# Quantum Algorithms for Computing Expectation Values and Partition Functions

Yassine Hamoudi

UC Berkeley

# Estimating expectation values

# Estimating expectation values

- Fundamental task for extracting classical information from quantum systems

- Entanglement allows for better accuracy in the estimation (Heisenberg vs shot-noise limits)

- Algorithmic perspective: focus on the statistical and computational challenges / limits

# Estimating expectation values

Given classical samples from a random variable $X$, compute

$$(1 \pm \epsilon)\ E[X]$$

$$\Downarrow$$

Given an observable $O$ and quantum-access to a state $|\psi\rangle$, compute

$$(1 \pm \epsilon)\ \langle \psi | O | \psi \rangle$$

# Estimating expectation values

What does it mean to have quantum-access to a state $|\psi\rangle$ ?

- We know a quantum circuit that implements the reflection $2|\psi\rangle\langle\psi| - I$

  (suffices to know a circuit that prepares $|\psi\rangle$)

- Assumption met by many state-preparation quantum algorithms

  (Hamiltonian simulation, quantum walks, …)

- Stronger than just having copies of $|\psi\rangle$ usually

# Estimating expectation values

Optimal complexity under minimal assumptions

$$(1 \pm \epsilon)\ E[X]$$

$$(1 \pm \epsilon)\ \langle \psi | O | \psi \rangle$$

$$\frac{\mathrm{Var}(X)}{\epsilon^2} \longrightarrow \frac{\sqrt{\mathrm{Var}(O)}}{\epsilon}$$

# classical samples

# quantum accesses

H. "Quantum Sub-Gaussian Mean Estimator". 2021.

Kothari, O'Donnell. "Mean Estimation when You Have the Source Code; Or, Quantum Monte Carlo Methods". 2023.

# Estimating expectation values

Based on encoding expectation value into an eigenphase

$$U|0\rangle = e^{f(\langle\psi|O|\psi\rangle)}|0\rangle$$

retrieved by quantum phase estimation.

**Challenge:** improving $\frac{\|O\|}{\epsilon}$ into $\frac{\sqrt{\mathrm{Var}(O)}}{\epsilon}$ for heavy-tailed distributions

Handled by combining old and new algorithmic techniques:

Quantiles estimation, QSVT, Grover's with complex phases, …

# Estimating expectation values

Results partially extended to multivariate estimation

$$\langle\psi|O_1|\psi\rangle, \ldots, \langle\psi|O_d|\psi\rangle$$

$\sqrt{d}$ overhead over univariate estimators

- For commuting observables: bounded covariance $\mathrm{Tr}(\Sigma)$ assumption
- For non-commuting observables: bounded norms $||O_i||$ assumption

Cornelissen, H., Jerbi. "Near-Optimal Quantum Algorithms for Multivariate Mean Estimation". 2022.
Huggins et al. "Nearly Optimal Quantum Algorithm for Estimating Multiple Expectation Values". 2022.

# Estimating partition functions

# Estimating partition functions

Given a classical Hamiltonian $H : \Omega \to \{0,1,\ldots,n\}$

and an inverse temperature $\beta$

approximate the partition function $Z(\beta) = \mathrm{Tr}\left(e^{-\beta H}\right)$

# Estimating partition functions

- Partition functions are ubiquitous
  - statistical physics
  - combinatorics (counting matchings, independent sets…)
  - linear algebra (permanents)
  - convex geometry (volume of a body)
  - machine learning (graphical models)
  - …

# Estimating partition functions

- Partition functions are ubiquitous
- Related to counting (generating functions) and phase transitions
- Exact computation is often #P-hard
- … but there exists efficient approximation methods (MCMC, Taylor’s approximation, correlation decay, …)

# Estimating partition functions

The classical Markov Chain Monte Carlo (MCMC) algorithms★ for estimating $Z(\beta)$ can be speed-up by quantum algorithms running in time

$$\approx \log^{1/4}|\Omega| \times \sqrt{\text{time of classical MCMC algo}}\,.$$

**This class of methods includes the best known algorithms for:**

- number of independent sets, colorings, matchings
- Ising, Potts, monomer-dimer,… models
- volume of convex bodies
- permanent of nonnegative matrices

★ Štefankovič, Vempala, Vigoda. "Adaptive Simulated Annealing: A Near-Optimal Connection between Sampling and Counting", 2009.
Cornelissen, H. "A Sublinear-Time Quantum Algorithm for Approximating Partition Functions". 2023.

# Estimating partition functions

Combines two branches of work:

**1**

Converting classical reversible Markov chains into quantum walks

**2**

"Enhanced" Quantum estimators

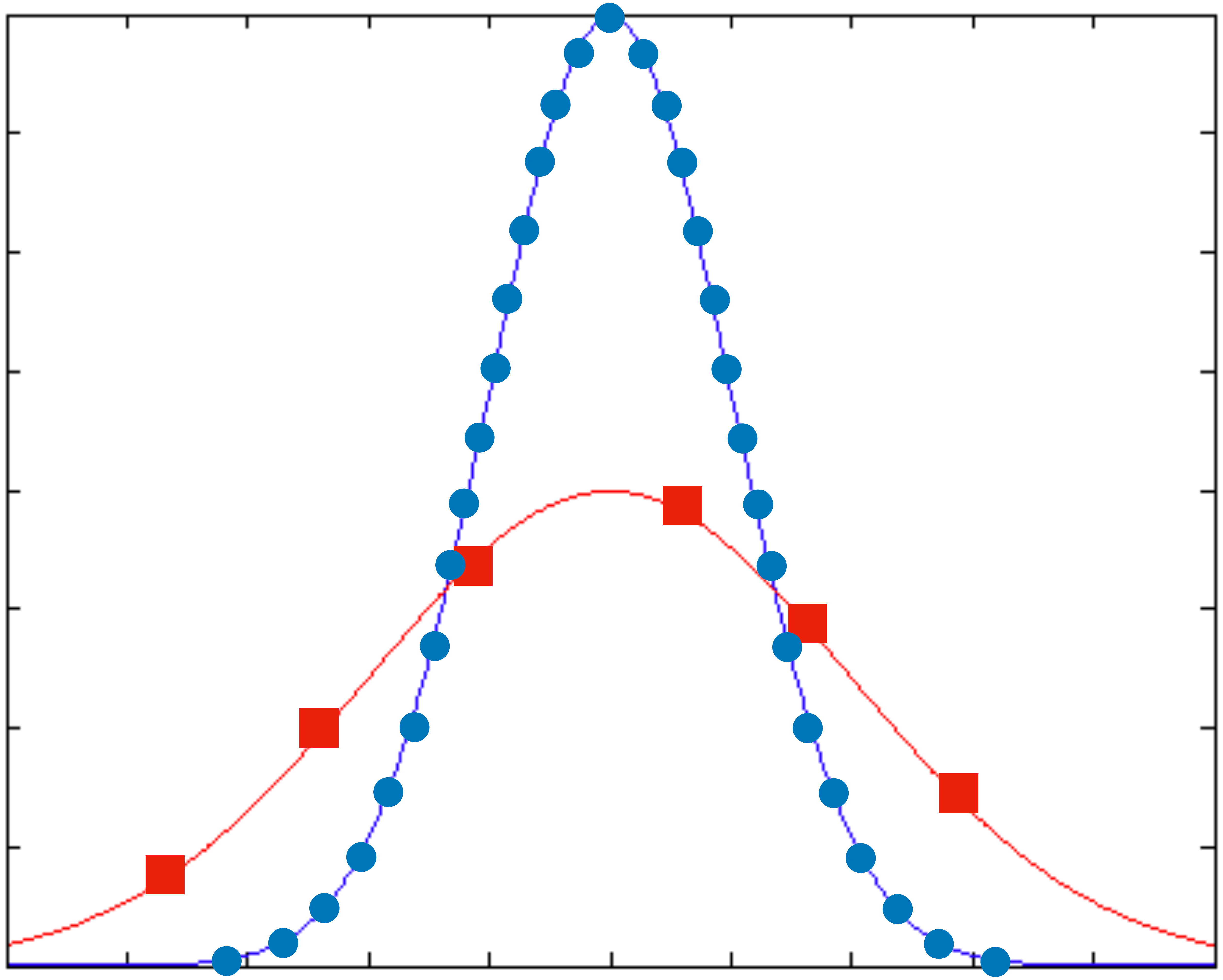
- Unbiased
  - ▶ Returns $\langle \psi | O | \psi \rangle$ in expectation
- Non-destructive
  - ▶ Restores $|\psi\rangle$ after estimation

Szegedy. "Quantum Speed-Up of Markov Chain Based Algorithms". 2004.
Harrow, Wei. "Adaptive Quantum Simulated Annealing for Bayesian Inference and Estimating Partition Functions". 2020.
Linden, de Wolf. "Average-Case Verification of the Quantum Fourier Transform Enables Worst-Case Phase Estimation". 2022.
Cornelissen, H. "A Sublinear-Time Quantum Algorithm for Approximating Partition Functions". 2023.

# New phase estimation primitive


Cornelissen, H. "A Sublinear-Time Quantum Algorithm for Approximating Partition Functions". 2023.

# New phase estimation primitive



Outcome distributions of:

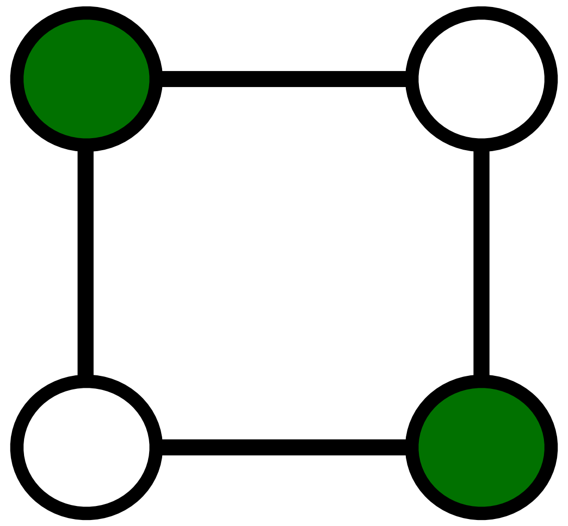
- Standard phase estimation

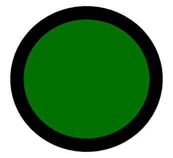
  (not exactly symmetric)

- Enhanced phase estimation

  (symmetric, lighter tail)

## Example 1:
## The hard-core gas model

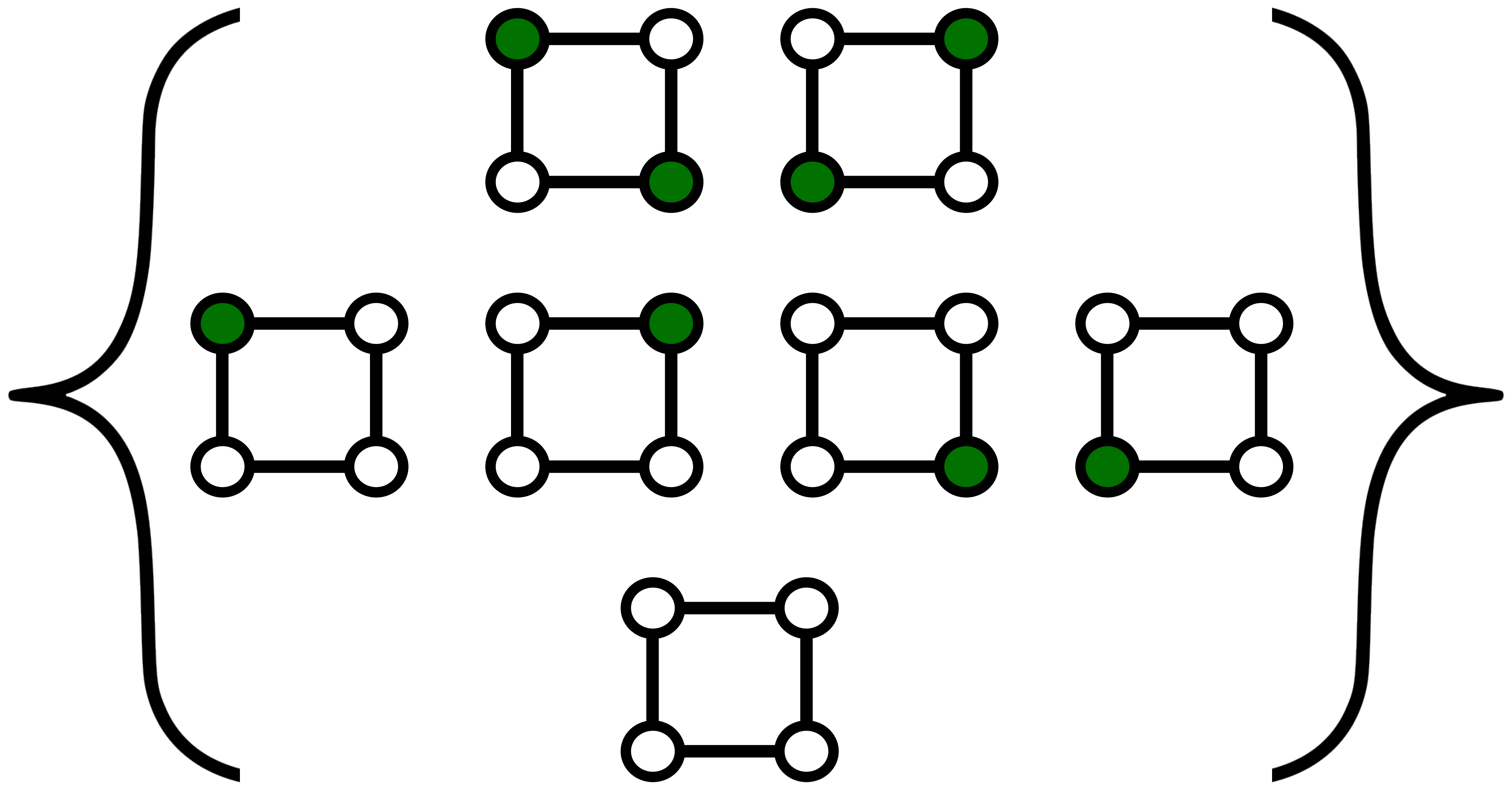


 = occupied

Independent set

(subset of non-adjacent vertices)

# Example 1:
# The hard-core gas model

$\Omega =$ 

$H(\sigma) =$ number of ● in $\sigma$

$Z(0) =$ number of ind. sets

Exponential size

# Example 1:
# The hard-core gas model

$$(1 \pm \epsilon)\ Z(0)$$

(for degree $\leq 5$ graphs)

Classical MCMC

$$\tilde{O}\left(\frac{(\#\text{vertices})^{2}}{\epsilon^{2}}\right)$$

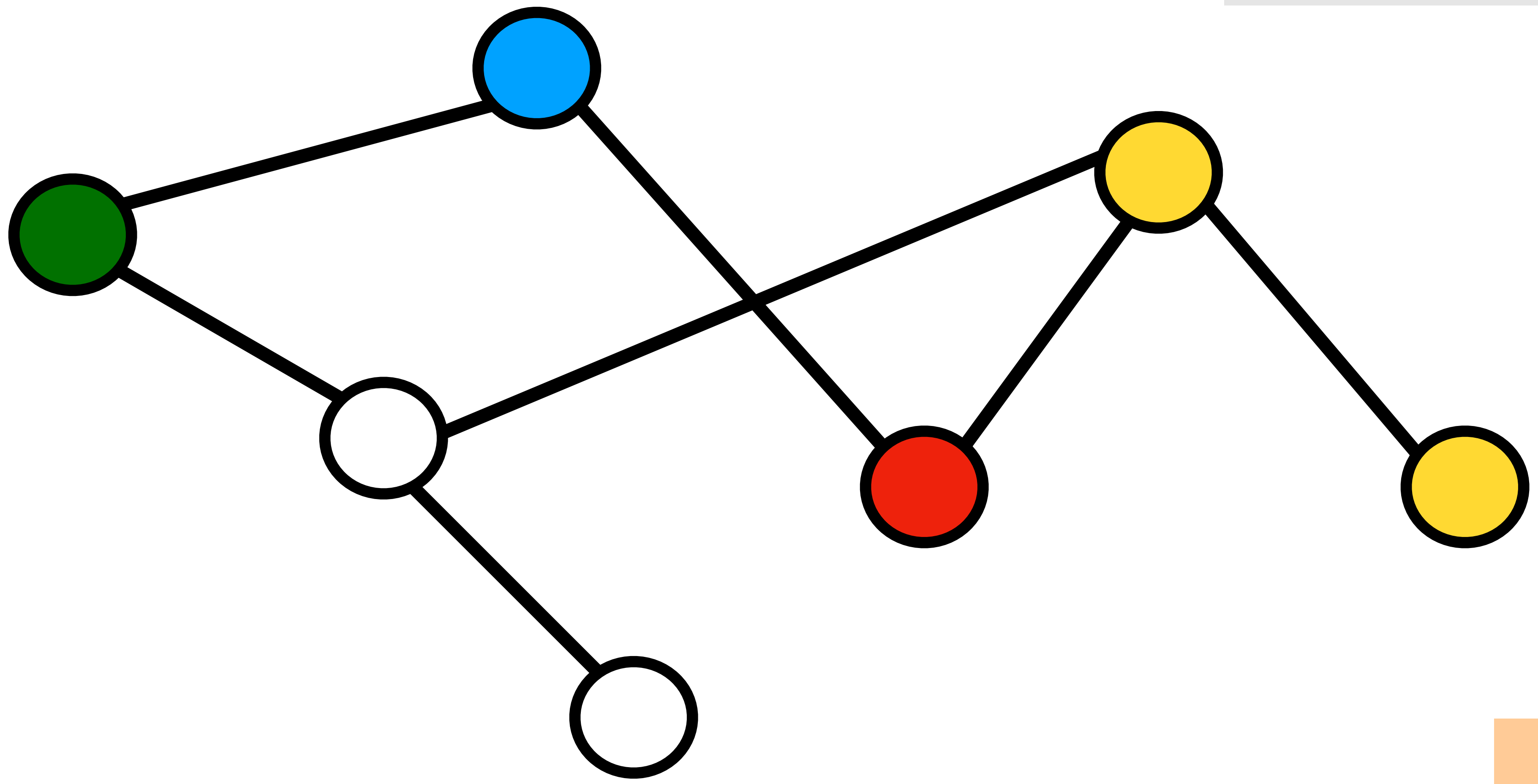
$\Rightarrow$

Quantum algorithm

$$\tilde{O}\left(\frac{(\#\text{vertices})^{5/4}}{\epsilon}\right)$$

Štefankovič, Vempala, Vigoda. “Adaptive Simulated Annealing: A Near-Optimal Connection between Sampling and Counting”, 2009.
Chen,Liu,Vigoda. “Optimal Mixing of Glauber Dynamics: Entropy Factorization via High-Dimensional Expansion”. 2021.
Cornelissen, H. “A Sublinear-Time Quantum Algorithm for Approximating Partition Functions”. 2023.

# Example 2:
# The Potts model



$H(\sigma)$ = number of monochromatic edges

$Z(\infty)$ = number of valid colorings

$$(1 \pm \epsilon)\, Z(\infty)$$

(for degree < #colors/2)

Classical MCMC

$$\tilde{O}\left(\frac{(\#\text{vertices})^{2}}{\epsilon^{2}}\right)$$

$$\Rightarrow$$

Quantum algo.

$$\tilde{O}\left(\frac{(\#\text{vertices})^{5/4}}{\epsilon}\right)$$

Jerrum. “A Very Simple Algorithm for Estimating the Number of k-Colorings of a Low-Degree Graph”. 1995.
Štefankovič, Vempala, Vigoda. “Adaptive Simulated Annealing: A Near-Optimal Connection between Sampling and Counting”, 2009.
Cornelissen, H. “A Sublinear-Time Quantum Algorithm for Approximating Partition Functions”. 2023.

# Future directions

- Quantum estimators with new features (robustness, differential privacy, …)
- Quantum estimators for NISQ devices (shadow tomography, …)
- Quantum estimators for high-dimensional statistics (applications in q. machine learning, q. linear algebra, …)
- Faster algorithms for (classical or quantum) partition functions