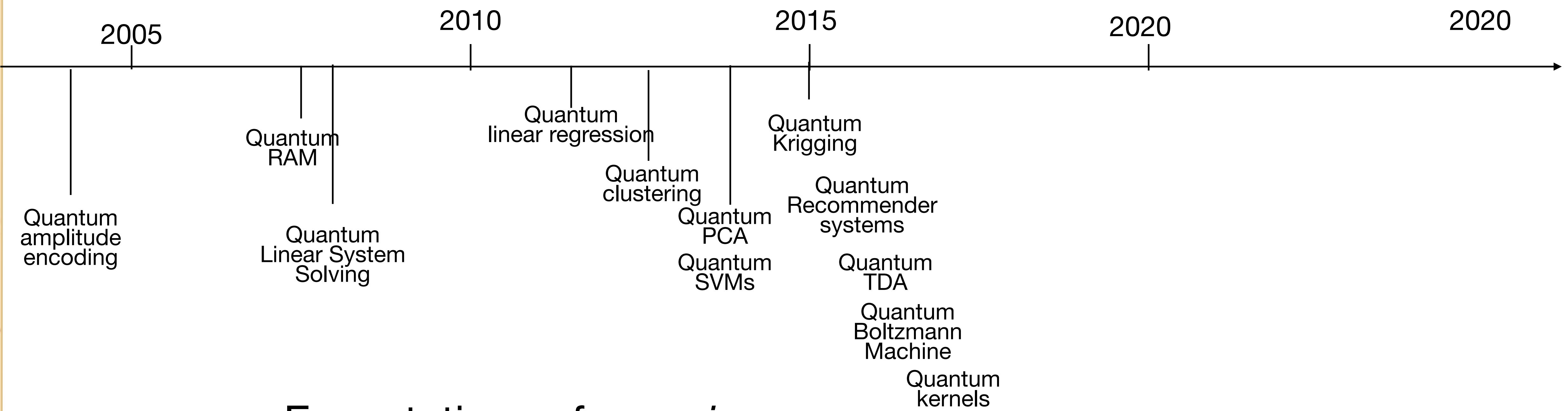
- 1) the motivation
- 2) the TDA problem and the algorithm(s)
- 3) TDA, bounds and complexity theory
- 4) QTDA versus current algorithms
- 5) Other open questions

# Timeline of QML



$\langle aQa \rangle$

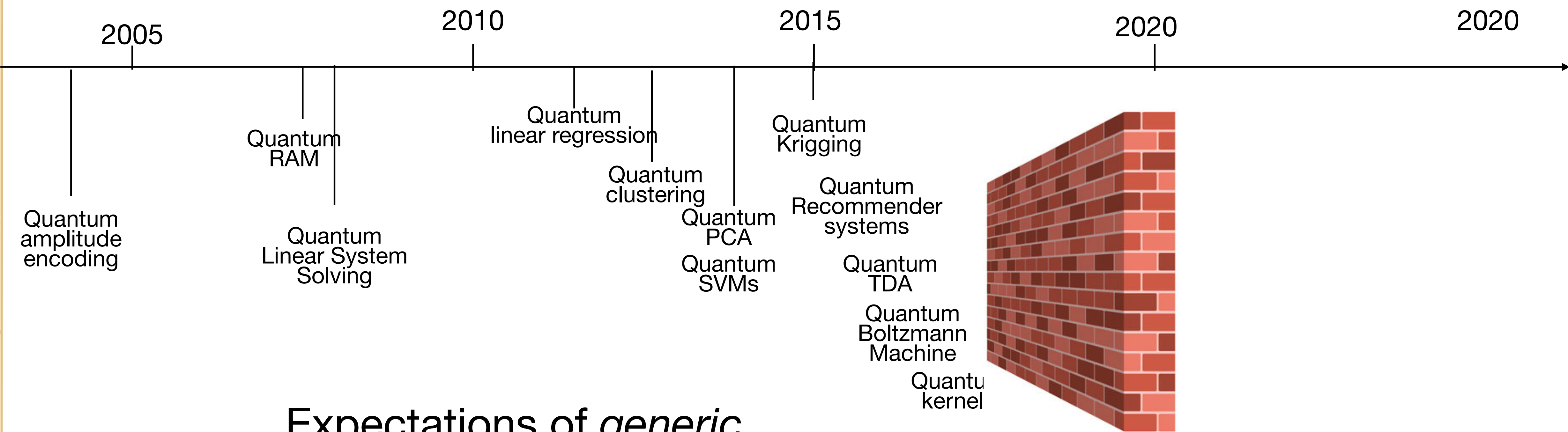
# Timeline of QML



Expectations of *generic* exponential speed-ups

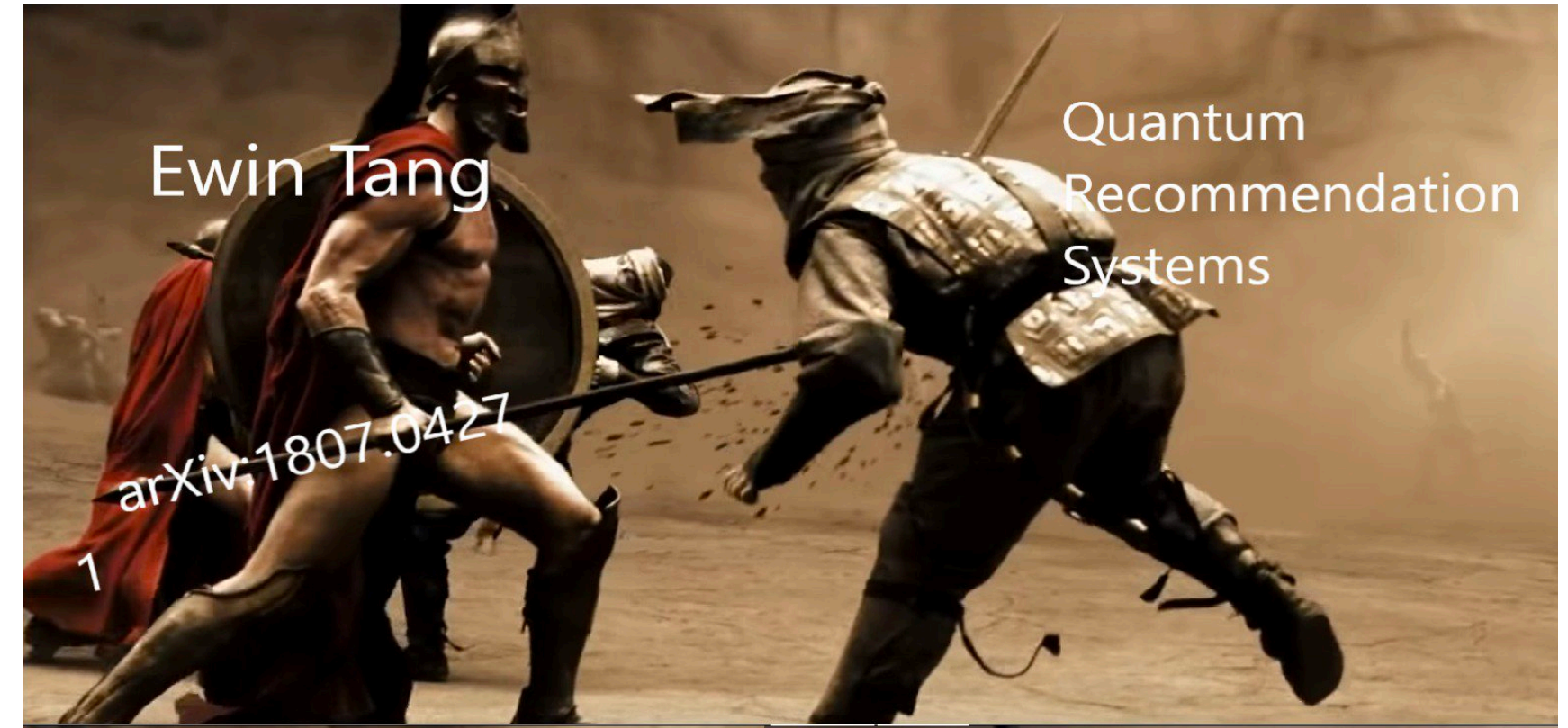
$\langle aQa \rangle$

# Timeline of QML



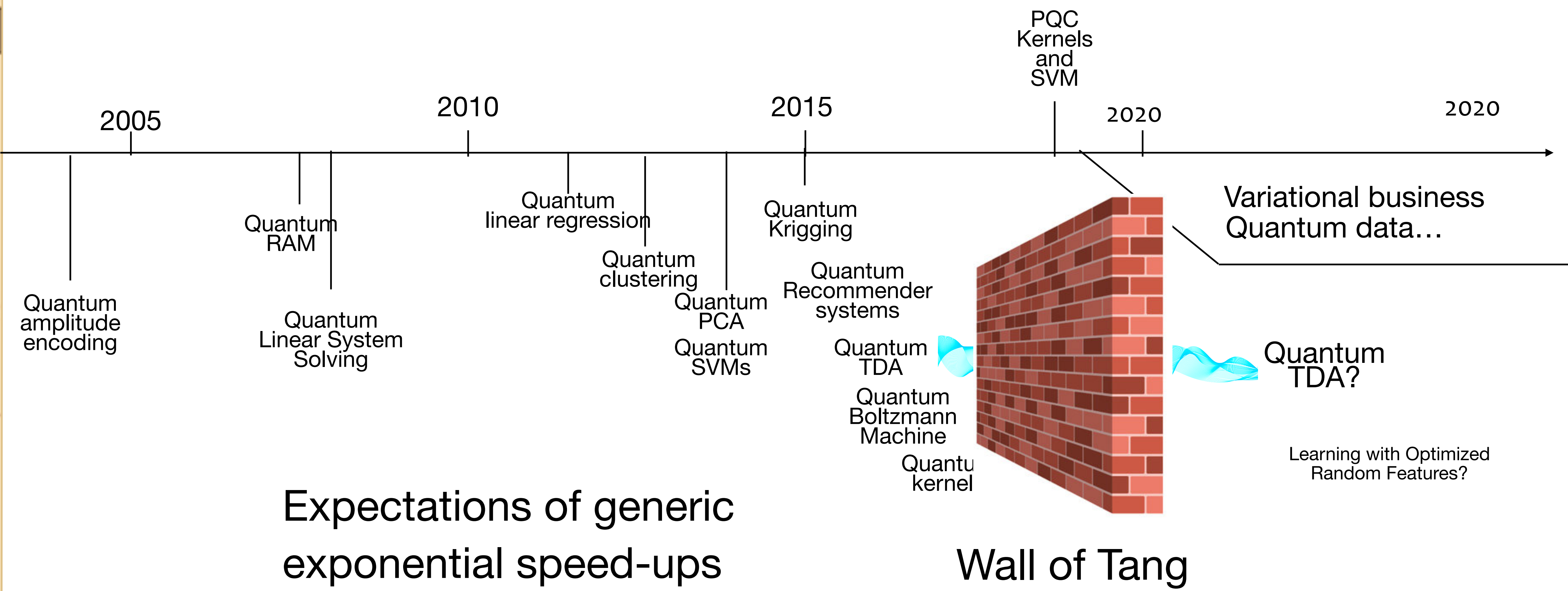
Expectations of *generic* exponential speed-ups

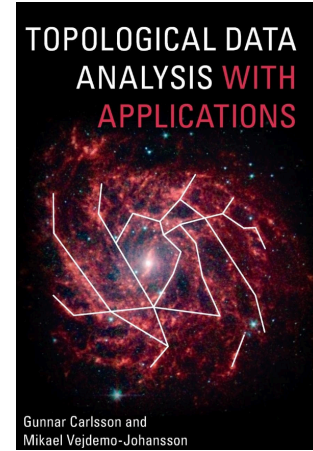
Wall of Tang



$\langle aQa \rangle$

# Timeline of QML

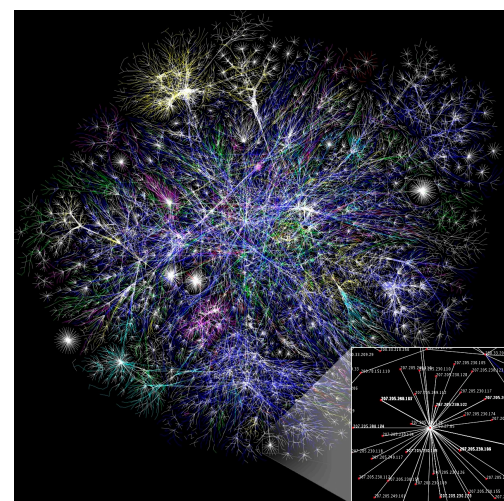




medicine, materials,  
entanglement, time-series...

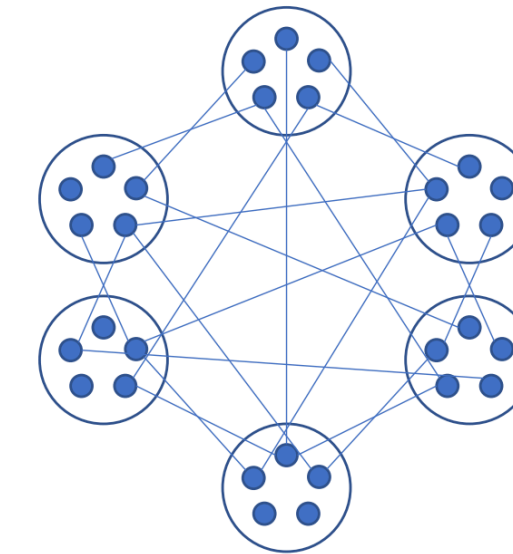
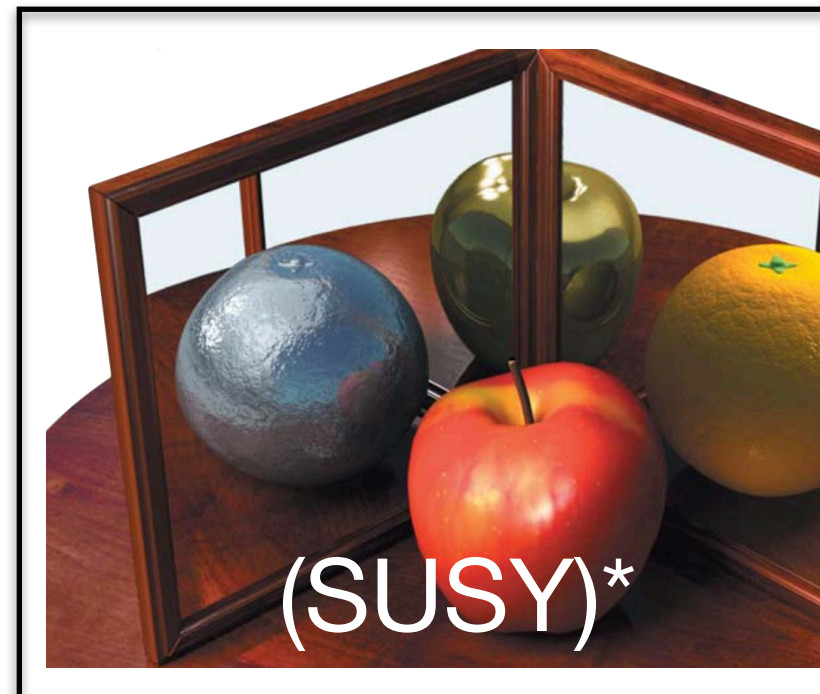
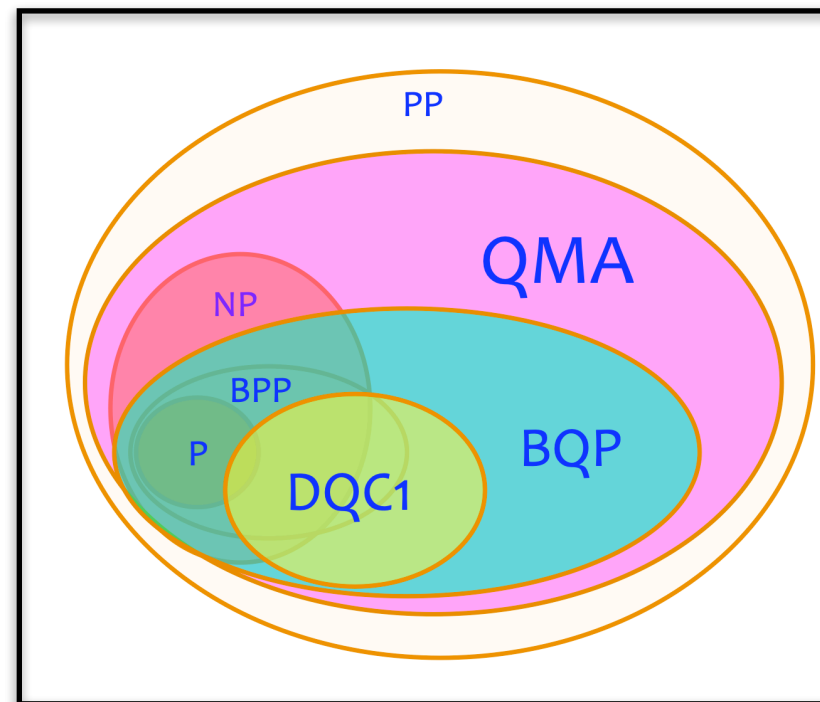


**SURVIVOR**



Complex network  
analysis

# (Q)TDA

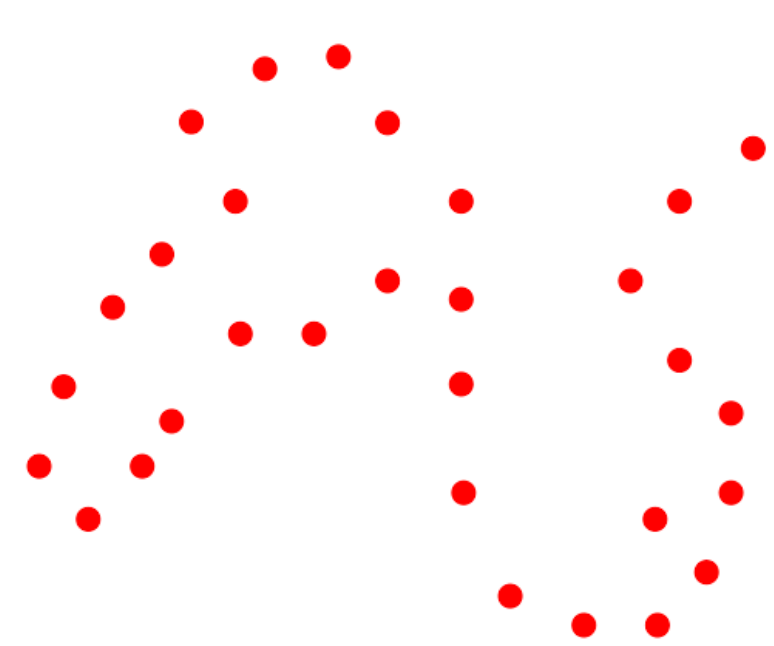


80 billion Toffolis in TDA...



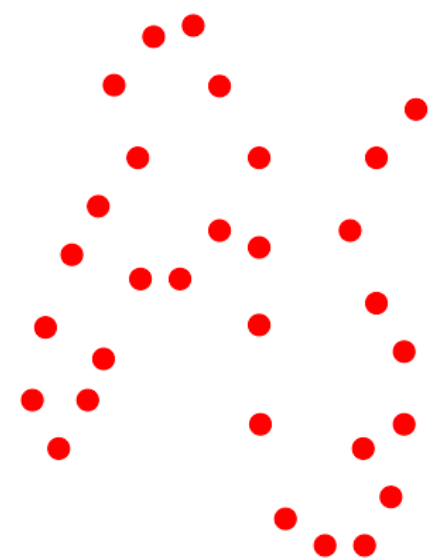
# Topological Data Analysis

Machine learning: about “robust” properties of data



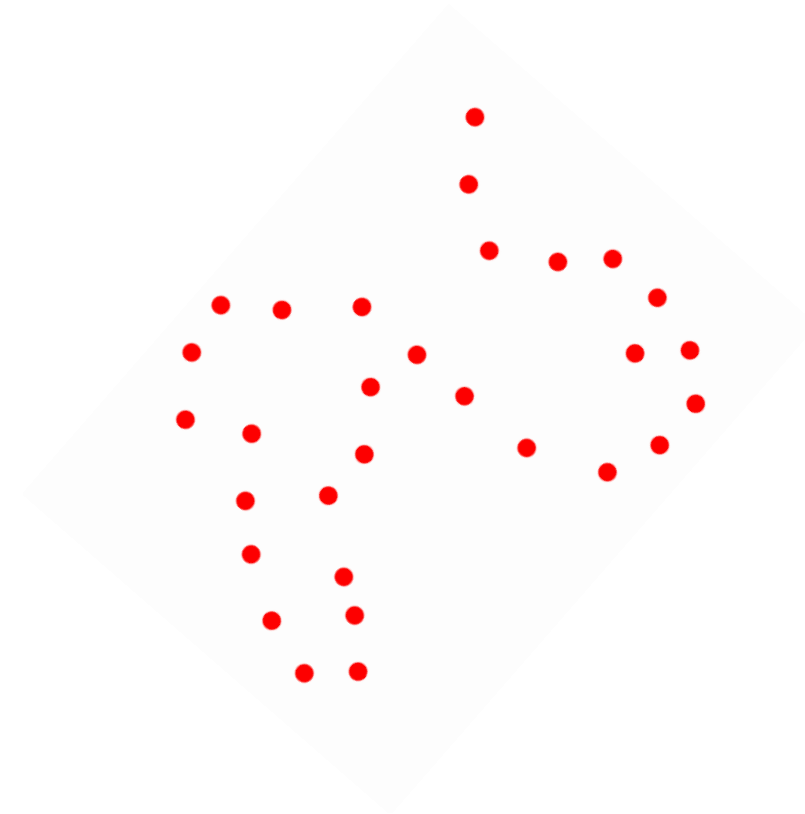
data

=



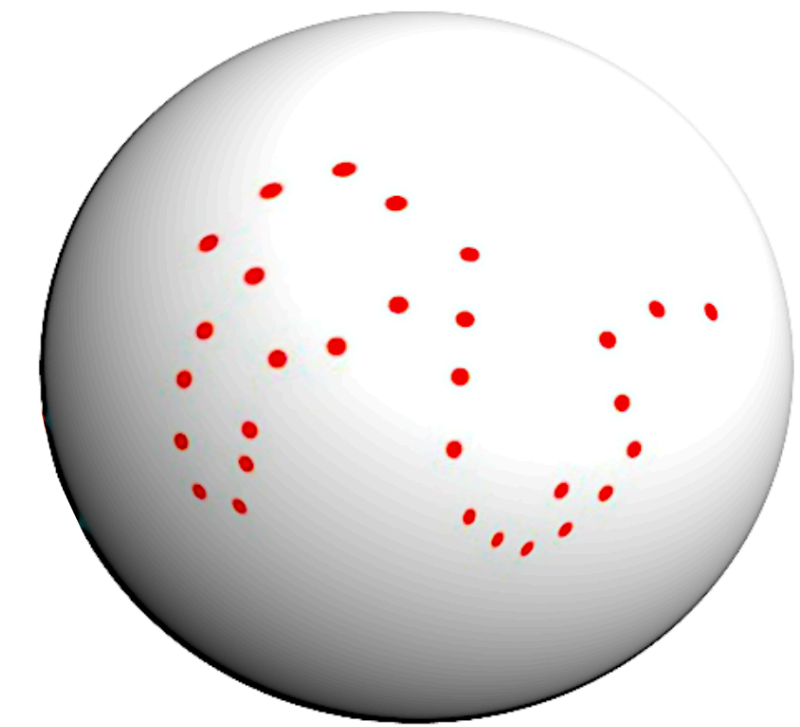
rescaling

=



rotating

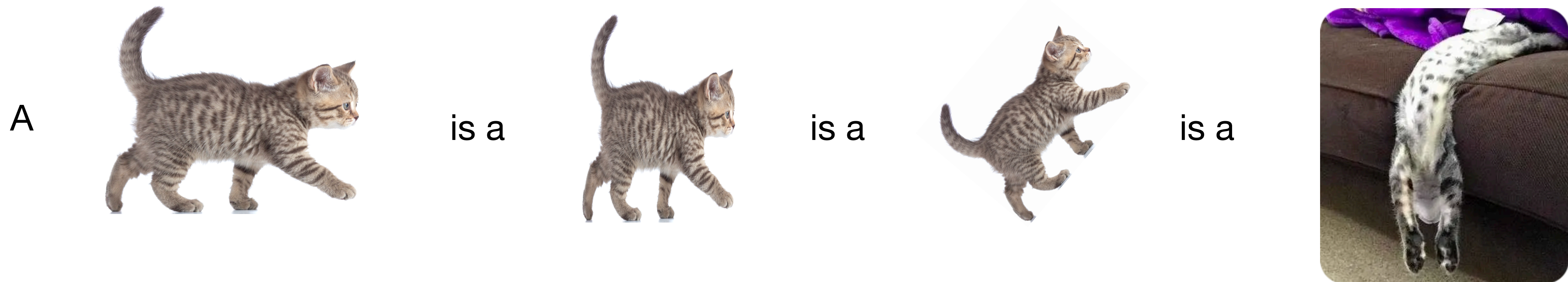
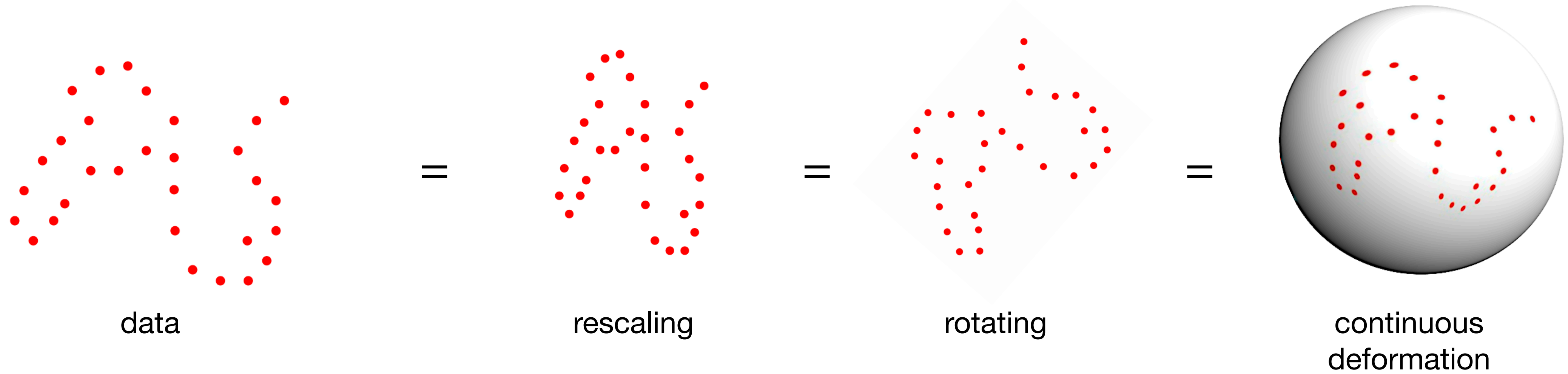
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continuous  
deformation

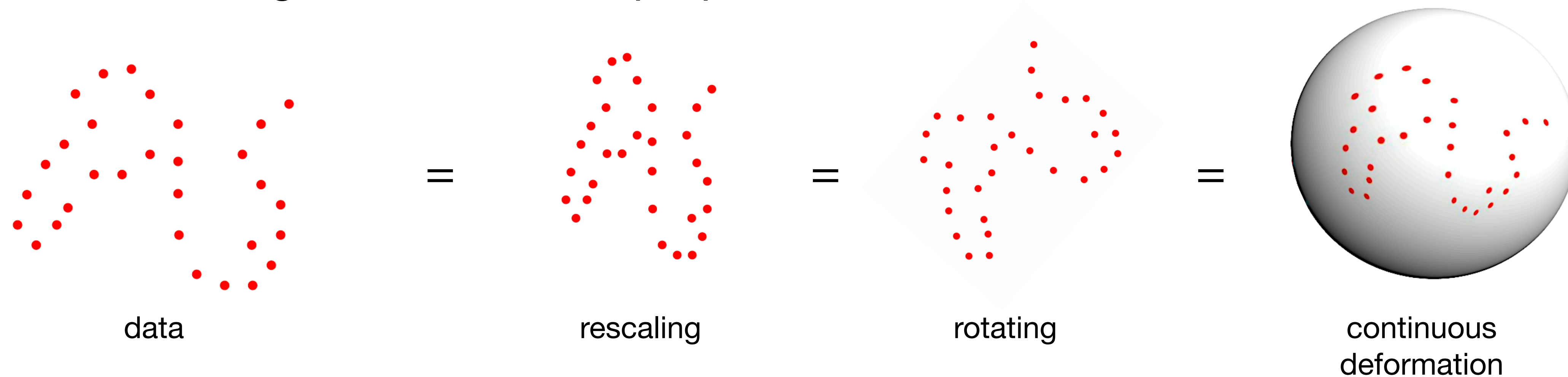
# Topological Data Analysis

Machine learning: about “robust” properties of data

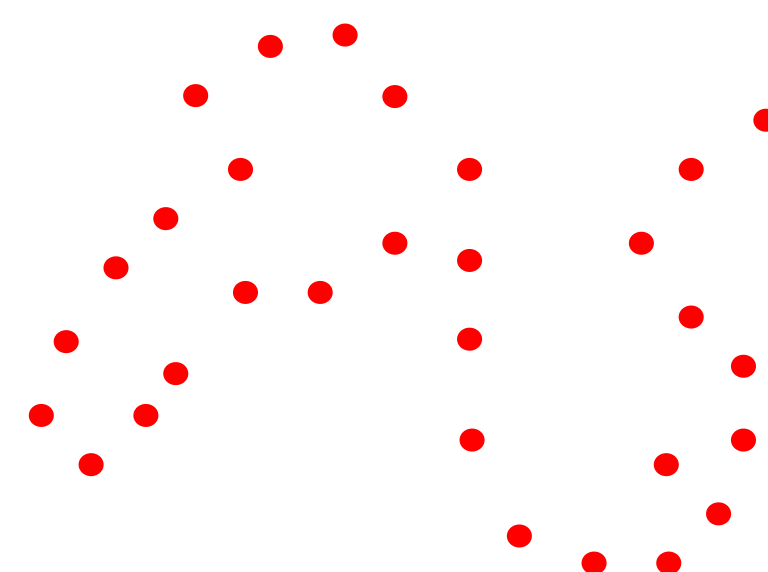
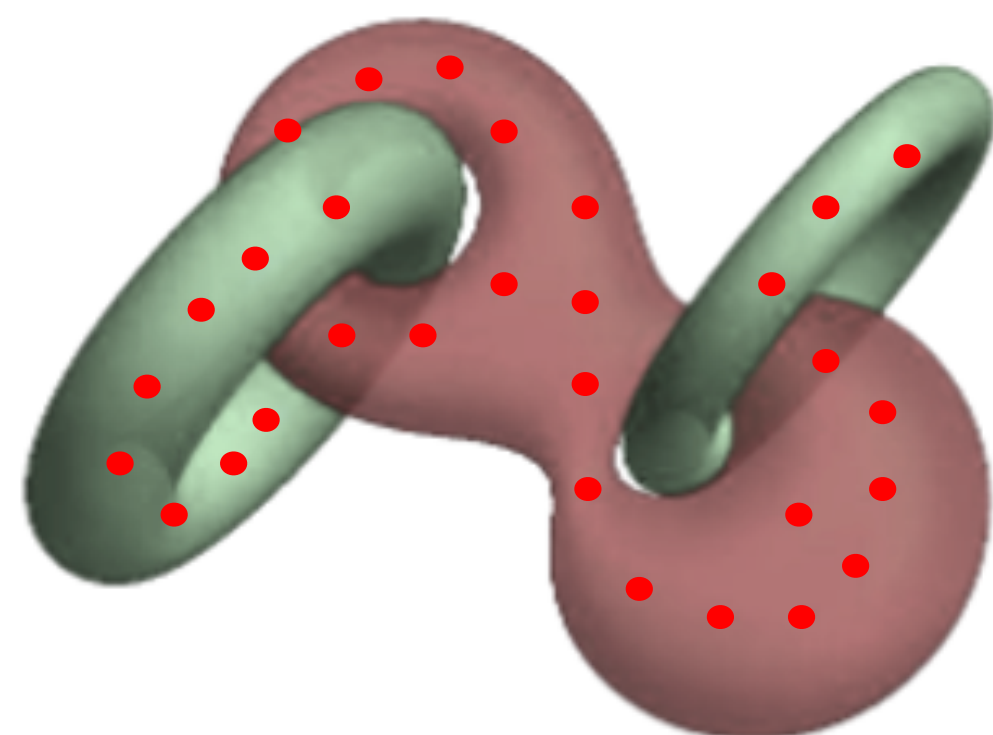


# Topological Data Analysis

Machine learning: about “robust” properties of data



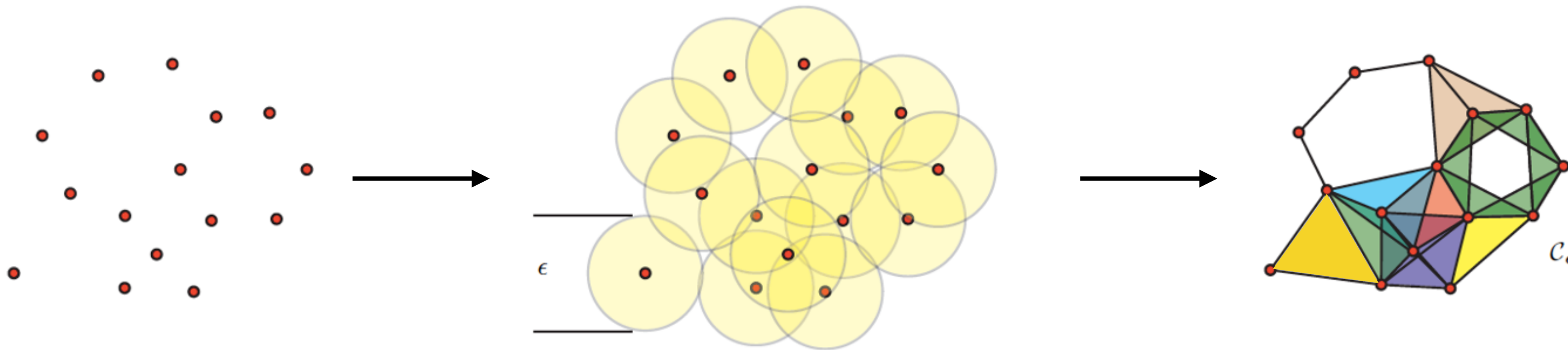
Remains:



*Topology of data*

# Topological Data Analysis

part of pipeline

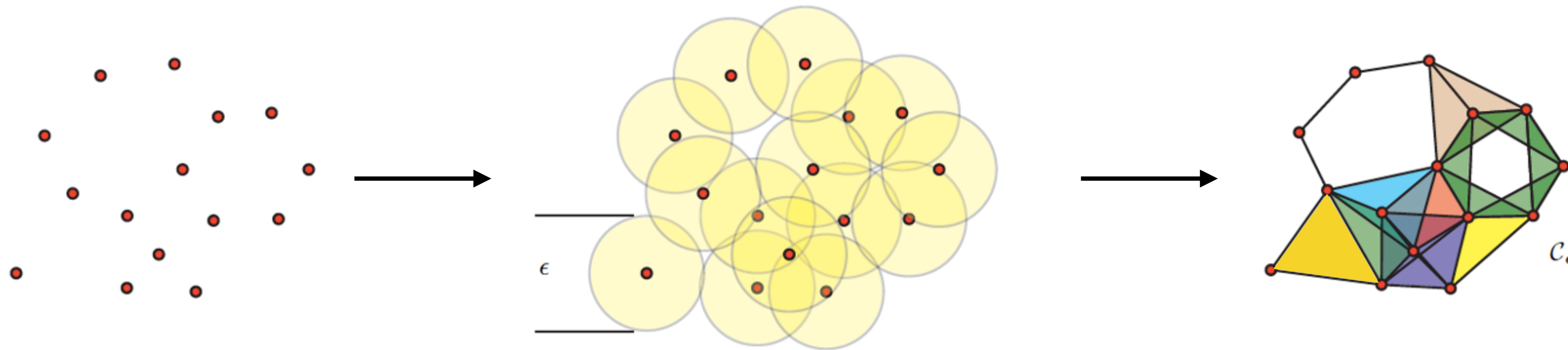


“connect if  
close”

clique complex (graph)  
“simplicial complex”

# Topological Data Analysis

part of pipeline

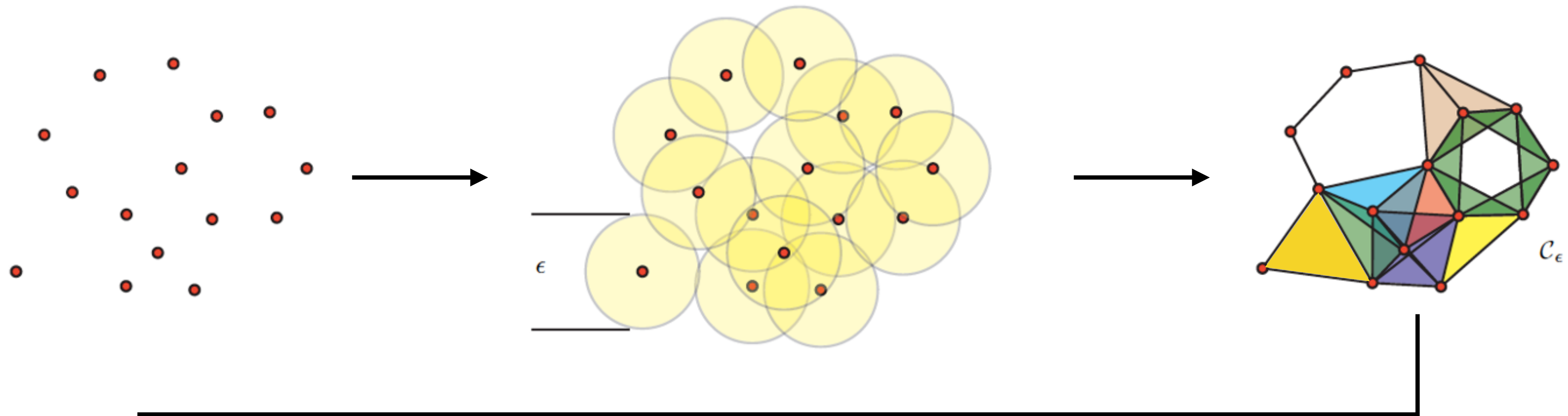


features = #  $k$ -dimensional *holes*  
=  $(\beta_k)_k$  (*Betti numbers*)

\*(persistent homology, barcodes, consider all  $\epsilon$ )

# Topological Data Analysis

part of pipeline



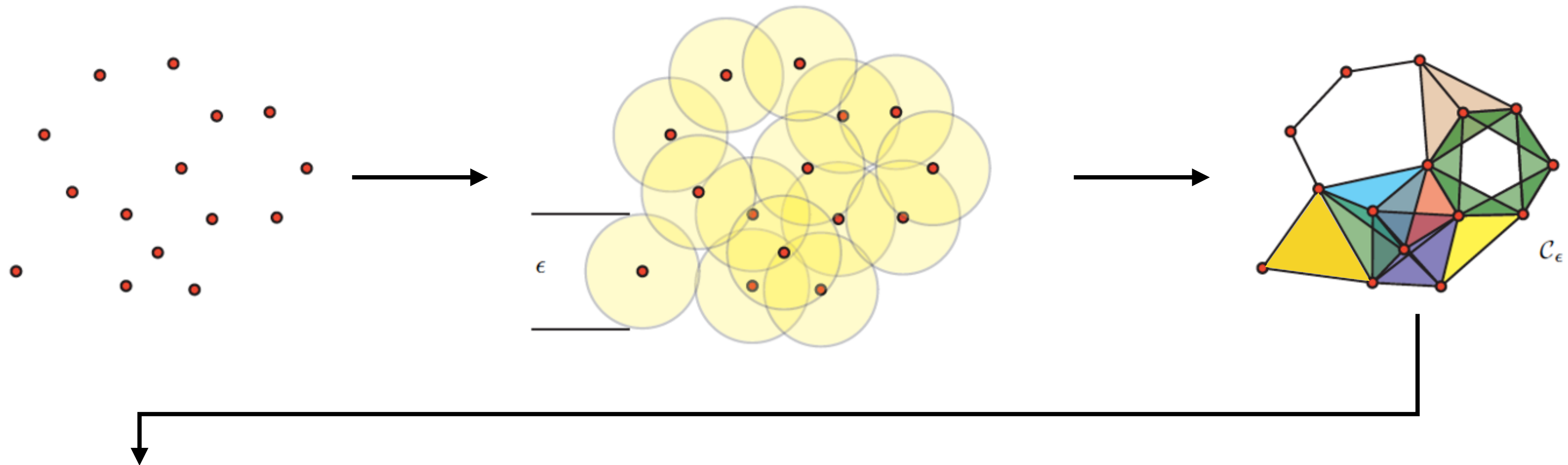
$$\Delta_k^G$$

“connectivity” of  $(k+1)$ -cliques

combinatorial Laplacian

# Topological Data Analysis

part of pipeline



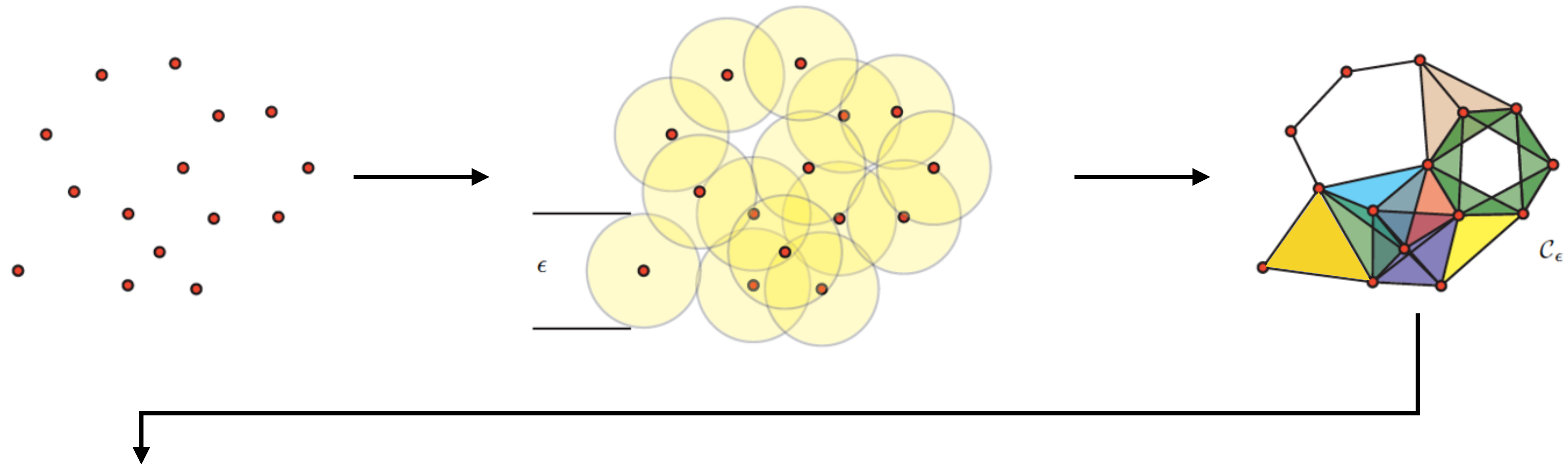
$$\Delta_k^G$$

“connectivity” of  $(k+1)$ -cliques for  $\beta_k$       $\beta_k = \dim(\text{Ker}(\Delta_k))$

combinatorial Laplacian

# Topological Data Analysis

part of pipeline



$$\Delta_k^G$$

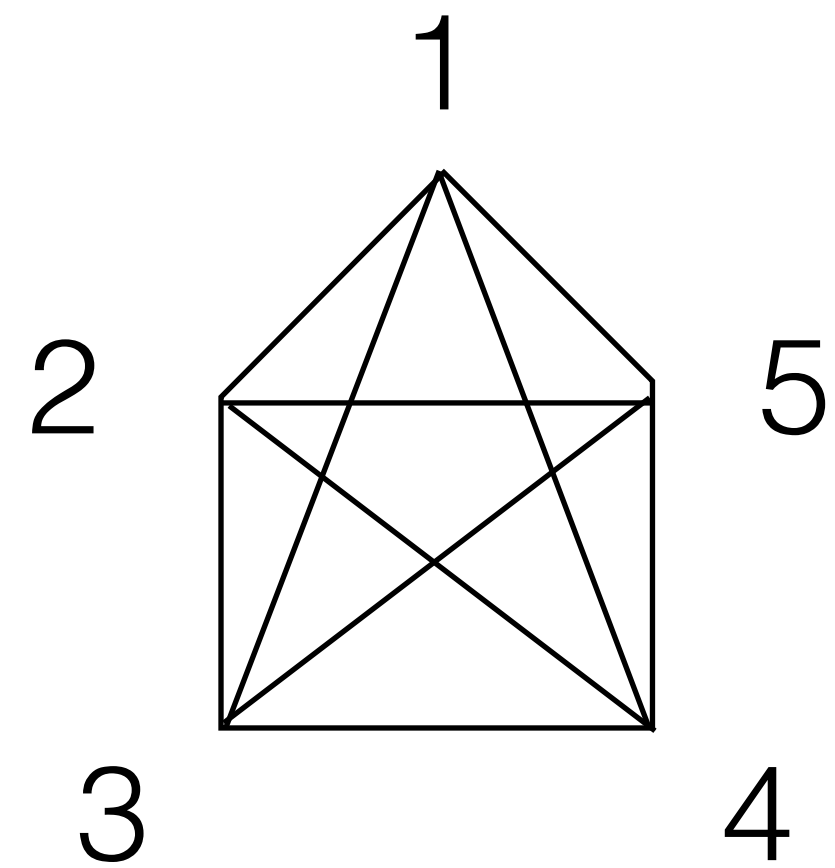
combinatorial Laplacian

$\binom{n}{k+1}$  – dimensional...  
Hermitian... sparse access...  
*Hint-hint*

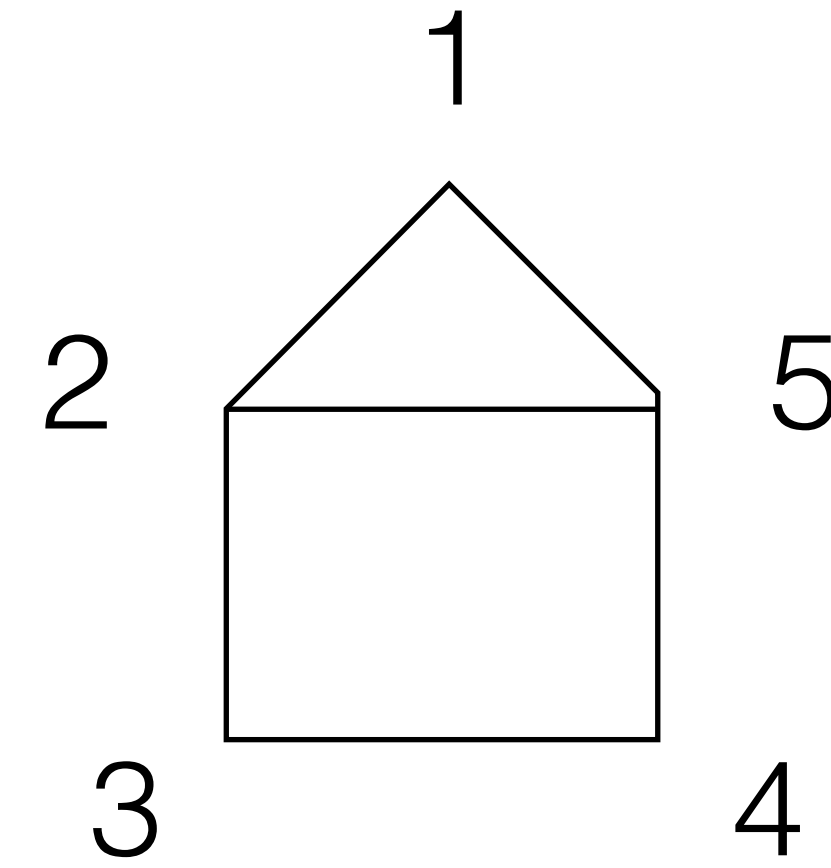
$$\beta_k = \dim(\text{Ker}(\Delta_k))$$



Input: Graph. Vertices = qubits.

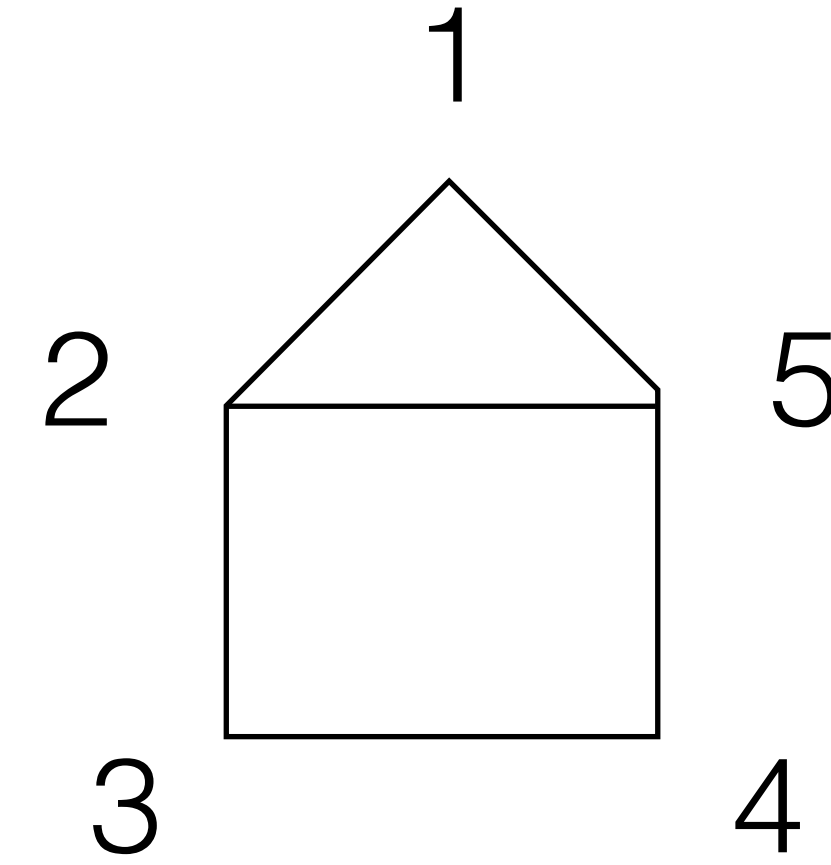
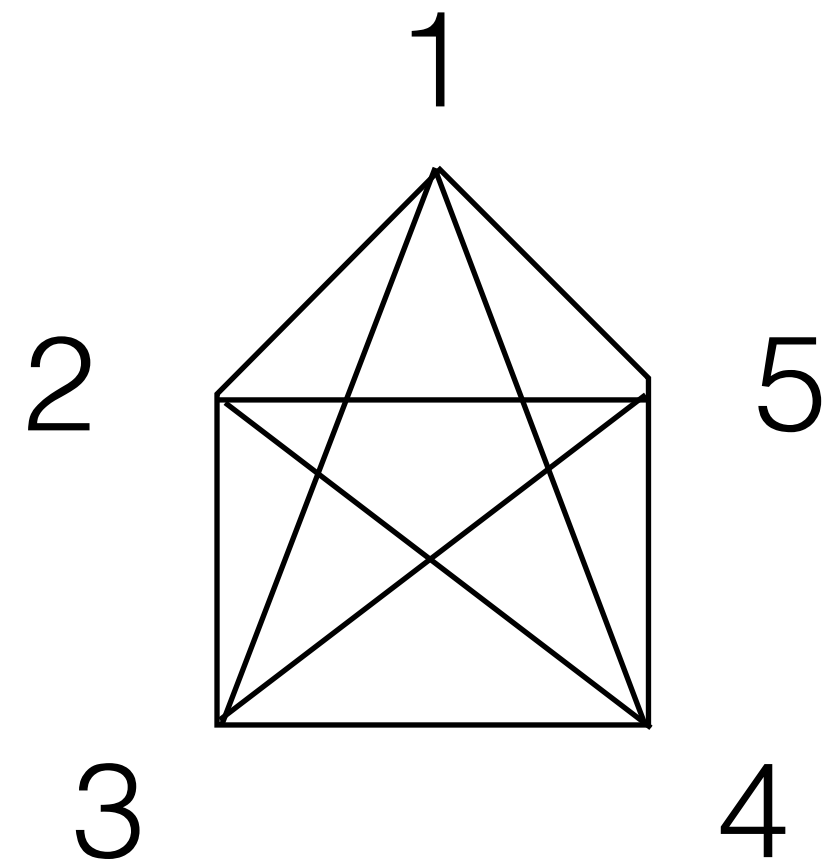


$|11100\rangle$  - 3 clique



$|11100\rangle$  - not a 3 clique

Boundary map  $(\partial_k^G : \mathcal{H}_{k+1}^G \rightarrow \mathcal{H}_k^G)$



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

$\uparrow$   
 set  $j$ -th to zero

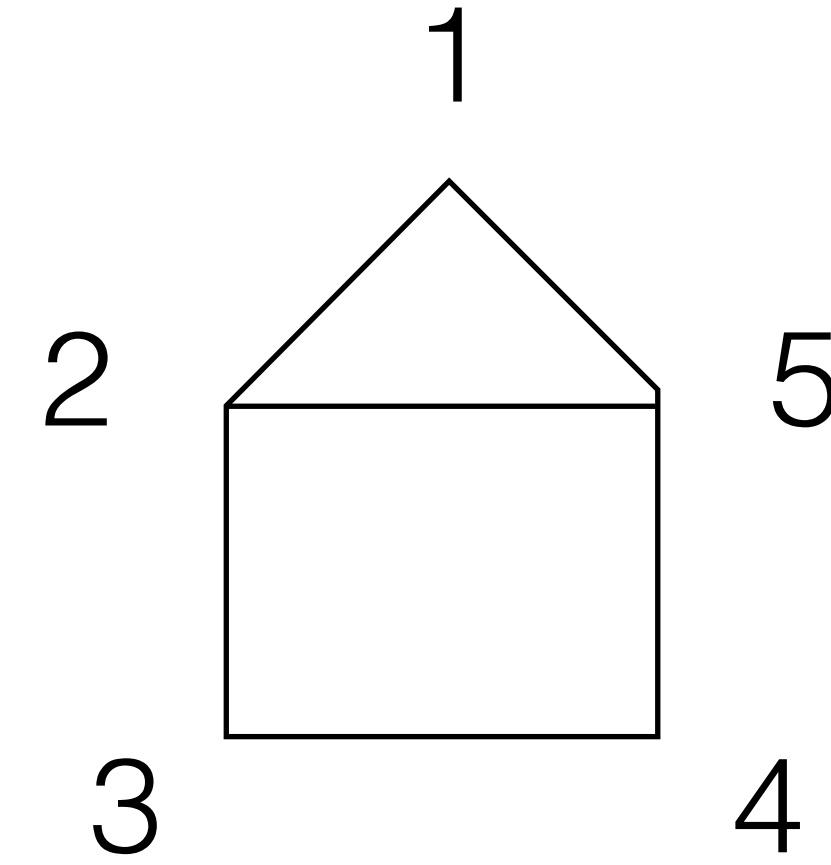
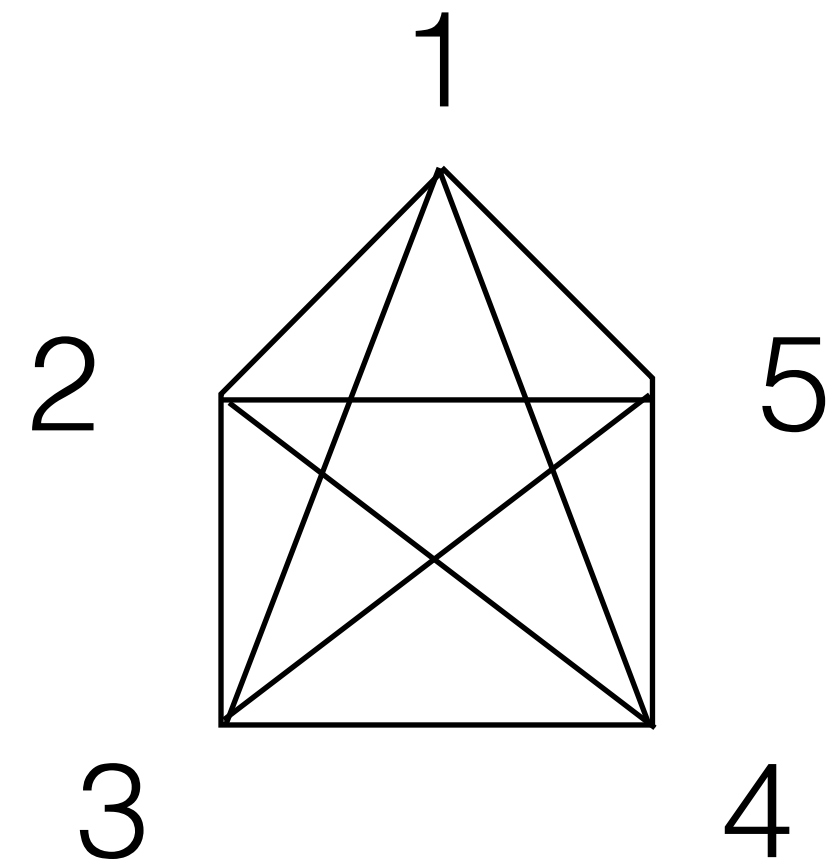
$$\partial_k^G = P_k^G (\partial_k) P_{k+1}^G$$

$$P_k^G = \sum_{c \in Cl_k(G)} |c\rangle \langle c|$$

$$|11100\rangle \rightarrow |01100\rangle - |10100\rangle + |11000\rangle$$

Restriction to  $G$  will be vital

# Boundary map and combinatorial Laplacian

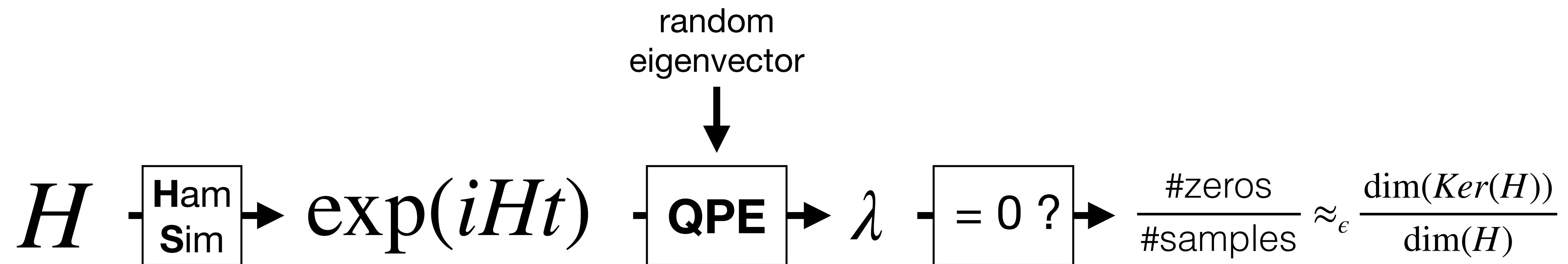


$$\Delta_k^G = \partial_k^{G^\dagger} \partial_k^G + \partial_{k+1}^G \partial_{k+1}^{G^\dagger}$$

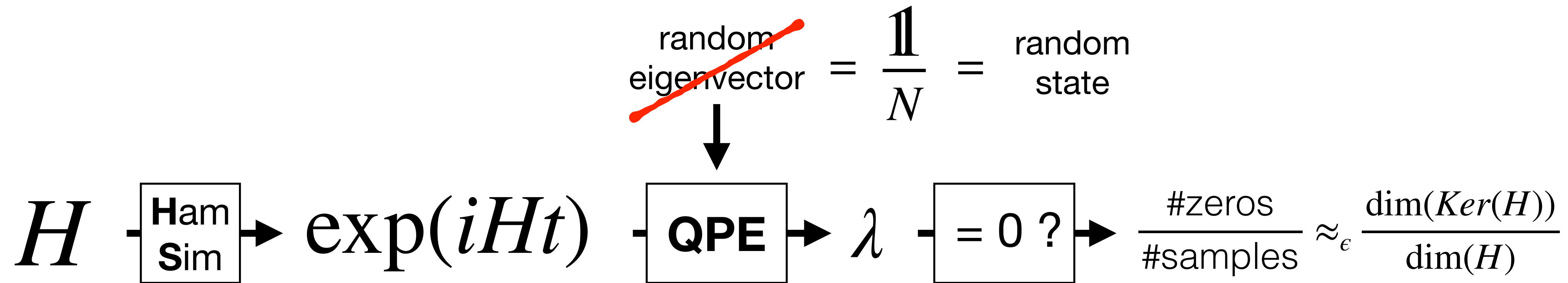
$$\dim(\text{Ker}(\Delta_k)) = \beta_k$$

compute on a QC!

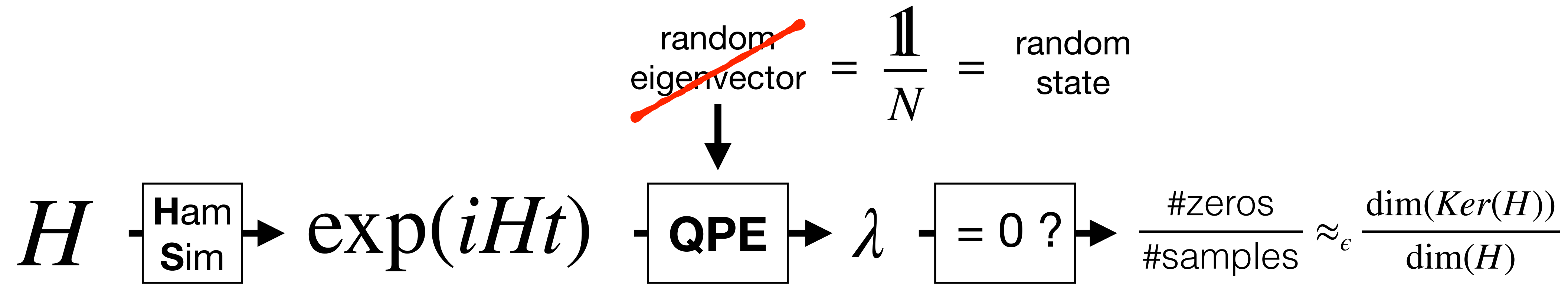
# Lloyd, Garnerone, Zanardi (LGZ)\* ideas



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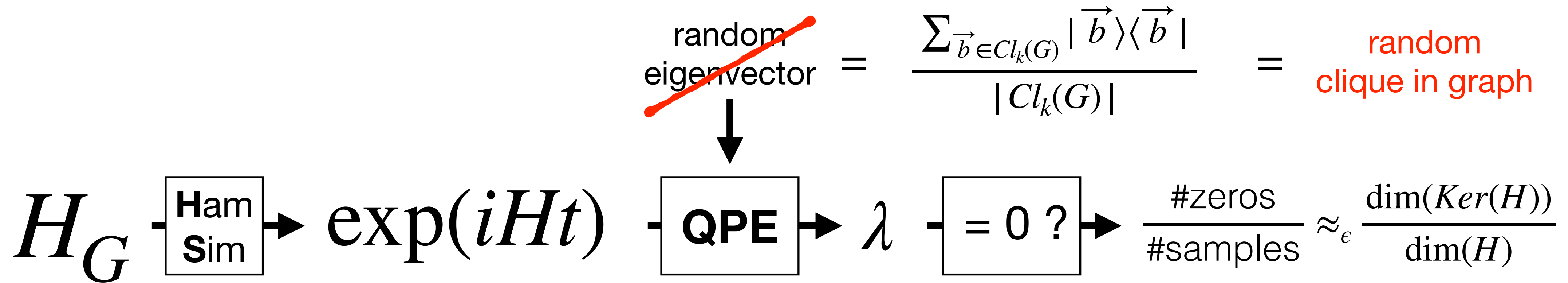


$$H \rightarrow \Delta^G$$

$$\partial_k^G = P_k^G (\partial_k) P_{k+1}^G$$

must only operate on *valid cliques*

# Lloyd, Garnerone, Zanardi (LGZ)\* ideas

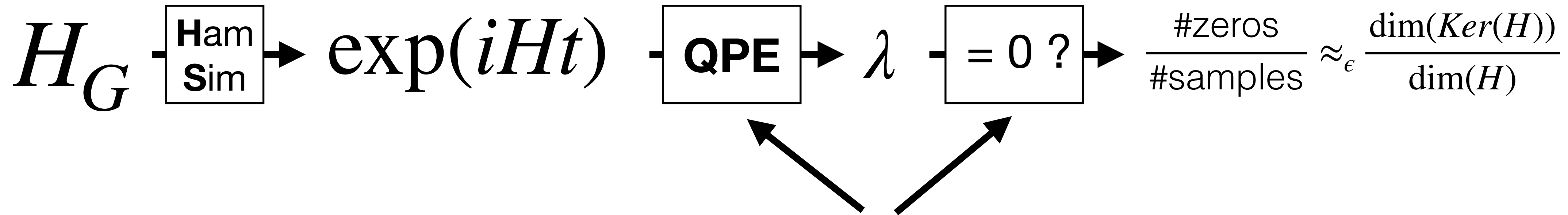


+ some projections needed

\*S. Lloyd, S. Garnerone & P. Zanardi, "Nat Commun. Vol. 7, Article no.: 10138 (2016)

# Lloyd, Garnerone, Zanardi (LGZ)\* ideas

~~random eigenvector~~ =  $\frac{\sum_{\vec{b} \in Cl_k(G)} |\vec{b}\rangle\langle\vec{b}|}{|Cl_k(G)|}$  = random clique in graph

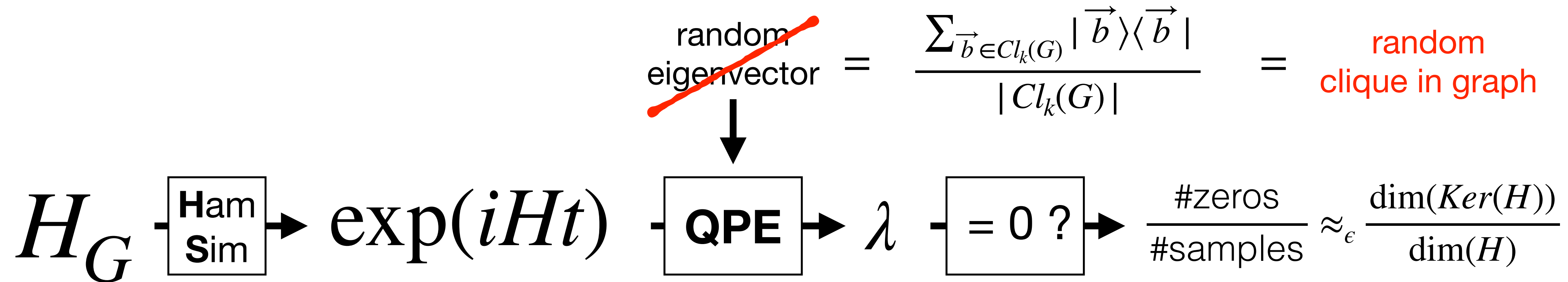


QPE to precision  
 $gap = \min\{|\lambda| \mid \lambda \neq 0\}$

\*S. Lloyd, S. Garnerone & P. Zanardi, "Nat Commun. Vol. 7, Article no.: 10138 (2016)"



# Lloyd, Garnerone, Zanardi (LGZ)\* ideas



## Quantum costs:

- Ham. sim. = cheap (*low-deg poly n*)
- QPE to prec. *gap* = *could be cheap*
- *random clique sampling*

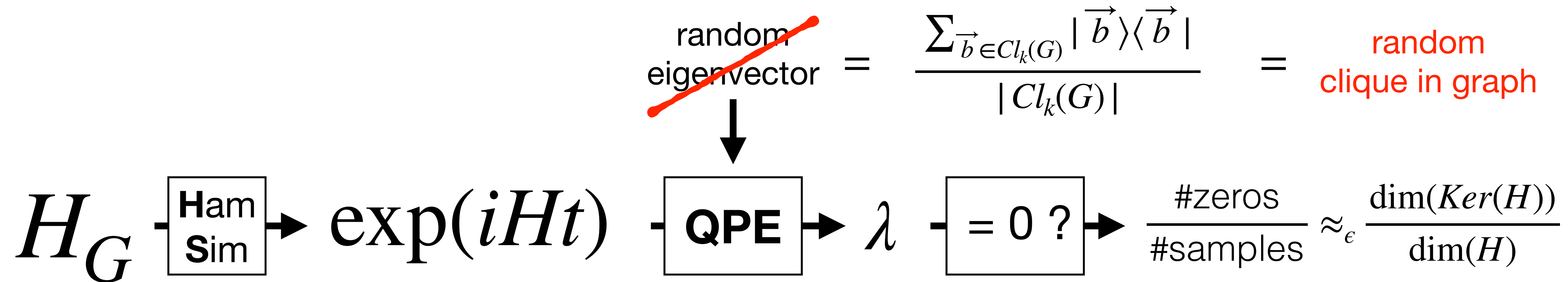
## Classical (vanilla) costs:

- $O(n^k)$
- note if  $k \sim n \rightarrow O(\exp(n))$

\*S. Lloyd, S. Garnerone & P. Zanardi, "Nat Commun. Vol. 7, Article no.: 10138 (2016)

*details matter*

# Lloyd, Garnerone, Zanardi (LGZ)\* ideas



## Quantum costs:

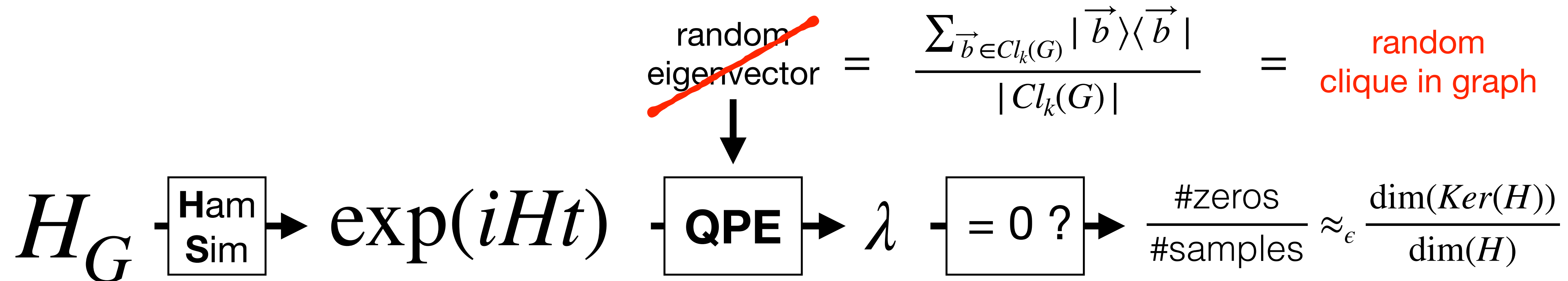
- Ham. sim. = cheap (*low-deg poly n*)
- QPE to prec. *gap* = *could be cheap*
- *random clique sampling = NP-hard*

## Classical (vanilla) costs:

- $O(n^k)$
- note if  $k \sim n \rightarrow O(\exp(n))$

\*S. Lloyd, S. Garnerone & P. Zanardi, "Nat Commun. Vol. 7, Article no.: 10138 (2016)

# Lloyd, Garnerone, Zanardi (LGZ)\* ideas



Quantum

*Efficient if clique sampling efficient*

**Dense graphs.**

Classical (vanilla) costs:

Vanilla algorithm still exponential

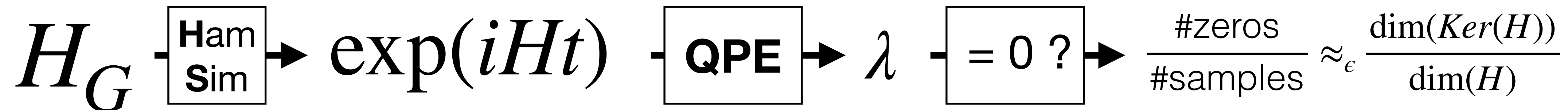
But this is certainly a *special case*

\*S. Lloyd, S. Garnerone & P. Zanardi, "Nat Commun. Vol. 7, Article no.: 10138 (2016)

# Lloyd, Garnerone, Zanardi (LGZ)\* ideas

~~random eigenvector~~ =  $\frac{\sum_{\vec{b} \in Cl_k(G)} |\vec{b}\rangle\langle\vec{b}|}{|Cl_k(G)|}$  = **random clique in graph**

↓



Quantum

*Estimates normalized*

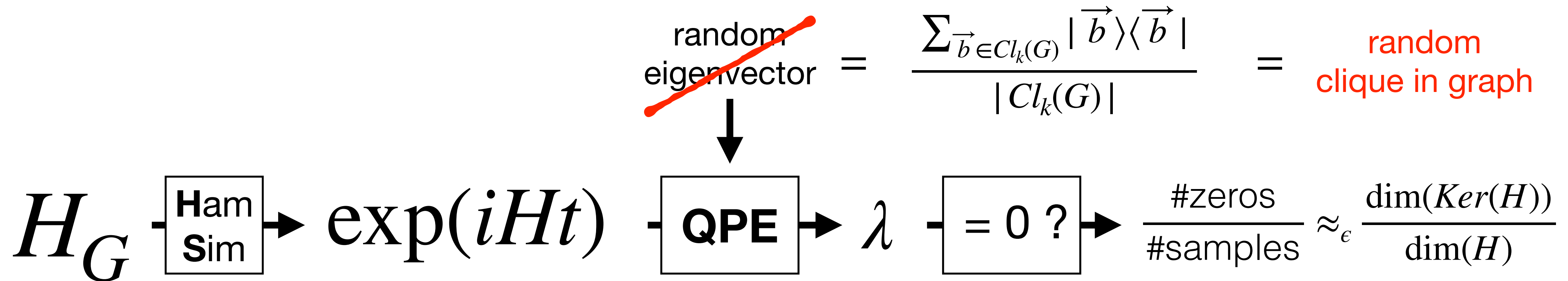
*Betti numbers =  $\frac{\beta_k}{\text{\#k-cliques}}$*

Classical (vanilla) costs:

Gets exact Betti!

\*S. Lloyd, S. Garnerone & P. Zanardi, "Nat Commun. Vol. 7, Article no.: 10138 (2016)

# Lloyd, Garnerone, Zanardi (LGZ)\* ideas

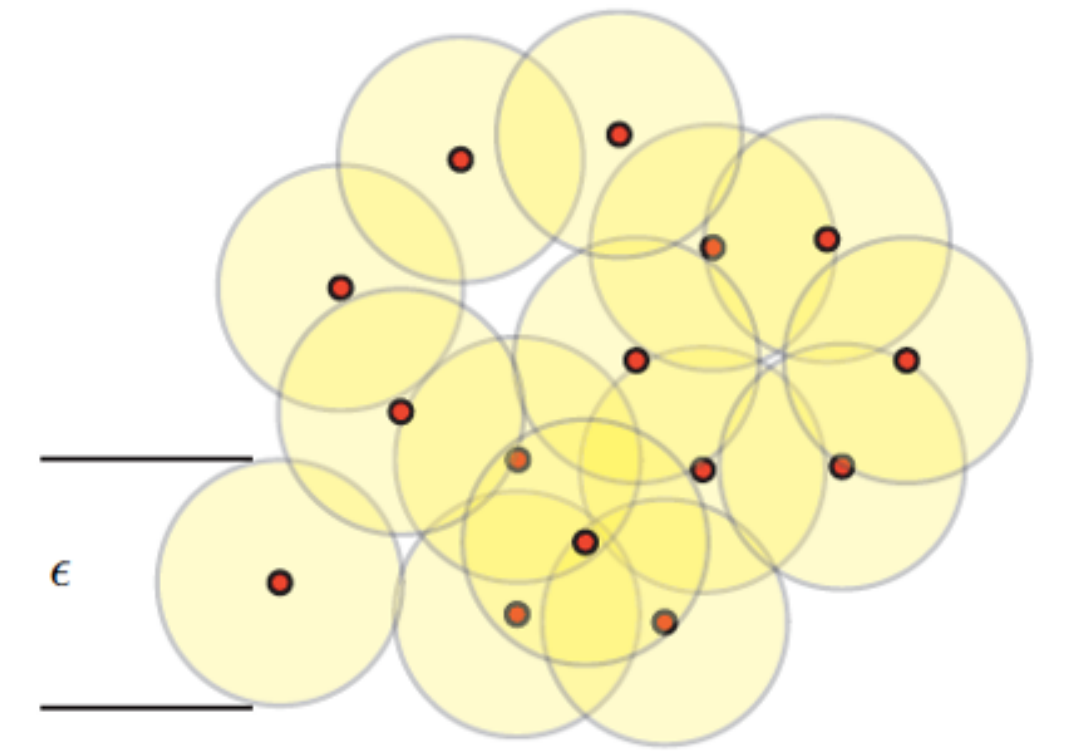
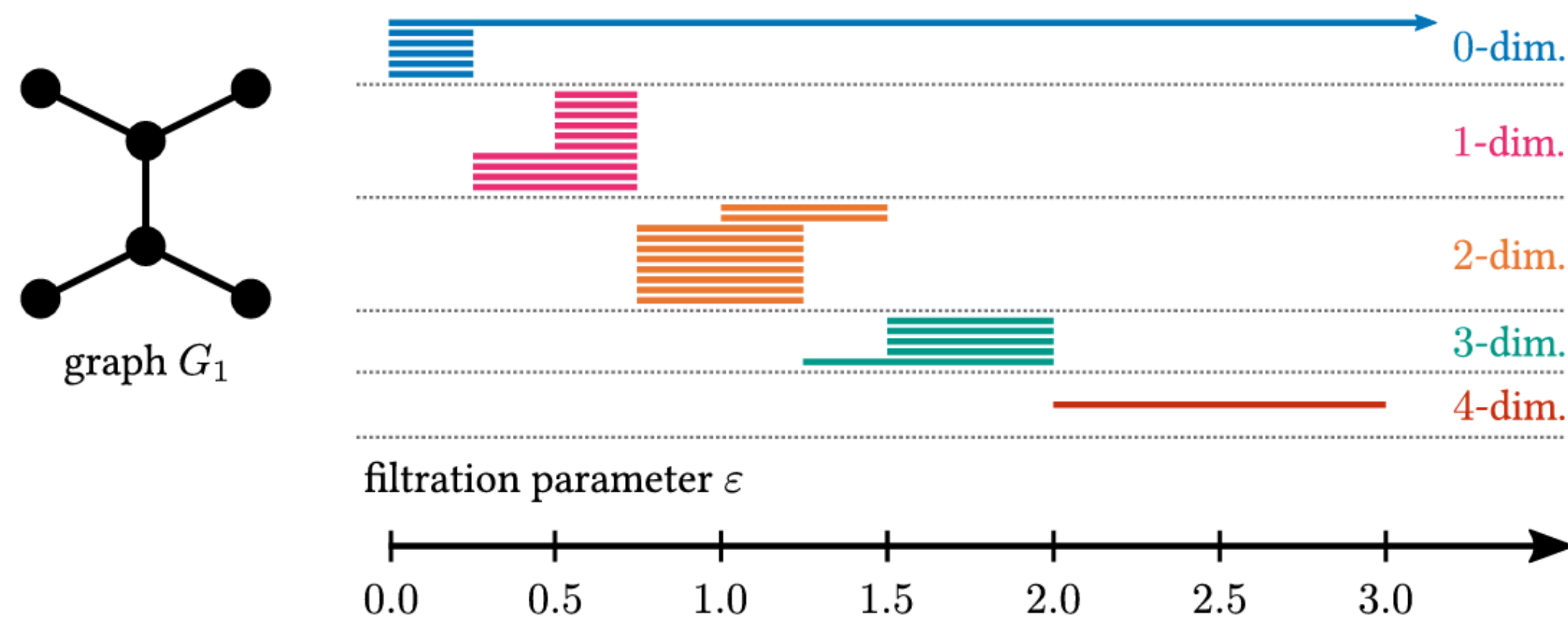


Quantum computers enable

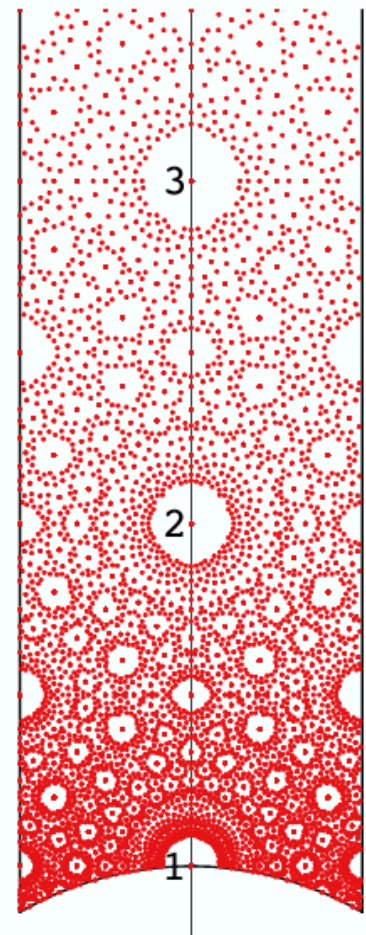
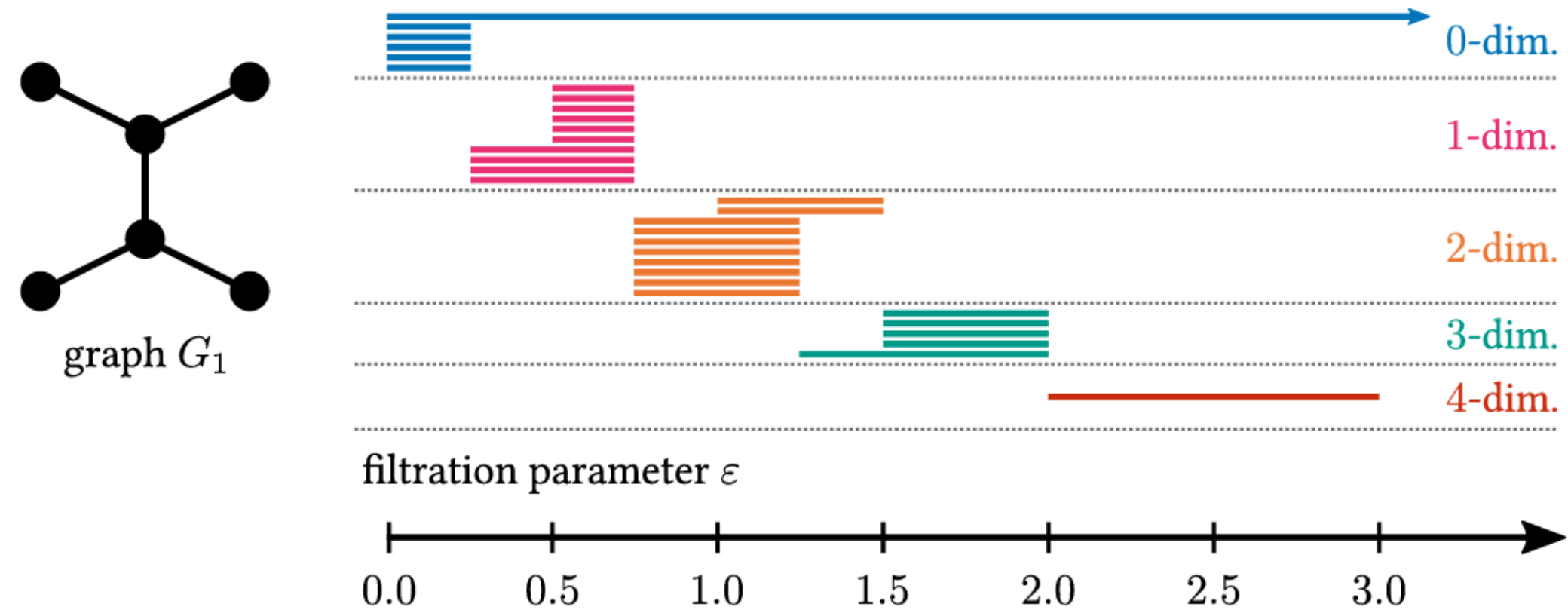
efficient (*additive error*) estimation of *normalized approximate Betti numbers* in regimes where clique sampling is efficient

\*S. Lloyd, S. Garnerone & P. Zanardi, "Nat Commun. Vol. 7, Article no.: 10138 (2016)

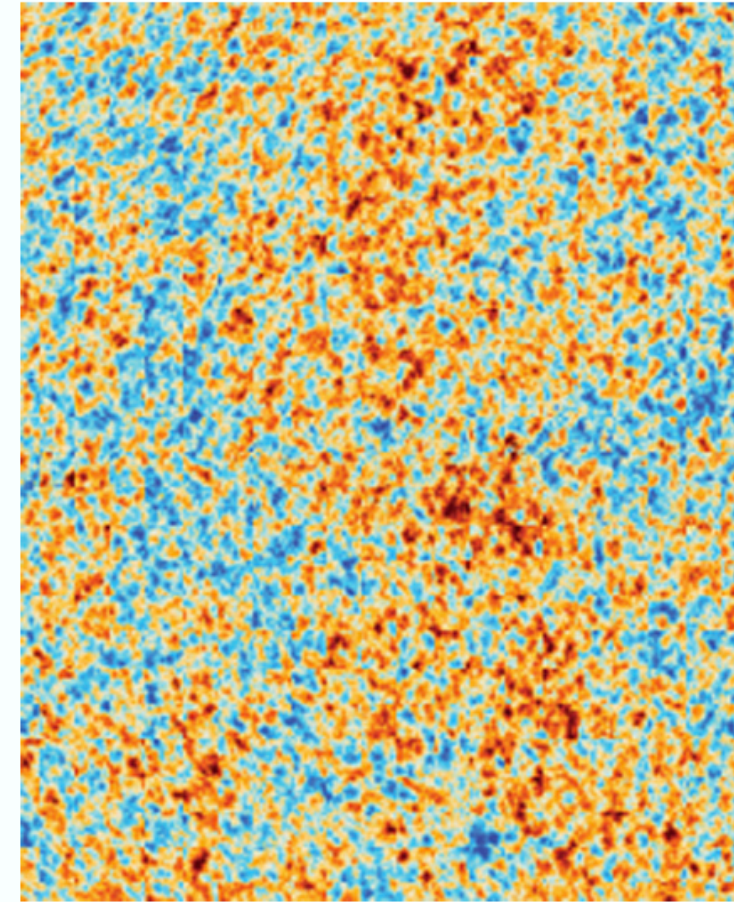
# What is the context! TDA v.s. QTDA



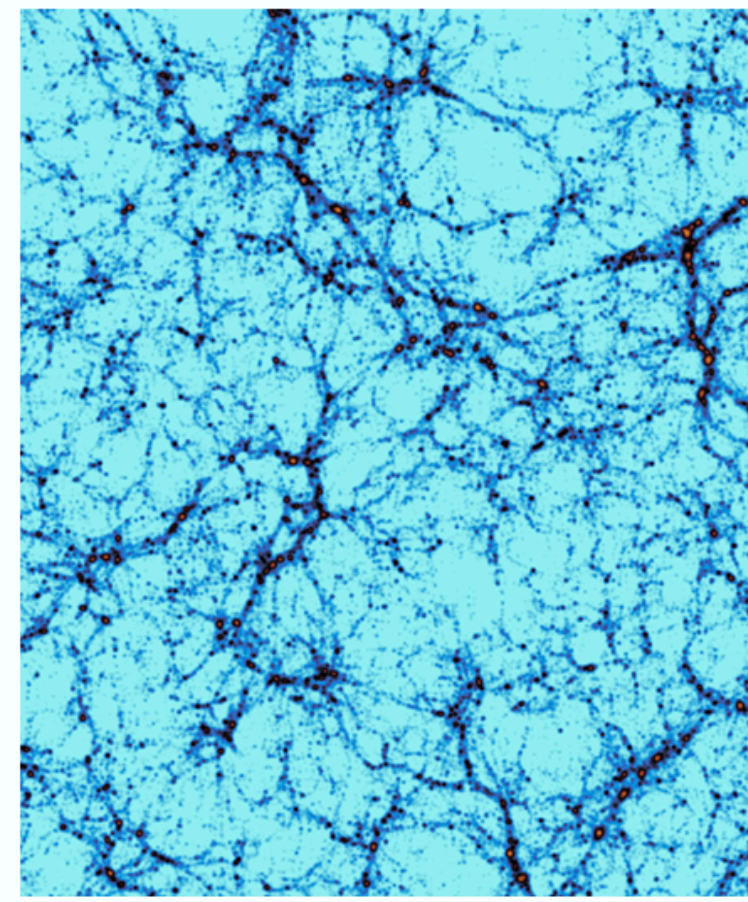
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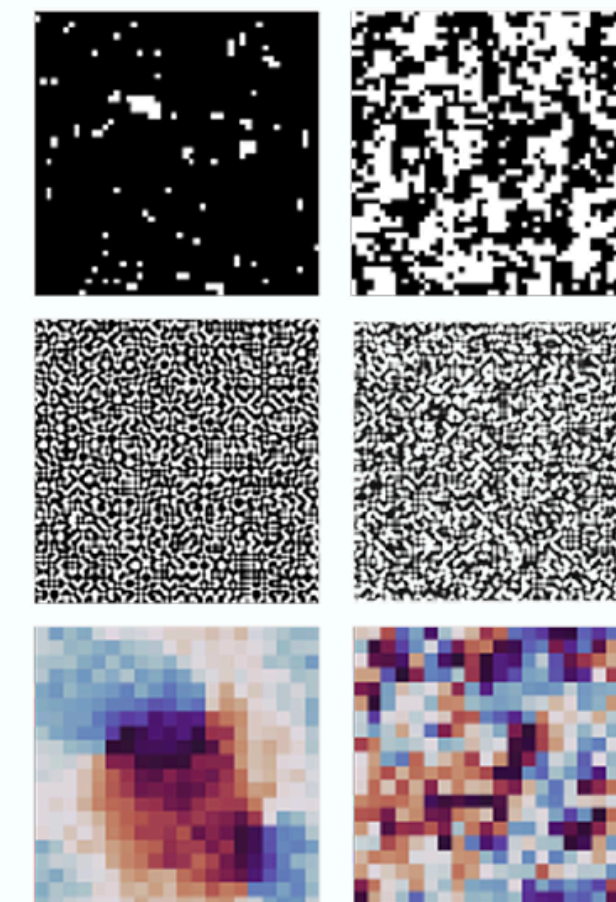
String Landscape



CMB



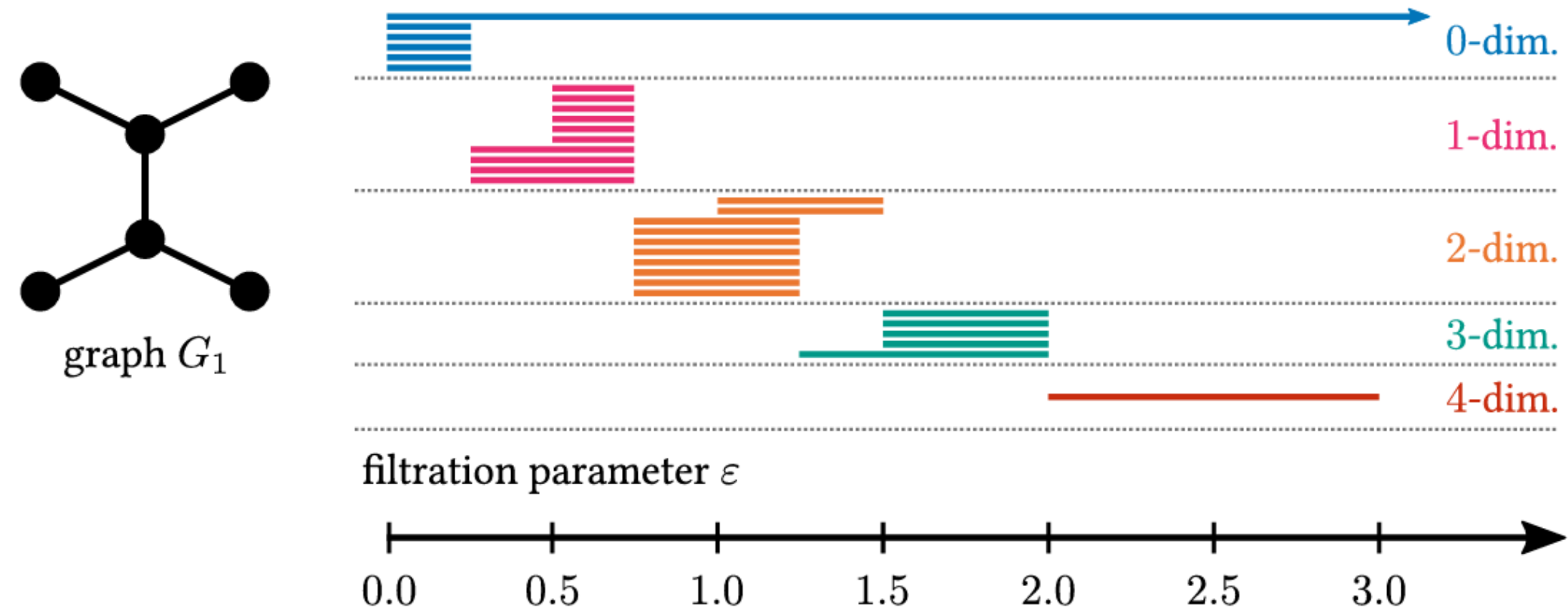
Large Scale Structures



Phases of Matter



# What is the context! TDA v.s. QTDA



## Persistent Homology of $\mathbb{Z}_2$ Gauge Theories

Dan Sehayek and Roger G. Melko

Department of Physics and Astronomy, University of Waterloo, Ontario, N2L 3G1, Canada and  
Perimeter Institute for Theoretical Physics, Waterloo, Ontario N2L 2Y5, Canada

(Dated: September 16, 2022)

Article | [Open access](#) | Published: 15 August 2022

## Precision dynamical mapping using topological data analysis reveals a hub-like transition state at rest

[Manish Saggar](#) , [James M. Shine](#), [Raphaël Liégeois](#), [Nico U. F. Dosenbach](#) & [Damien Fair](#)

*Nature Communications* **13**, Article number: 4791 (2022) | [Cite this article](#)

Article | Published: 21 July 2015

## Topological data analysis of contagion maps for examining spreading processes on networks

[Dane Taylor](#) , [Florian Klimm](#), [Heather A. Harrington](#), [Miroslav Kramár](#), [Konstantin Mischaikow](#), [Mason A. Porter](#) & [Peter J. Mucha](#)

*Nature Communications* **6**, Article number: 7723 (2015) | [Cite this article](#)

## Probing center vortices and deconfinement in SU(2) lattice gauge theory with persistent homology

Nicholas Sale\* and Biagio Lucini†

Department of Mathematics, Swansea University, Bay Campus, SA1 8EN, Swansea, Wales, UK

Jeffrey Giansiracusa

Department of Mathematical Sciences, Durham University,  
Upper Mountjoy Campus, Durham, DH1 3LE, UK

(Dated: January 16, 2023)

Article | [Open access](#) | Published: 11 April 2018

## Towards a new approach to reveal dynamical organization of the brain using topological data analysis

[Manish Saggar](#) , [Olaf Sporns](#), [Javier Gonzalez-Castillo](#), [Peter A. Bandettini](#), [Gunnar Carlsson](#), [Gary Glover](#) & [Allan L. Reiss](#)

*Nature Communications* **9**, Article number: 1399 (2018) | [Cite this article](#)

## Topological Data Analysis of Financial Time Series: Landscapes of Crashes

Marian Gidea

Yeshiva University, Department of Mathematical Sciences, New York, NY 10016, USA

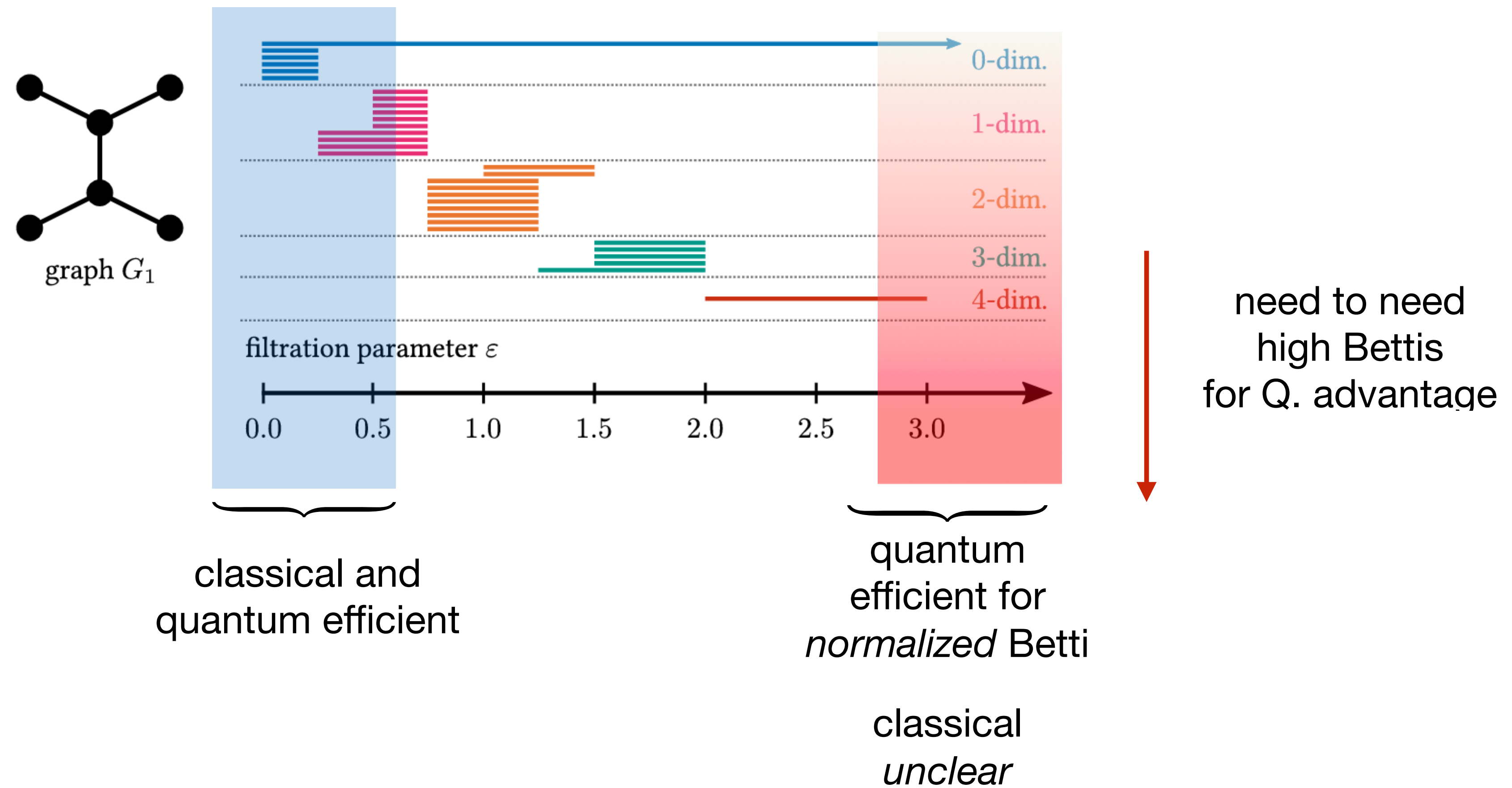
Yuri Katz

S&P Global Market Intelligence, 55 Water Str., New York, NY 10040, USA

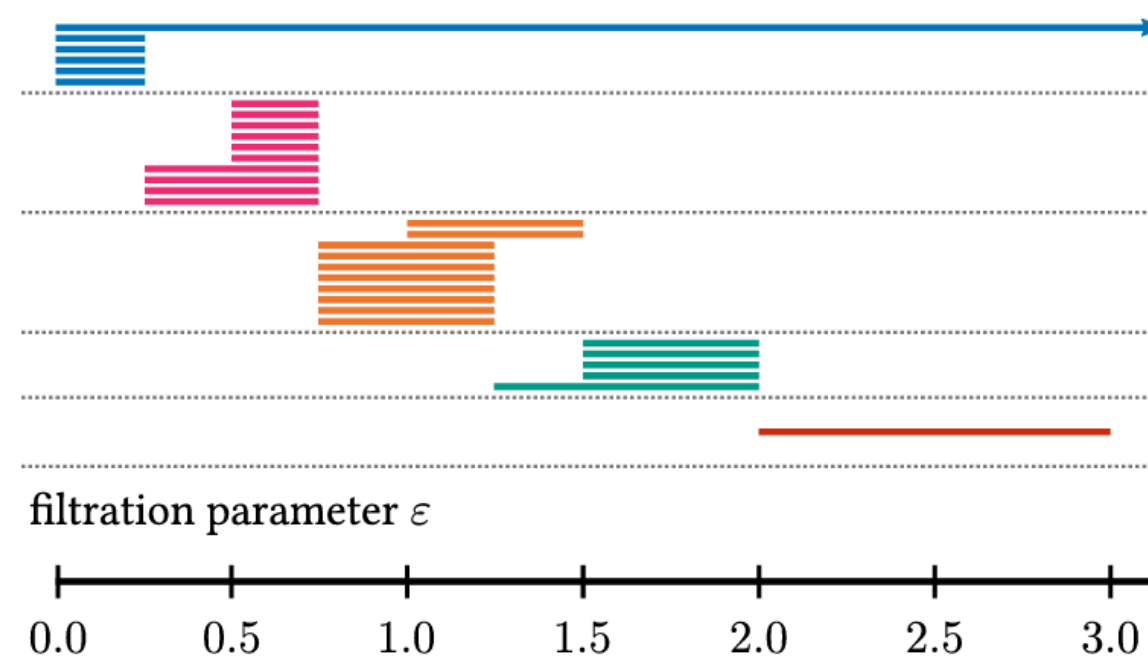
G. A. Hamilton, F. Leditzky, arXiv:2307.07492 (2023)

Image source: <https://indico.cern.ch/event/958074/contributions/4133637/attachments/2163528/3652970/Shiu-sd2020.pdf>

# What is the context! TDA v.s. QTDA



## Questions



1) can we do *significantly better* on a QC?

- *better precision?*
- *full range of densities?*

2) is there a *guaranteed* quantum advantage *for what we do have*, and can it be relevant?

- *hardness of TDA?*
- *when is the QC algorithm truly faster against vanilla...*
- *...and new classical algorithms?*

3) **Beyond basic TDA applications, or**

- are there better applications we are missing

## **Can we do *significantly better* on a QC?**

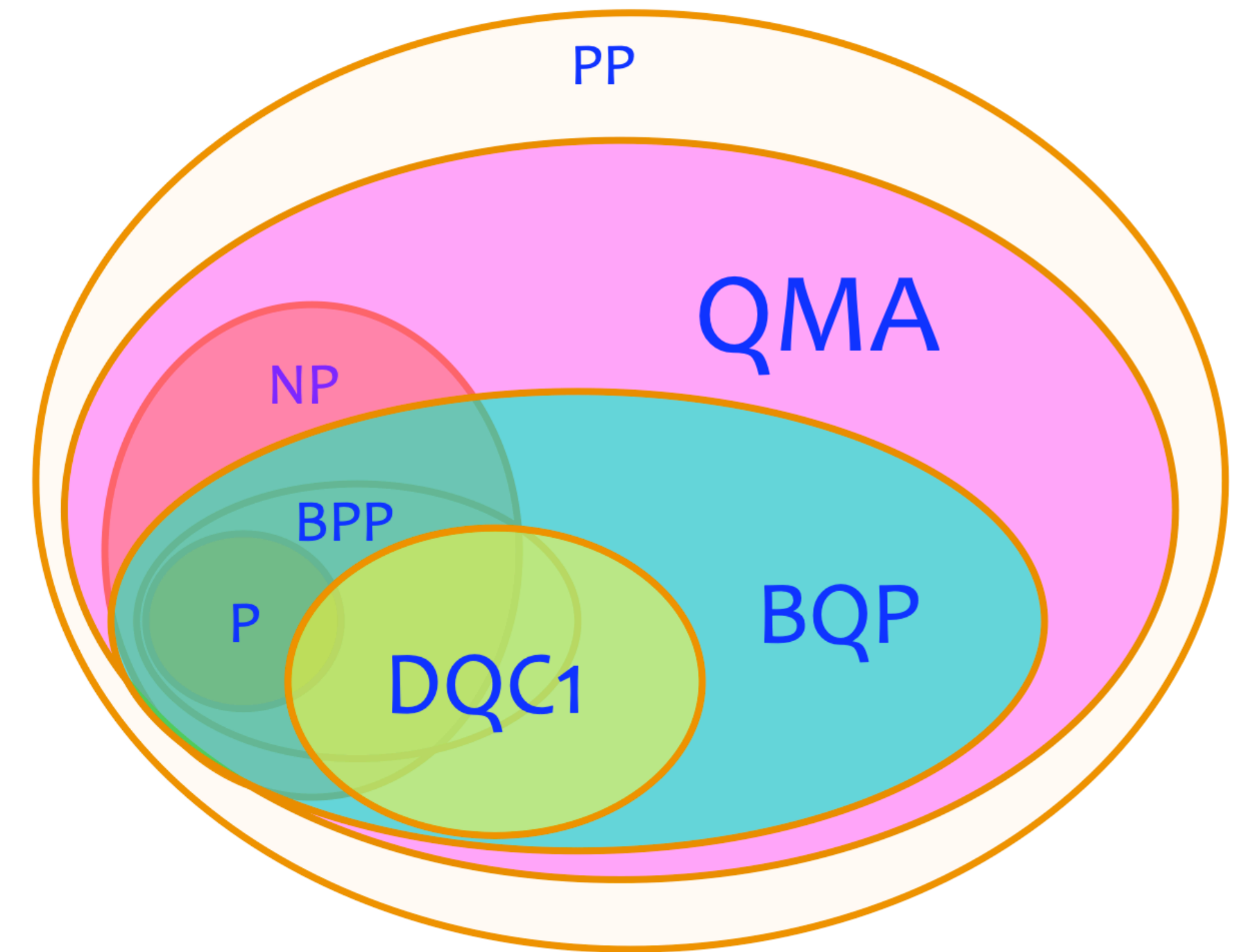
- *better precision?*
- *full range of densities?*

No.

No.

*Multiplicative estimation of Betti numbers is QMA1-hard (2022)*

New (King, Kohler, '23-ish):  
*under promised eigenvalue gap, QMA1-hard and in QMA*



M. Crichigno, T. Kohler, Clique Homology is QMA1-hard (2022)

R. King, T. Kohler, ??? (in 1 week?)

No.

*Multiplicative* estimation of Betti numbers  
is QMA1-hard (2022)

New (King, Kohler, '23-ish):  
under *promised eigenvalue gap*,  
QMA1-hard and in QMA

PP

Quantum costs:

- Ham. sim. = cheap (*low-poly  $n$* )
- QPE to prec. gap = *could be cheap*
- *random clique sampling = NP-hard*

No.

*Multiplicative* estimation of Betti numbers  
is QMA1-hard (2022)

New (King, Kohler, '23-ish):  
under *promised eigenvalue gap*,  
QMA1-hard and in QMA

*Lemma: it is also hard when the graph  
is **clique-dense***

➔ *Hardness is NOT in clique sampling*

➔ *“Homology is quantum”*

PP

Quantum costs:

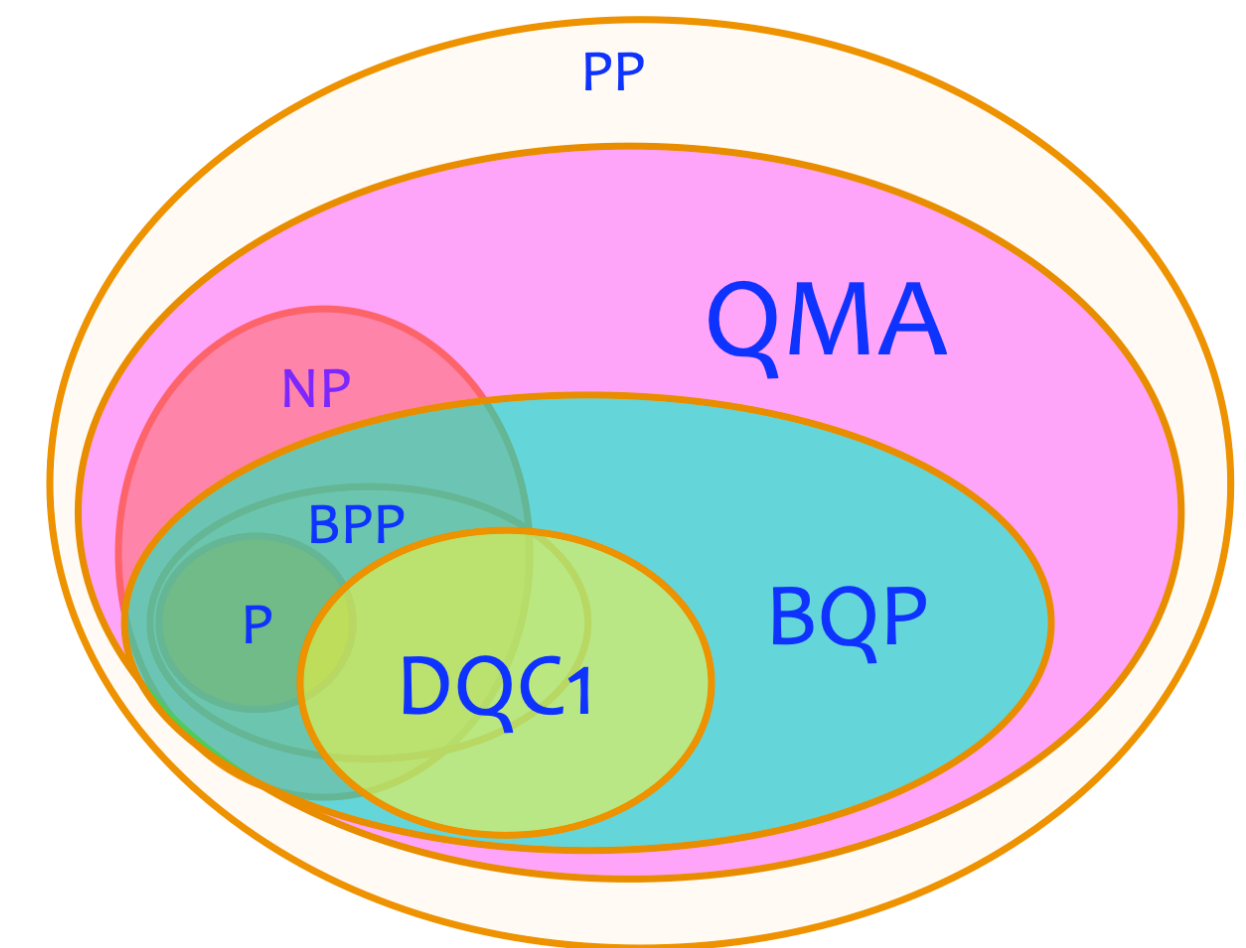
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**Is there a *guaranteed* quantum advantage  
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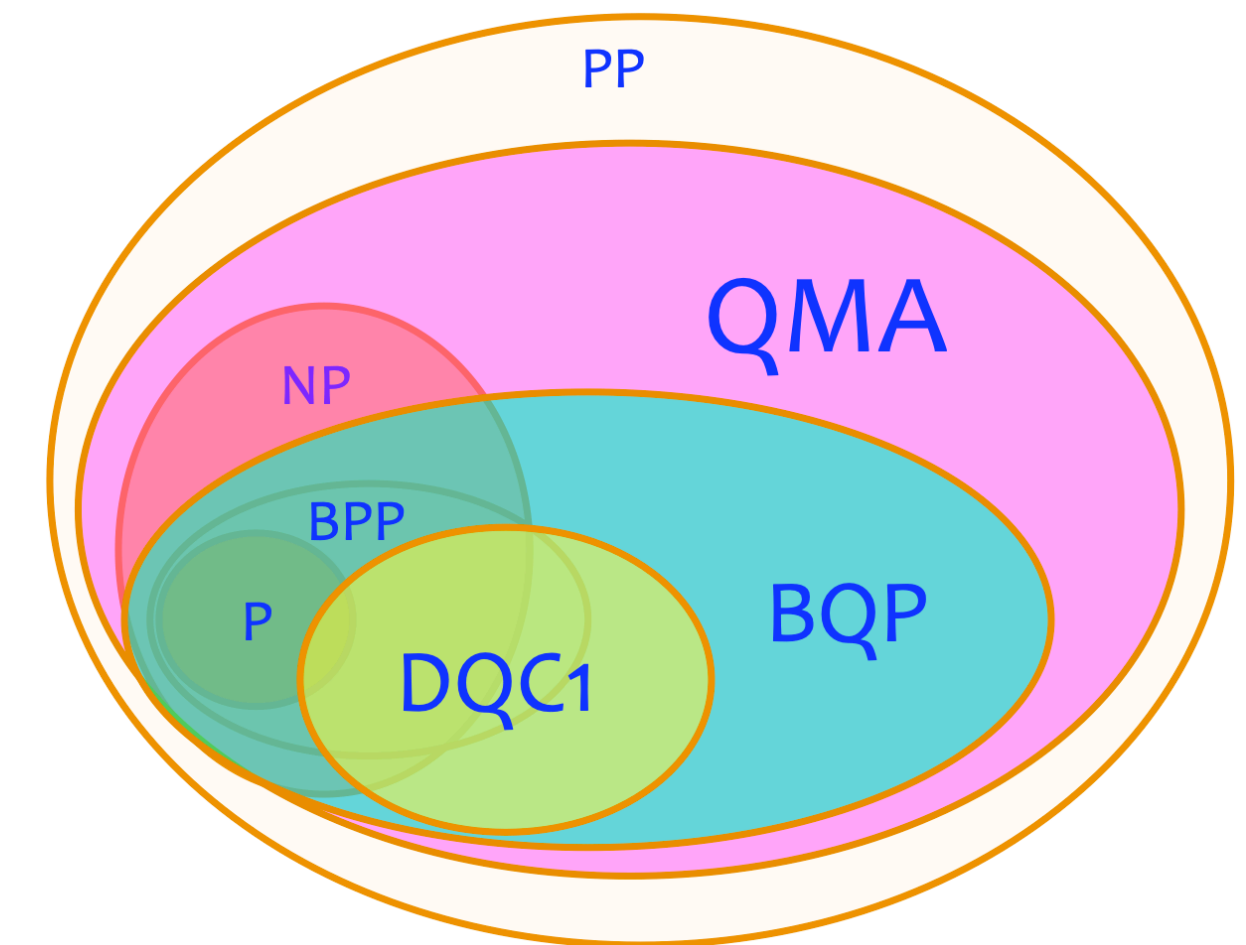
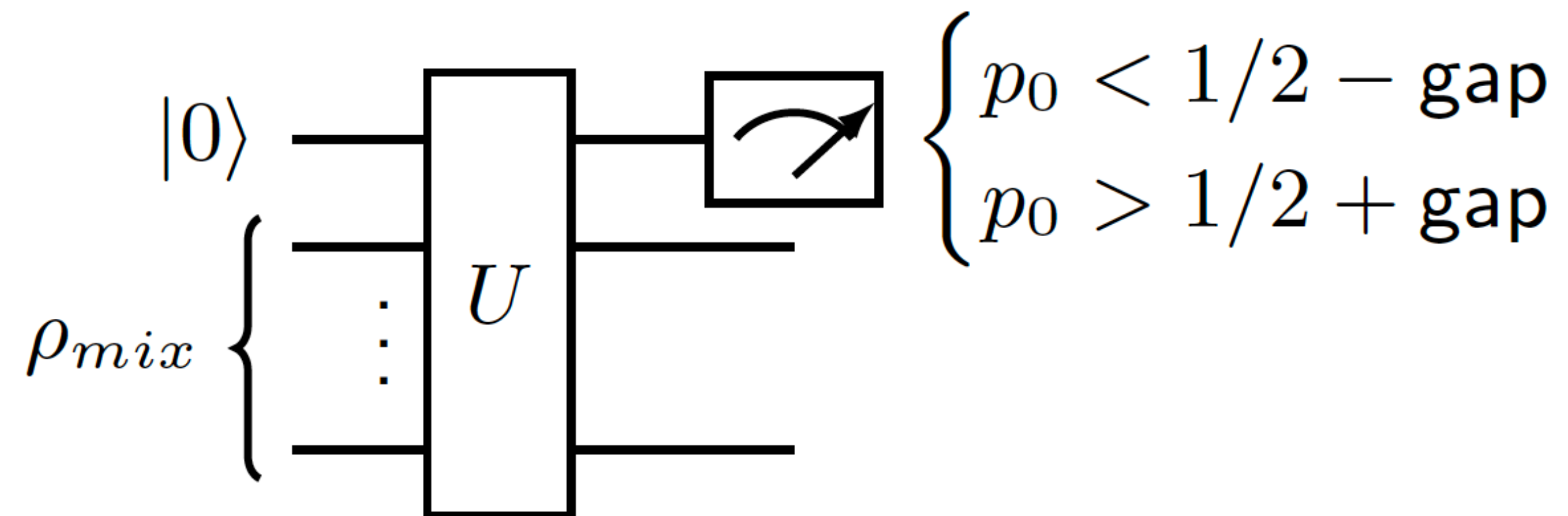
- ***hardness of TDA?***
- *when is the QC algorithm truly faster against “vanilla”...*
- *...and new classical algorithms?*

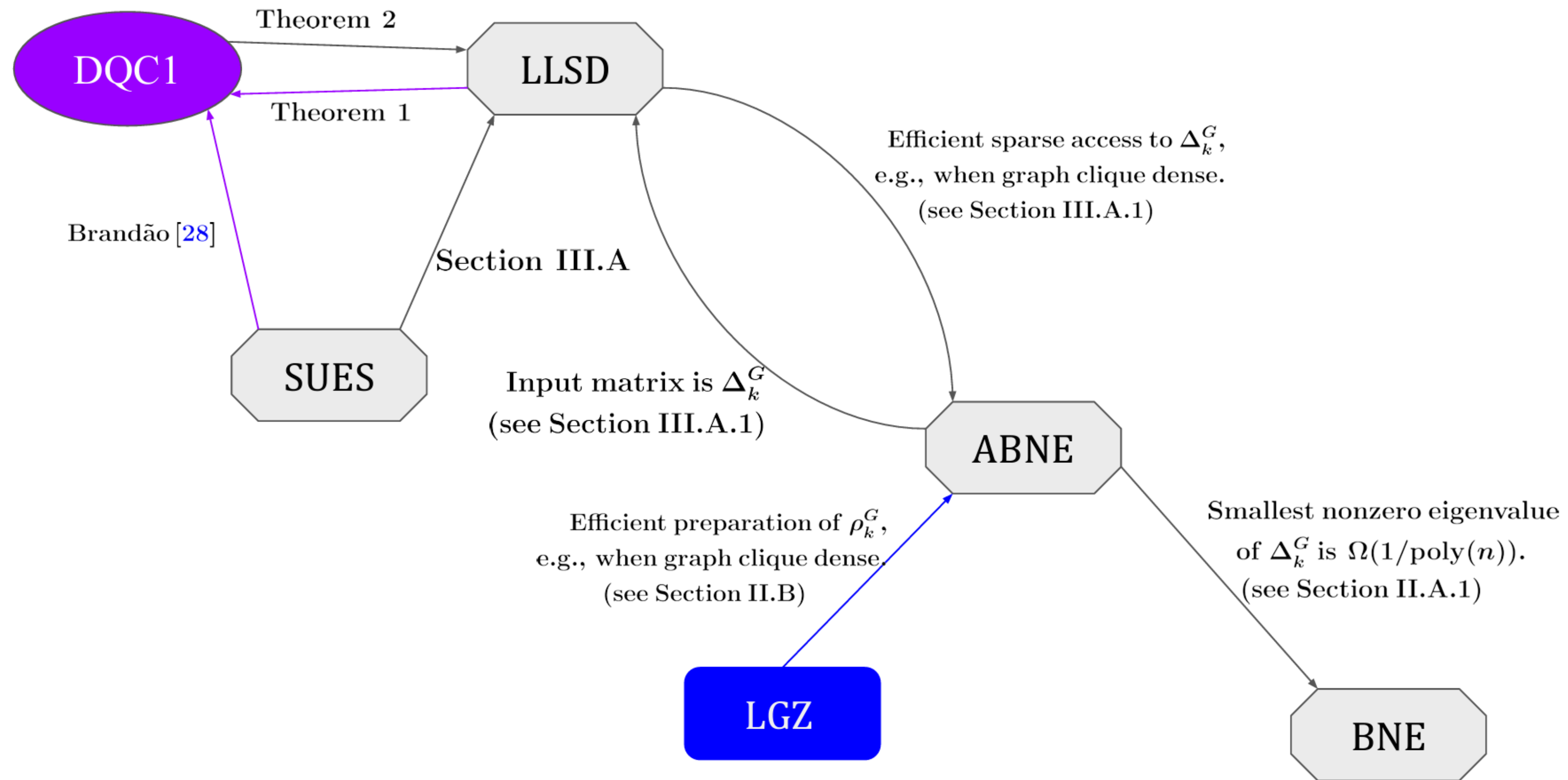
Generalizations of normalized-Betti-estimation are *DQC1-hard*



Generalizations of normalized-Betti-estimation are *DQC1-hard*

*DQC1 model of computation:*

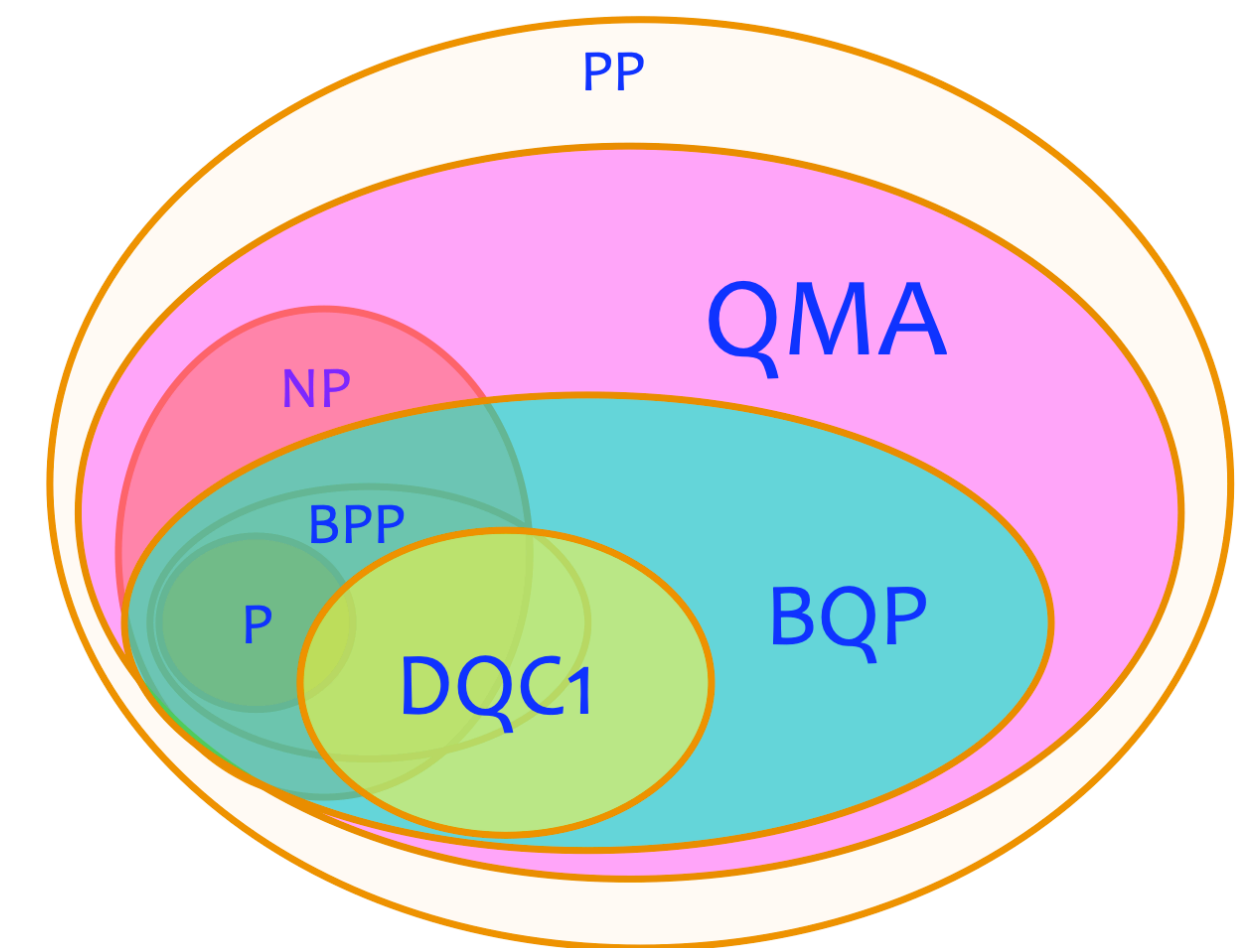
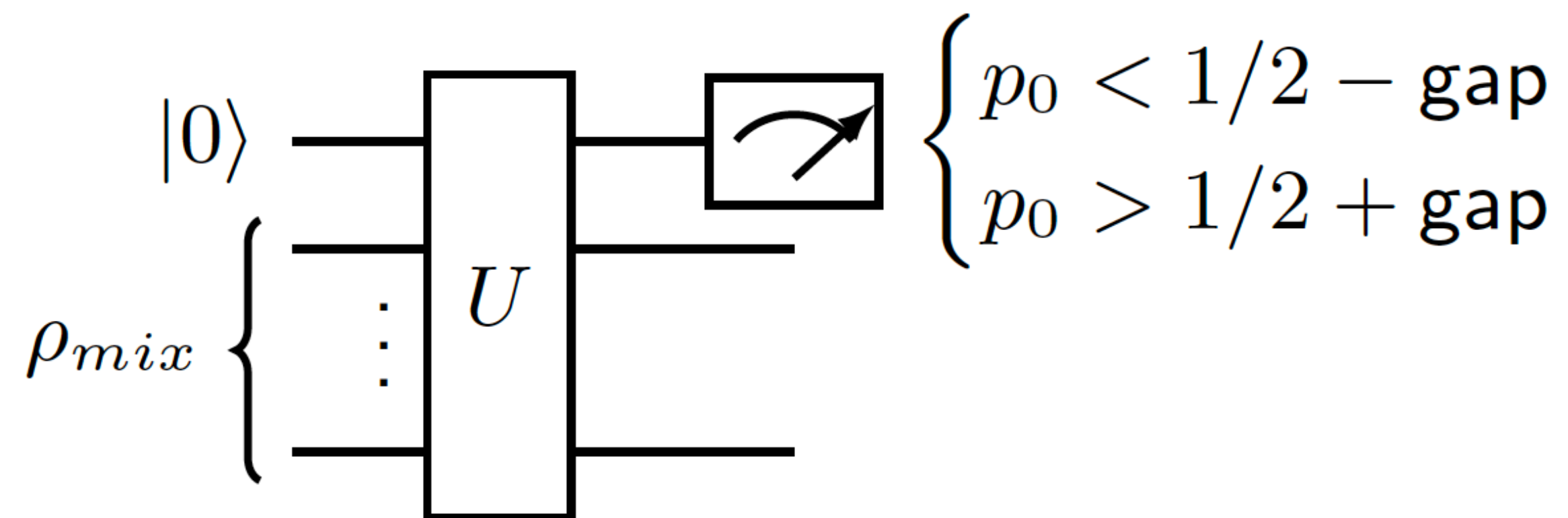




Marcos and Chris different (better) generalization

## Generalizations of normalized-Betti-estimation are *DQC1-hard*

*DQC1* model of computation:



However, generalizations quite substantial. Also, not **in BQP** for full range.  
Interestingly, QMA1 hardness of multiplicative error does not give DQC1 result.  
**Question unresolved.** Better classical algorithms emerging for **regions of interest**.

**Happy? Unhappy?**

## There is a reason to be worried\*

efficient (**additive** error) estimation of *normalized approximate Betti numbers* in regimes *where clique sampling is efficient*

(\*but I think in some cases we will be fine

\*\* arboricity properties will do, but let's not complicate)

## There is a reason to be worried\*

efficient (**additive** error) estimation of *normalized approximate Betti numbers* in regimes **where clique sampling is efficient**

**normalized** = *Betti / total-clique-number*

**sampling is efficient** = dunno, have many cliques out of all possible, probably\*\*?

→ *total-clique-number* is  $\Omega(n^k / \text{poly}(n))$ ....

(\*but I think in some cases we will be fine

\*\* arboricity properties will do, but let's not complicate)



**There is a reason to be worried\***

**Known results: Betti numbers tend to scale linearly with  $n$**

**Normalized Betti ... is zero** (to inverse sub-exponential additive error).

*(\*but I think in some cases we will be fine*

*\*\* arboricity properties will do, but lets not complicate)*

**Is there a *guaranteed* quantum advantage  
for *what we do have*, and can it be relevant?**

- *hardness of TDA?*
- ***when is the QC algorithm truly faster against vanilla...***
- ***...and new classical algorithms?***

## Analyzing Prospects for Quantum Advantage in Topological Data Analysis

Dominic W. Berry,<sup>1,\*</sup> Yuan Su,<sup>2</sup> Casper Gyurik,<sup>3</sup> Robbie King,<sup>2,4</sup> Joao Basso,<sup>2</sup> Alexander Del Toro Barba,<sup>2</sup> Abhishek Rajput,<sup>5</sup> Nathan Wiebe,<sup>5,6</sup> Vedran Dunjko,<sup>3</sup> and Ryan Babbush<sup>2,†</sup>

arXiv:2209.13581

Polynomial improvements in:

- (i) Dicke state preparation, clique checking, (ii) filtering for Kernel projection,
- (iii) better amplitude estimation for **optimal Toffoli gate count**

**also moved to relative error scalings for the estimation of Betti numbers!**

## Analyzing Prospects for Quantum Advantage in Topological Data Analysis

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Cost for relative error  $r$  for  $\beta_{k-1}$ :

Amplitude estimation

$$2 \frac{\ln(1/\delta)}{r} \sqrt{\frac{\#\text{k-cliques}}{\beta_{k-1}^G}}$$

×

Amplification

$$\frac{\pi}{4} \sqrt{\frac{\binom{n}{k}}{\#\text{k-cliques}}}$$

×

Preparing cliques

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

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Classical vanilla cost: #k-cliques  $\leq \binom{n}{k}$

Do graphs which are “**Betti dense**” (quantum easy)  
but still **large in clique numbers** (classically hard) even exist?

(= can the **red** be superpolynomially larger than the **blue**?)

## Do there exist graphs allowing a superpolynomial advantage?

reminder  $k$  = dimension of holes we are counting (which Betti?)

$n$  = # vertices

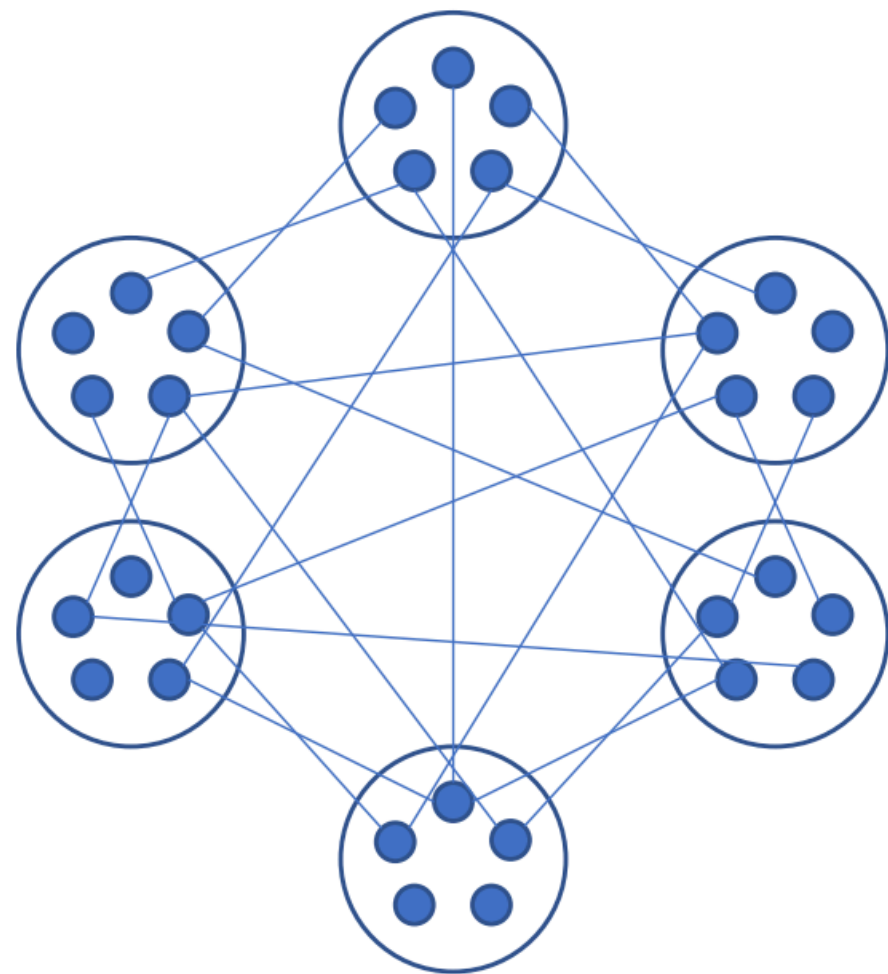
Regime  $k \in O(1)$  - classical runtime is poly, no superpolynomial speed-up

Regime  $k = cn, c \in [0,1)$  - classical runtime is exponential... ***but so is the quantum***



## Do there exist graphs allowing a superpolynomial advantage?

Regime  $k \in \Theta(\text{polylog}(n))$ .



$K(n/k, k)$

Künneth formulas

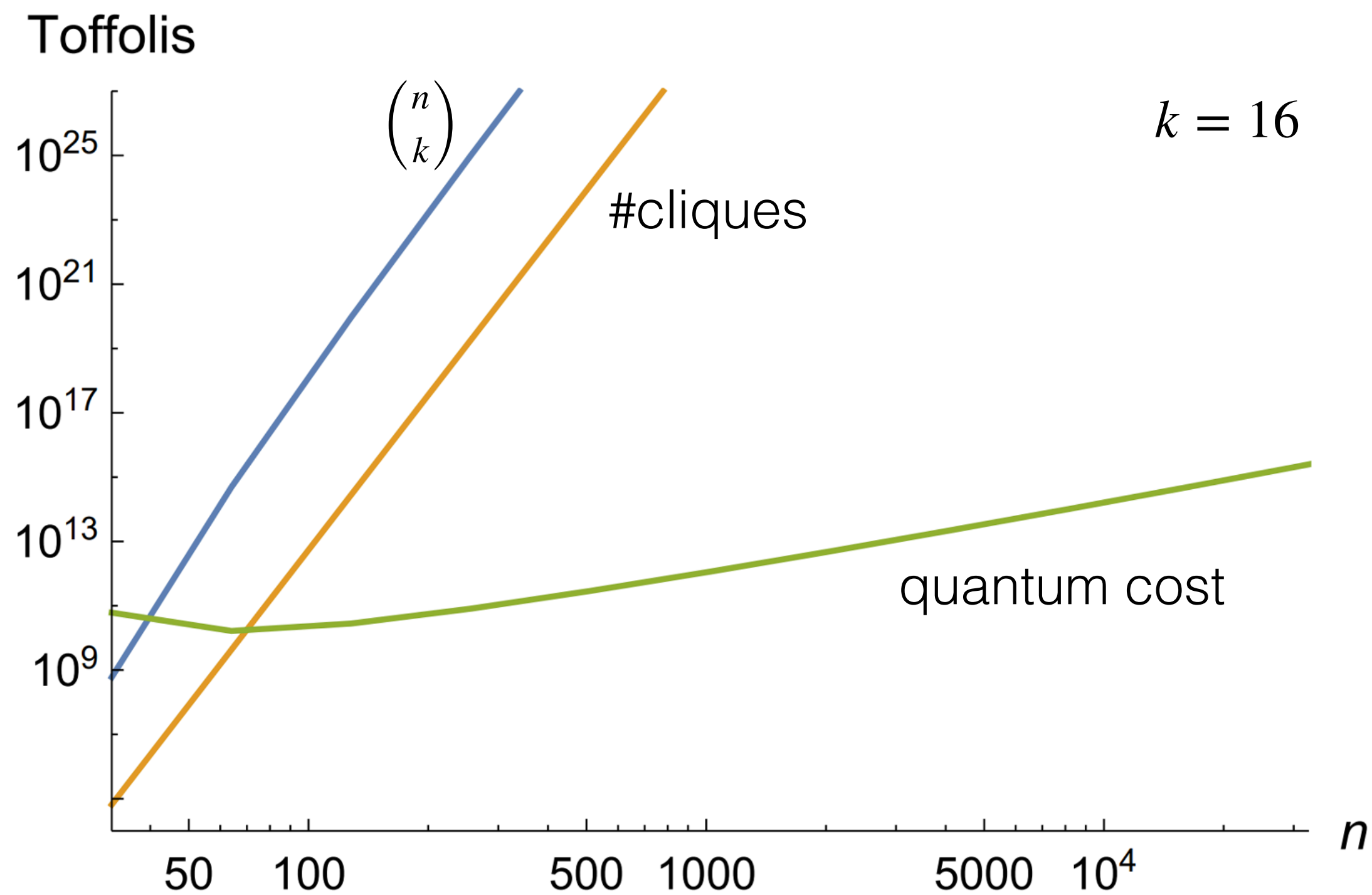
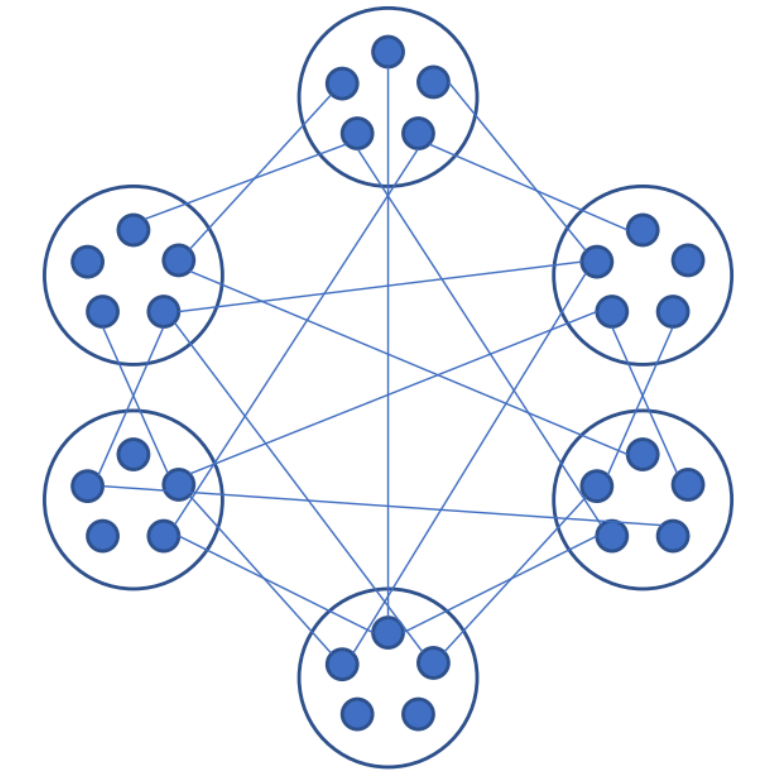
$$T_c \sim \exp(k \times (1 + \ln n/k))$$

$$T_q \sim \exp(k(1 + k/n)/2)$$

$$\alpha \text{ s.t. } T_c = T_q^\alpha; \quad \alpha \in \Theta(\log(n))$$

**Superpolynomial speed-up**

# Computing actual numbers...



$k=16, n=256$

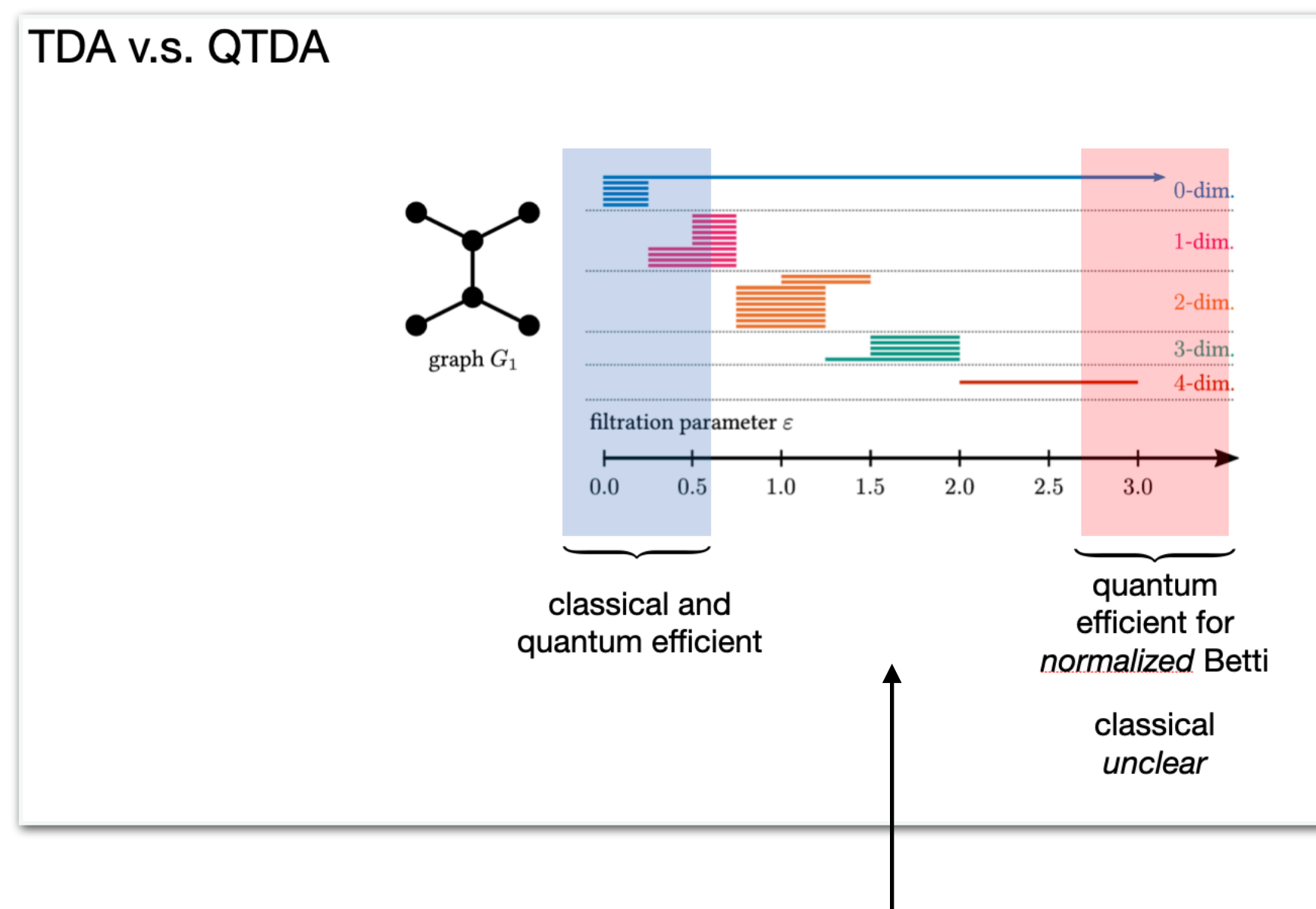
“speed-up” ~ 7.5<sup>th</sup> power

Dimension  $\binom{n}{k} \sim 10^{25}$

Classical: #cliques ~  $10^{19}$

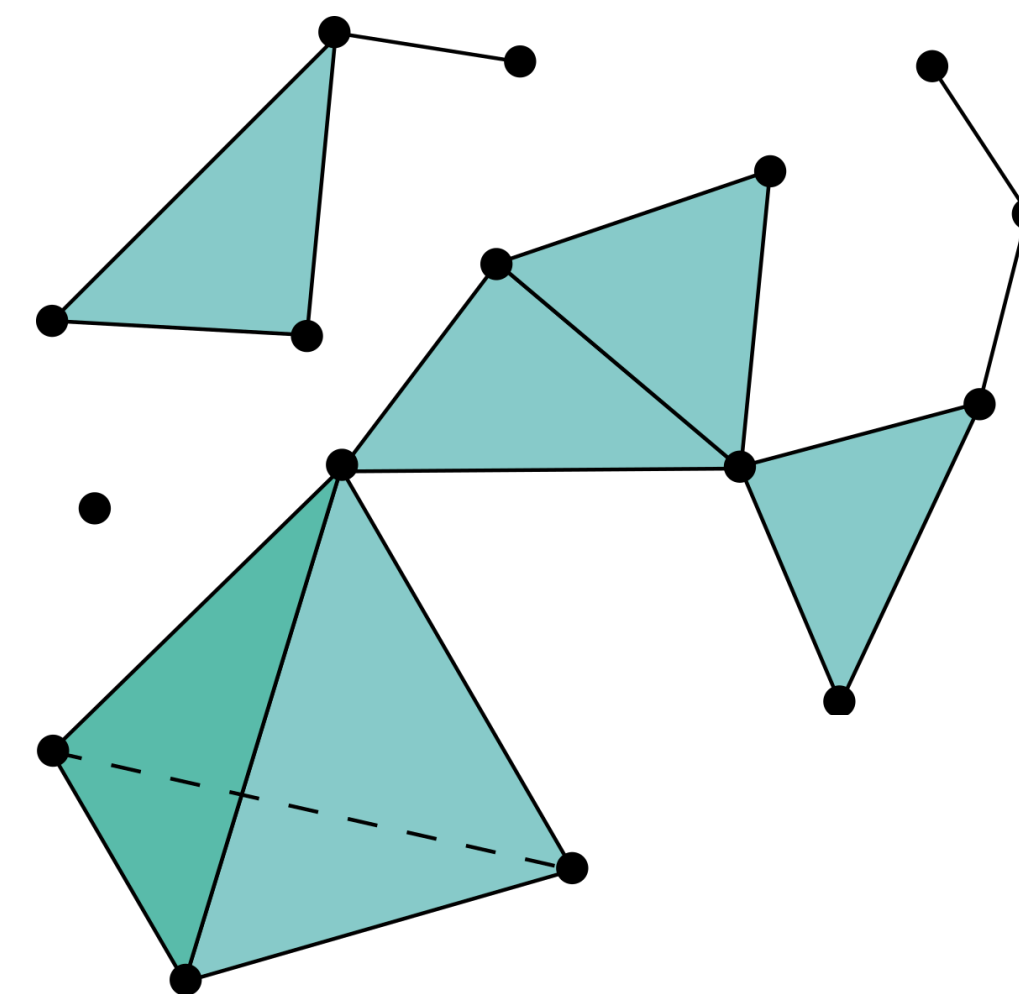
Quantum: 80 billion Toffolis

# Clique sampling *circumvented*



Not accessible due to no efficient generic sampling method of cliques from graphs

“Maximal faces” representation:



QMA1 hardness persists.  
Likely DQC1 hardness as well.

# In the meantime...

A (simple) classical algorithm for estimating Betti numbers

Simon Apers<sup>1</sup>, Sander Gribling<sup>1</sup>, Sayantan Sen<sup>2</sup>, and Dániel Szabó<sup>1</sup>

<sup>1</sup>Université Paris Cité, CNRS, IRIF, Paris, France

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## Abstract

We describe a simple algorithm for estimating the  $k$ -th normalized Betti number of a simplicial complex over  $n$  elements using the path integral Monte Carlo method. For a general simplicial complex, the running time of our algorithm is  $n^{\mathcal{O}(\frac{1}{\sqrt{\gamma}} \log \frac{1}{\varepsilon})}$  with  $\gamma$  measuring the spectral gap of the combinatorial Laplacian and  $\varepsilon \in (0, 1)$  the additive precision. In the case of a clique complex, the running time of our algorithm improves to  $(n/\lambda_{\max})^{\mathcal{O}(\frac{1}{\sqrt{\gamma}} \log \frac{1}{\varepsilon})}$  with  $\lambda_{\max} \geq k$ , where  $\lambda_{\max}$  is the maximum eigenvalue of the combinatorial Laplacian. Our algorithm provides a classical benchmark for a line of quantum algorithms for estimating Betti numbers. On clique complexes it matches their running time when, for example,  $\gamma \in \Omega(1)$  and  $k \in \Omega(n)$ .

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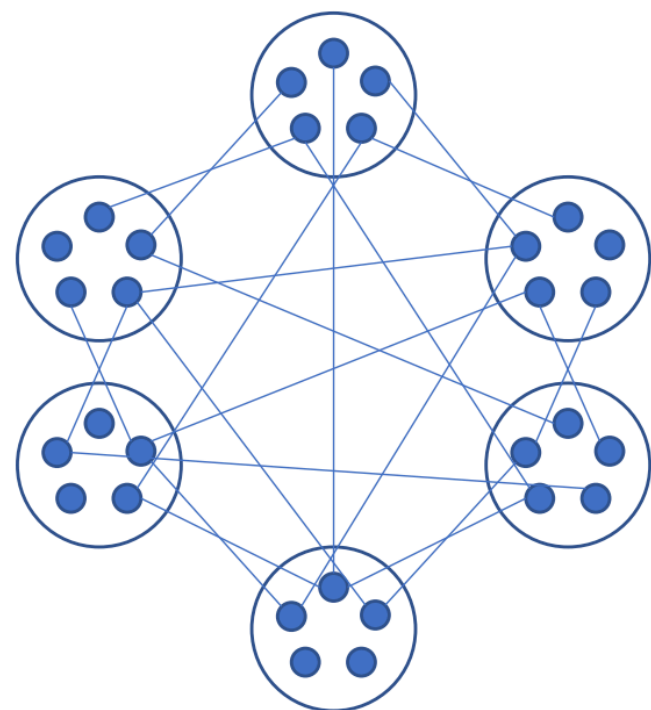
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$$(n/\lambda_{\max})^{\mathcal{O}\left(\frac{1}{\sqrt{\gamma}} \log \frac{1}{\varepsilon}\right)}$$

**Gap**   **Error**



**has constant gap  $\gamma \in \Theta(1)$ .**

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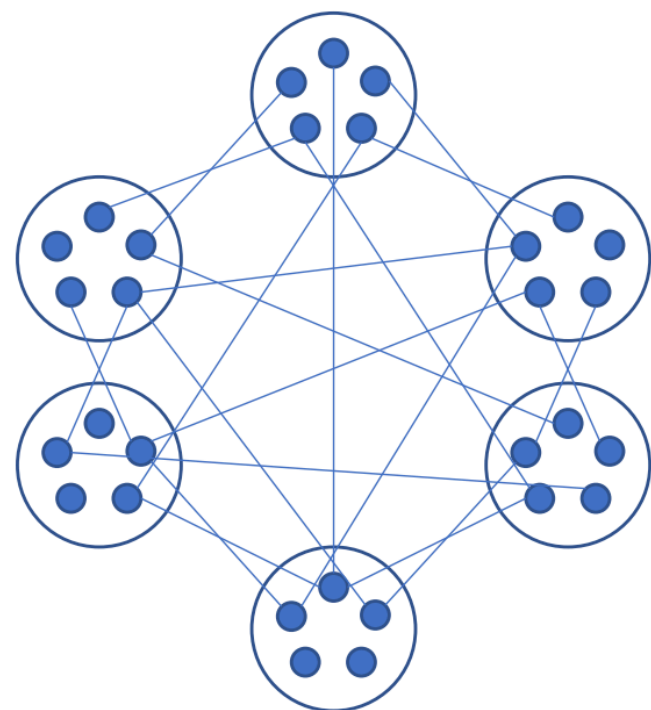
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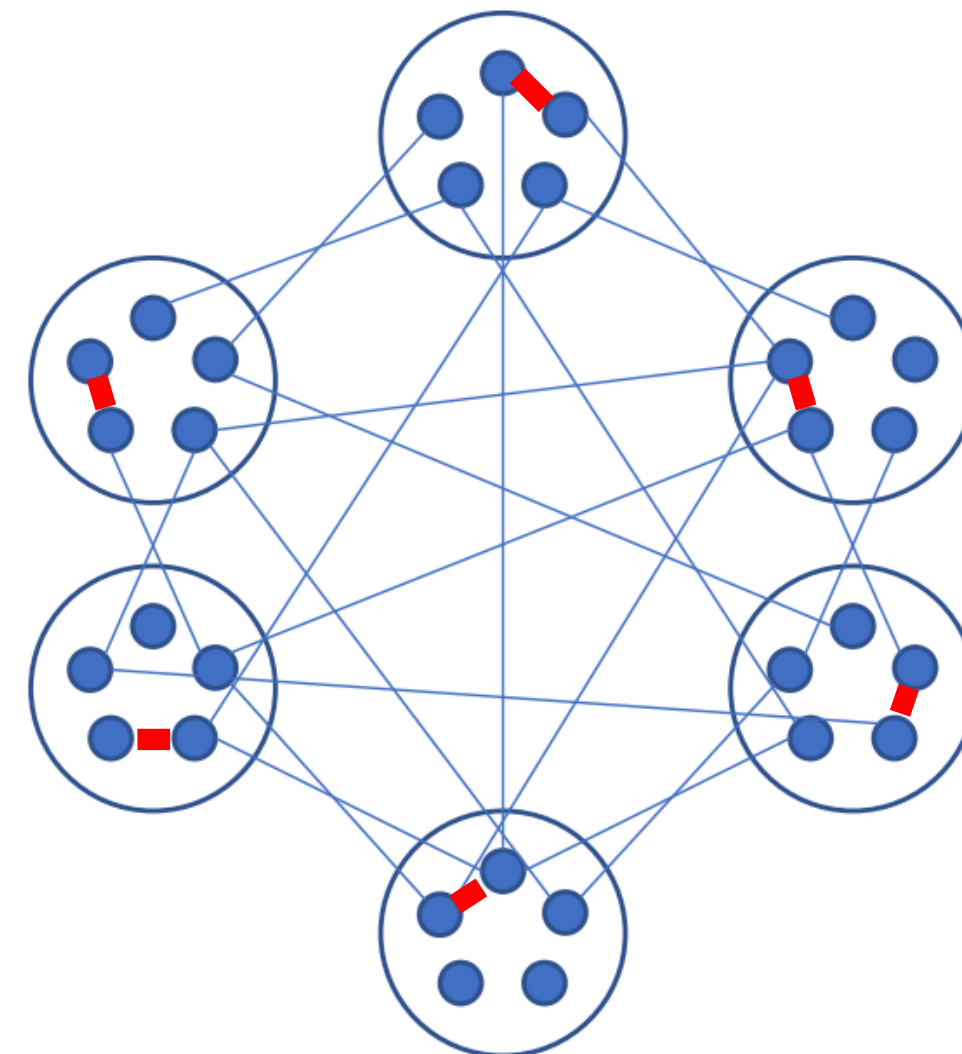
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$$(n/\lambda_{\max})^{\mathcal{O}(\frac{1}{\sqrt{\gamma}} \log \frac{1}{\varepsilon})}$$

$\xrightarrow{\text{Gap}}$       $\xrightarrow{\text{Error}}$



**has constant gap  $\gamma \in \Theta(1)$ .**



**perturbation has  $\gamma \leq \frac{1}{n}$**   
**superpoly speed-up**

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$$(n/\lambda_{\max})^{\mathcal{O}\left(\frac{1}{\sqrt{\gamma}} \log \frac{1}{\varepsilon}\right)}$$

Diagram showing the equation with arrows pointing to the terms  $\gamma$  and  $\varepsilon$  in the exponent, labeled "Gap" and "Error" respectively.

Gap Error

normalized ***approximate*** Betti numbers

approximate = counting *small* eigenvalues (not *silly* due to Cheeger-like arguments)

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Diagram showing the equation with arrows pointing from the words "Gap" and "Error" to the terms  $\gamma$  and  $\varepsilon$  respectively in the exponent.

normalized ***approximate*** Betti numbers

approximate = counting *small* eigenvalues (not *silly* due to Cheeger-like arguments)

small = small constant or  $\log^{-1}(n) \rightarrow$  no quantum advantage

small =  $\text{poly}^{-1}(n) \rightarrow$  maybe quantum advantage



## Meta-problem

we prove separations... by computing Betti number  
so there exists **an** efficient algorithm, *and we know it!*

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so there exists **an** efficient algorithm, *and we know it!*

but if we cannot compute it... we cannot claim quantum speed-up

**Solution:** prove certain perturbations sometimes perturb the Betti *measurably* by a small amount without *explicitly* computing it

(Likely) can be done, as alternatively adding edges could always fully uncontrollably change Betti numbers, or do nothing...

To be sure-sure: prove DQC1-hardness!

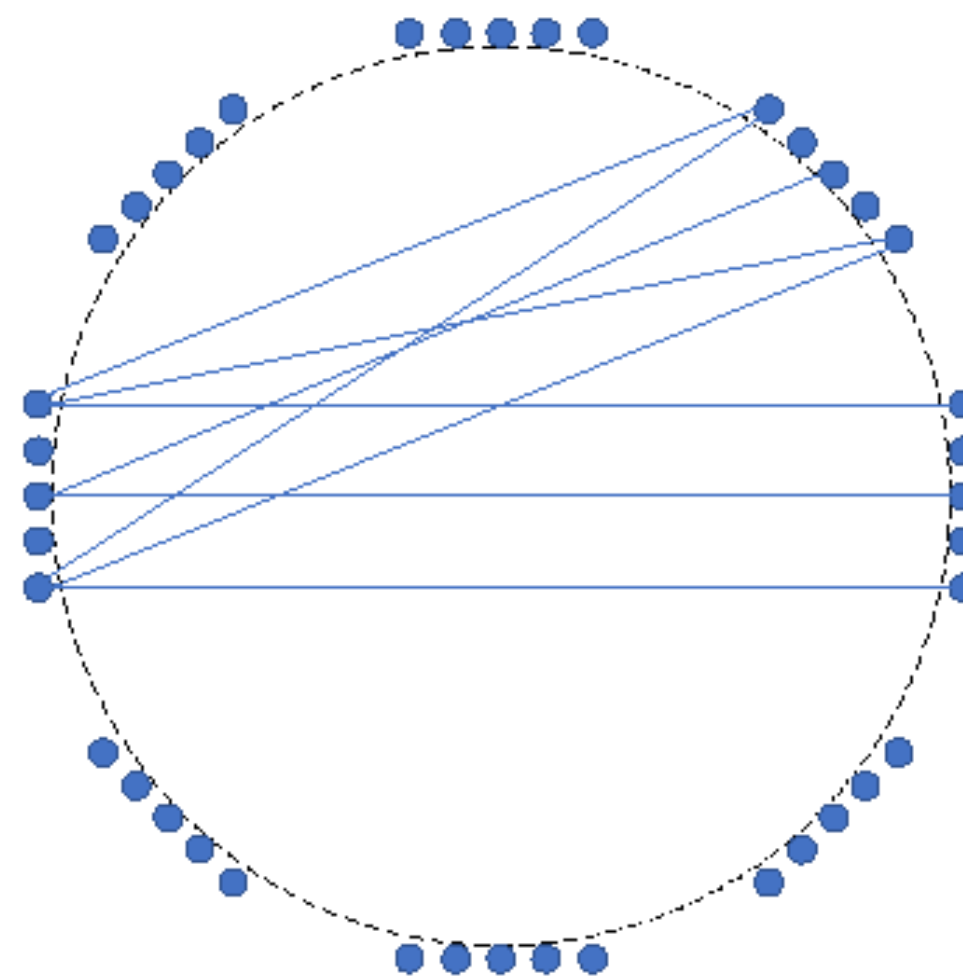
## Are superpolynomial speedups for TDA likely generic?

Likely not. For *generic* graphs, we do not have the nice properties....

For Erdős-Renyi graphs, there are regions with expected **quartic** speed-ups

For Vietoris-Rips complexes (i.e., the way I described the pipeline from point clouds) for data from *i.i.d.* distributions, **avg.** Betti numbers do not scale fast enough.

But already in 2D (worst) case:



Large Betti and small gap....

## Small summary

DQC1 hardness needed

high Betti problems needed

huge v.s. tiny Betti problems needed

non-iid point-clouds needed

graph density / max face input settings needed

good *approximate* Betti needed

but superpoly speed-ups still plausible

some high-poly speed-ups even *likely*

*and there is much more to the overall topic*

## Beyond *obvious* TDA applications



Betti numbers  
Persistence properties

Other complexes  
Other homology problems



Supersymmetry



Homology

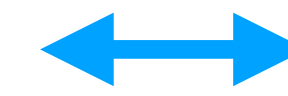


SUSY QM on lattices

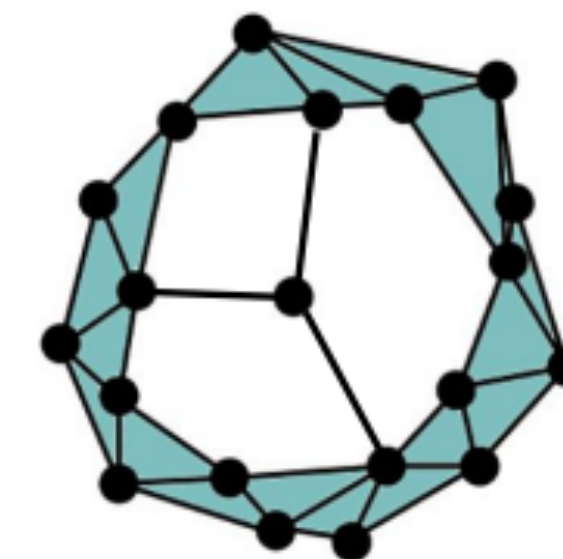


Homology on  
(simplicial) complexes

$$H = \{Q, Q^\dagger\}$$



supercharge operators





$$H = \{Q, Q^\dagger\} \quad Q = \sum_i a_i^\dagger P_i$$

$$H = \sum_{(i,j) \in E} P_i a_i^\dagger a_j P_j + \sum_{i \in V} P_i \quad P_i = \prod_{j|(i,j) \in E} (1 - a_j^\dagger a_j)$$

# $\ell$ -dim holes = # $\ell$ -fermion ground states

fine print: the above is for the *independence complex*

Witten '89  
<https://arxiv.org/pdf/2107.00011.pdf>





$$H = \{Q, Q^\dagger\} \quad Q = \sum_i a_i^\dagger P_i$$

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$\#\ell$ -dim holes =  $\#\ell$ -fermion ground states

quantum computational physics  $\leftrightarrow$  computational physics  $\leftrightarrow$  theory  $\leftrightarrow$  quantum TDA methods

# Combinatorial Laplacians for complex networks



Quantity: 
$$S_\alpha(\Delta_k^G) = \frac{1}{1-\alpha} \log \left( \sum_{j=0}^{d_k-1} p(\lambda_j)^\alpha \right)$$

Generalizations hard as Renyi entropies known to be DQC1-hard

Precision not as obviously problematic

Clique sampling still an issue, depending on the model

spectral entropy of higher-order  
representations of networks

## Some topics in group + friends

Computational many-body methods & comp. topology

Heuristic and QML algorithms for comp. topology

Applications of (Q)TDA to HEP and other physics

Applications in biology (networks)

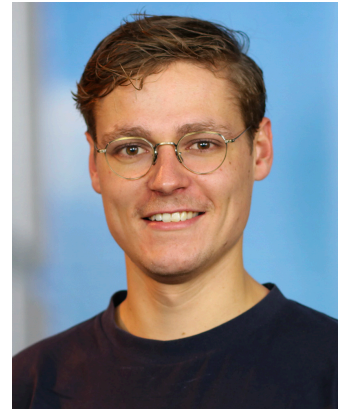
Other developments in complexity and new algos



*Patrick*



*Alice*



*Casper*



*Mahtab*



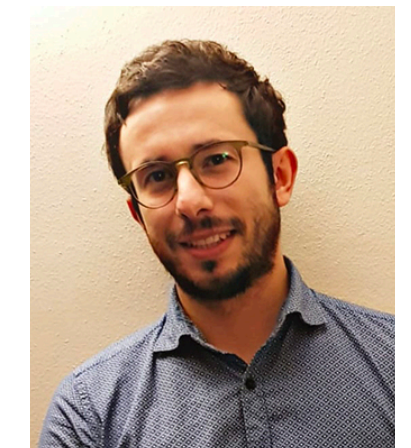
*Vincent*



*Waheeda*



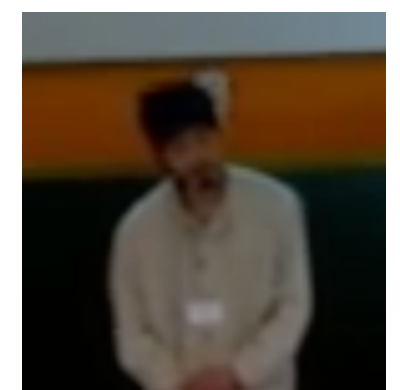
*Sofia*



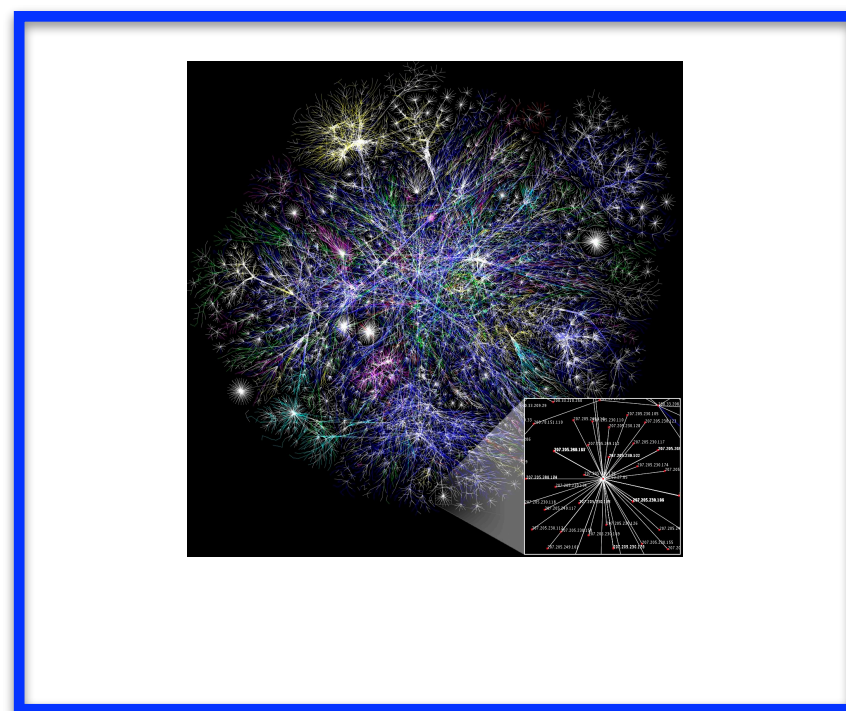
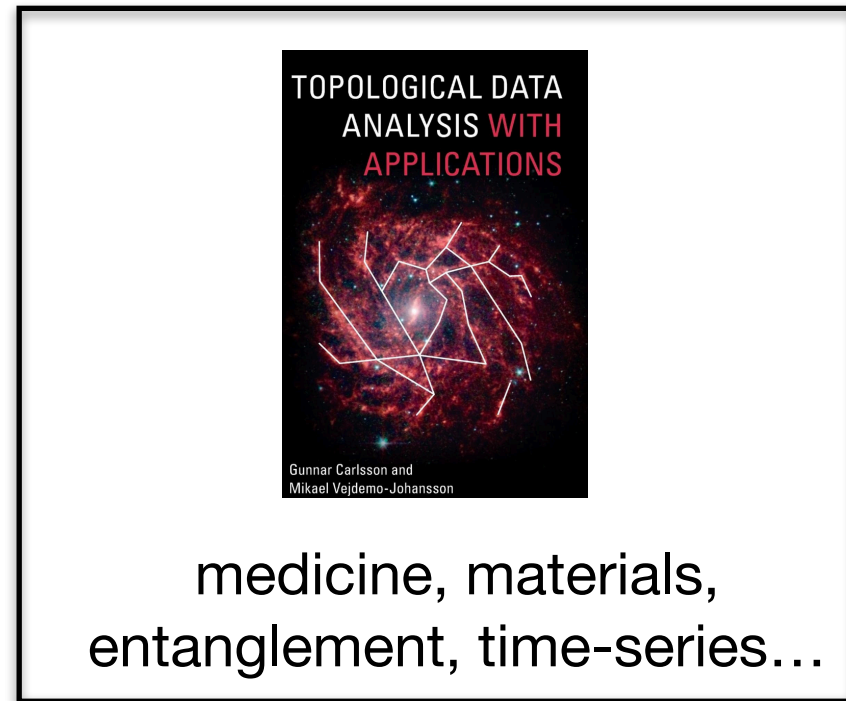
*Michele*



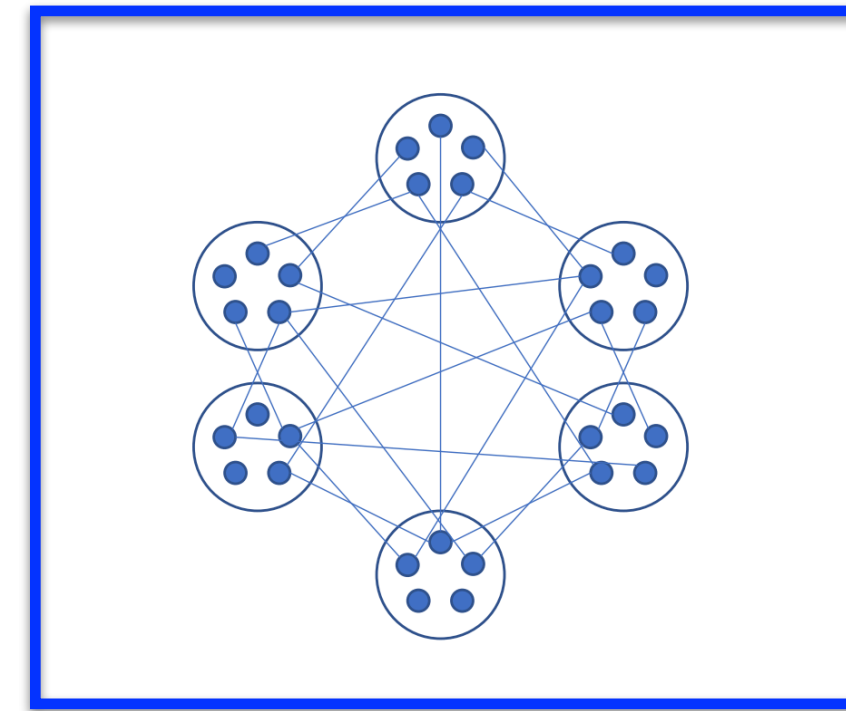
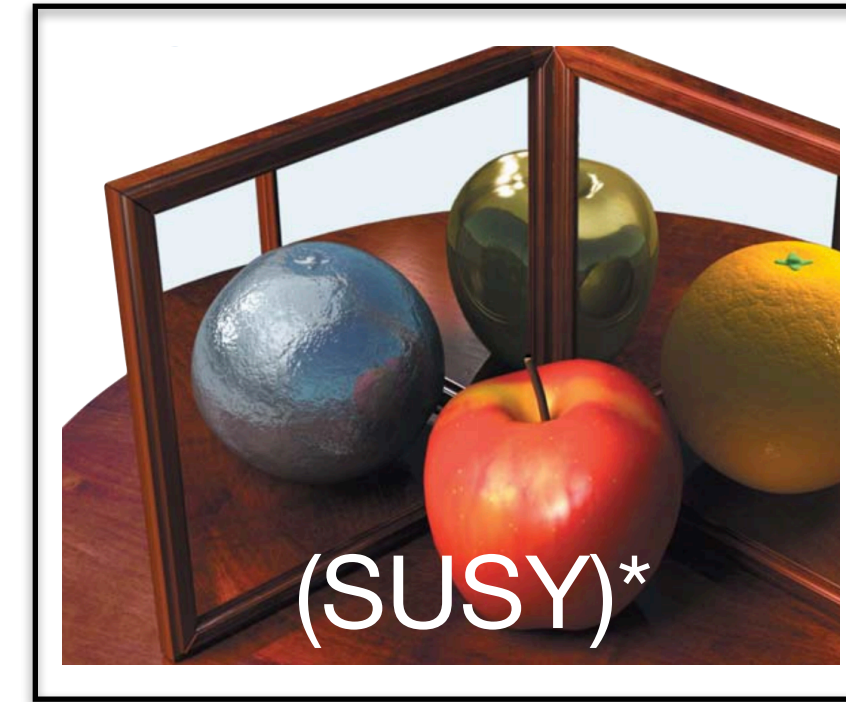
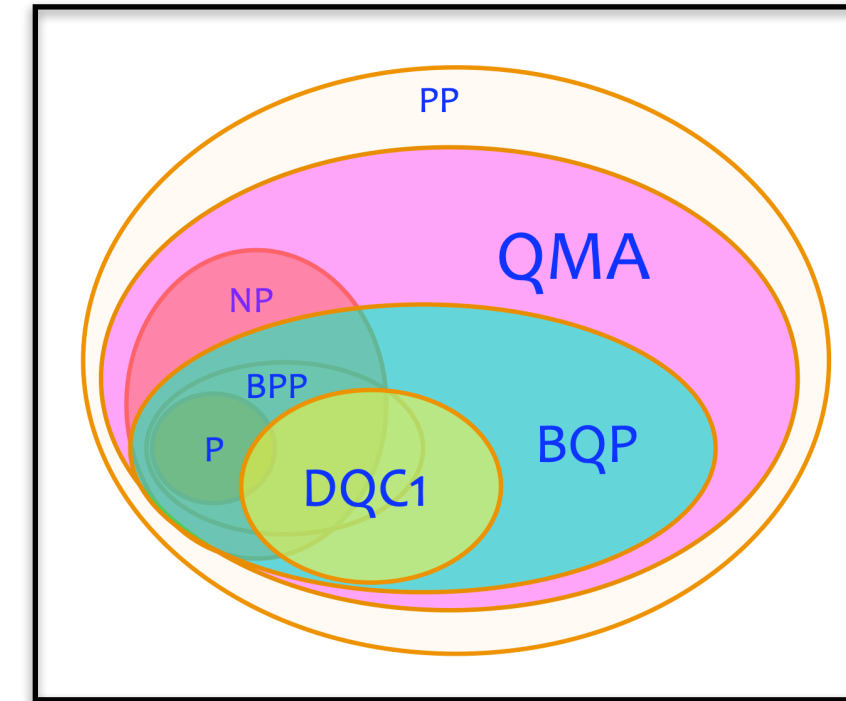
*Robbie*



*Hayakawa*



(Q)TDA



Quantum+Topology\*\* is well-connected and *rich*

\*Image credit: Scientific American, JSTOR

\*\* Don't get me started on TQFT and knots!

Big thanks to coauthors:

Casper Gyurik, Chris Cade, Dominic Berry, Yuan Su, Robbie King, Joao Basso, Alexander Del Toro Barba, Abhishek Rajput, Nathan Wiebe, Ryan Babbush



**Applied Quantum Algorithms Leiden:**  
**Open PhD and PostDoc positions**

