Quantum Algorithms for the Monte Carlo Method

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Soutenance de thèse présentée
le 7 juillet 2021

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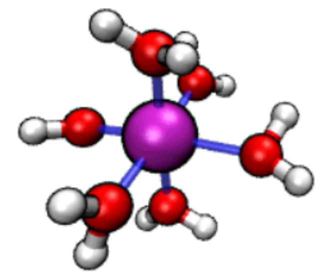
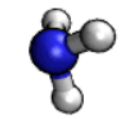
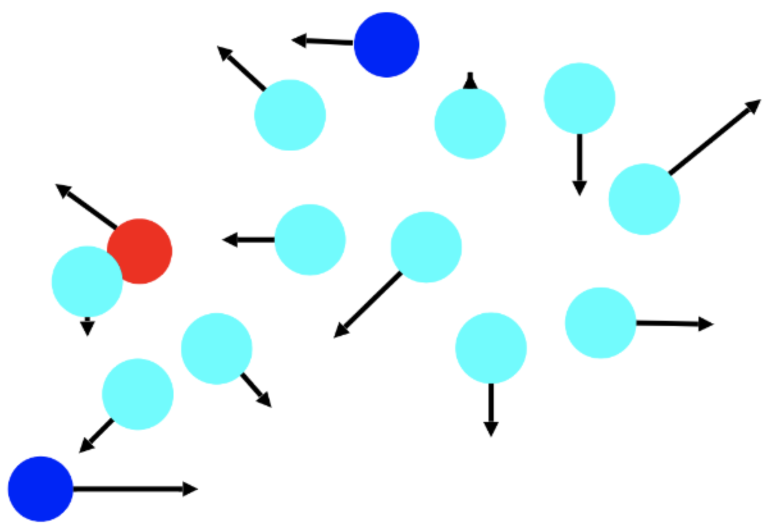
DE RECHERCHE
EN INFORMATIQUE
FONDAMENTALE

A concrete example: Molecular Dynamics





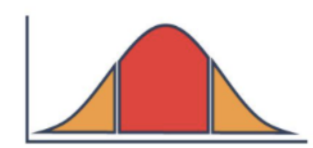
- Protein folding
- Drug design
- Nanotechnologies
- …



Simulate trajectories and interactions of molecules

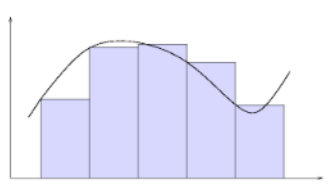
Monte Carlo

Statistical analysis

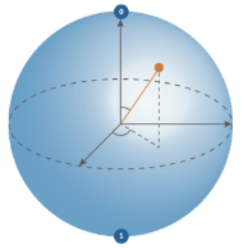


Random sampling

Approximation methods



Quantum computing



Bottleneck: performances (time, memory, …) scale **exponentially** with number of particles

→ Classical computers are not suited to simulate the laws of quantum mechanics (*language barrier*)

→ New algorithmic methods adapted to **quantum computers**

Estimating Statistics

- Y. Hamoudi and F. Magniez. “Quantum Chebyshev’s Inequality and Applications”, ICALP 2019.
- Y. Hamoudi. “Quantum Sub-Gaussian Mean Estimator”, ESA 2021.
- Y. Hamoudi and F. Magniez. “Quantum Approximate Triangle Counting”. In submission.

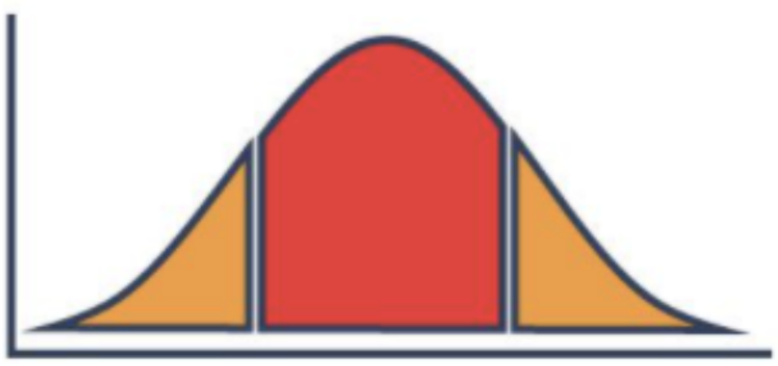
Random Sampling

- Y. Hamoudi, P. Rebentrost, A. Rosmanis, and M. Santha. “Quantum and Classical Algorithms for Approximate Submodular Function Minimization”, *Quantum Information & Computation*.
- P. Rebentrost, Y. Hamoudi, M. Ray, X. Wang, S. Yang, M. Santha. "Quantum algorithms for hedging and the learning of Ising models", *Physical Review A.*

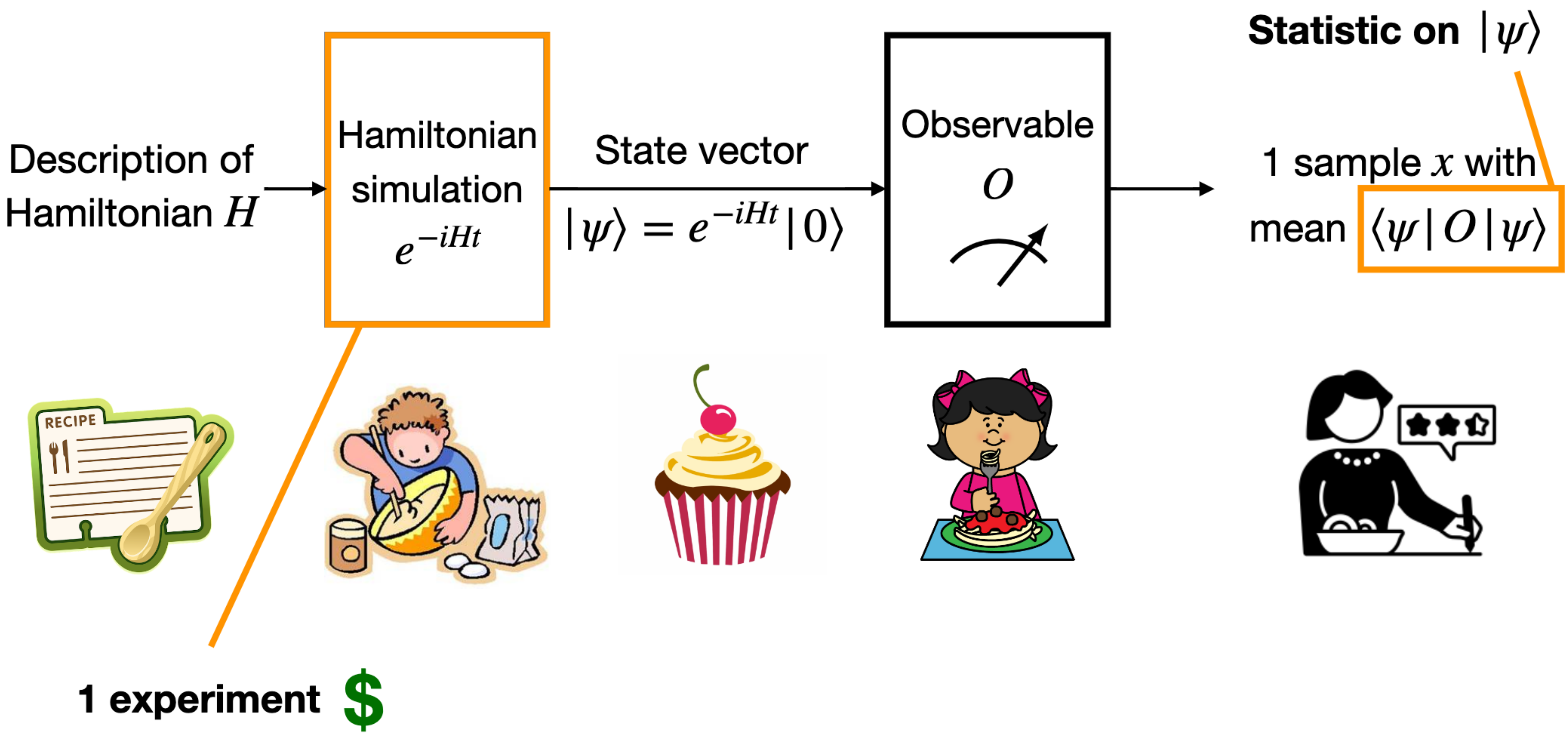
Small-Memory Algorithms

- Y. Hamoudi and F. Magniez. “Quantum Chebyshev’s Inequality and Applications”, ICALP 2019.
- Y. Hamoudi and F. Magniez. “Quantum Time-Space Tradeoff for Finding Multiple Collision Pairs”, TQC 2021.

Estimating Statistics



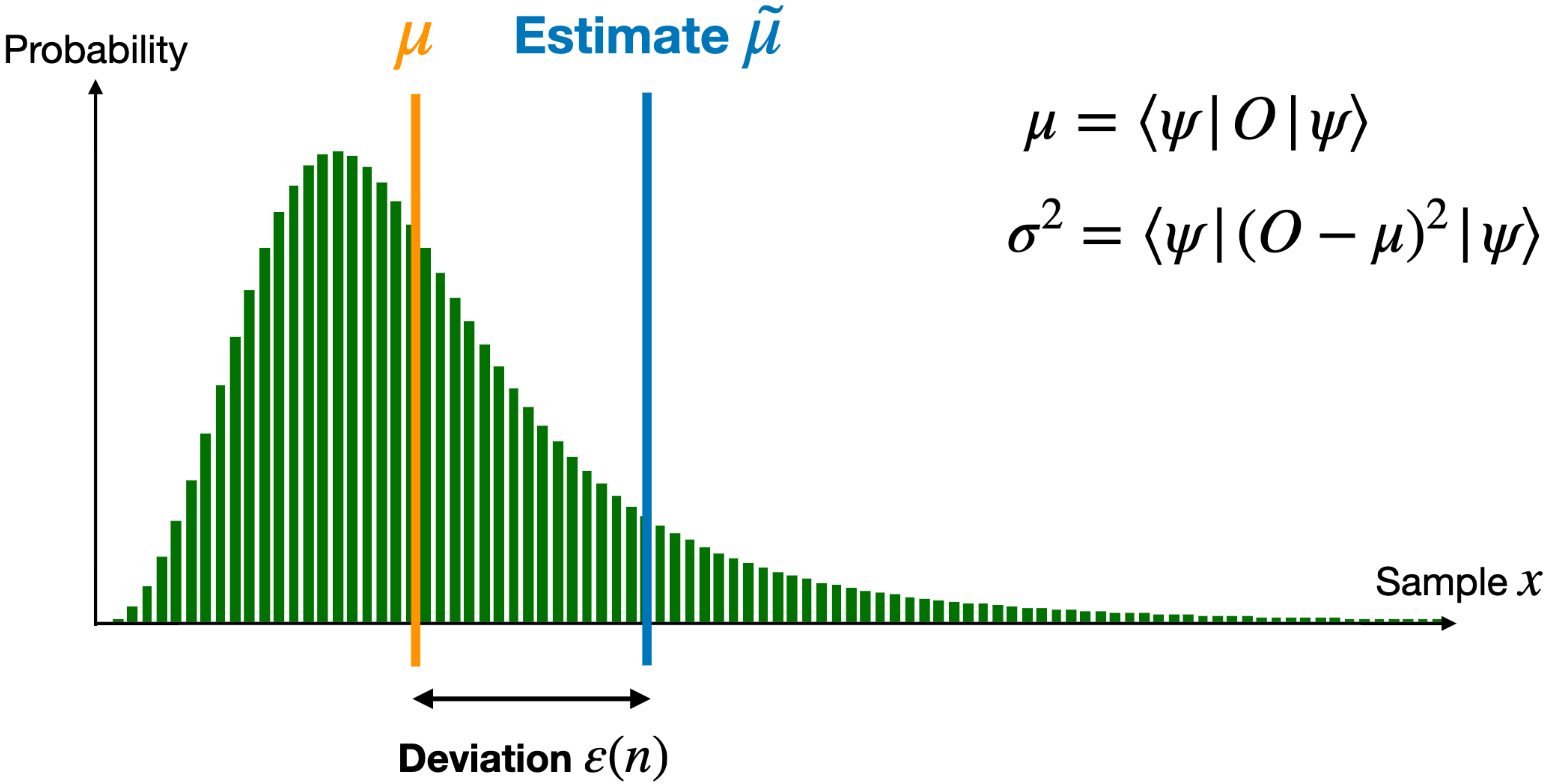
Quantum simulation & Expectation estimation



What is the best possible estimate $\tilde{\mu}$ of $\langle\psi|O|\psi\rangle$

that can be computed by running n experiments?

Output sample distribution

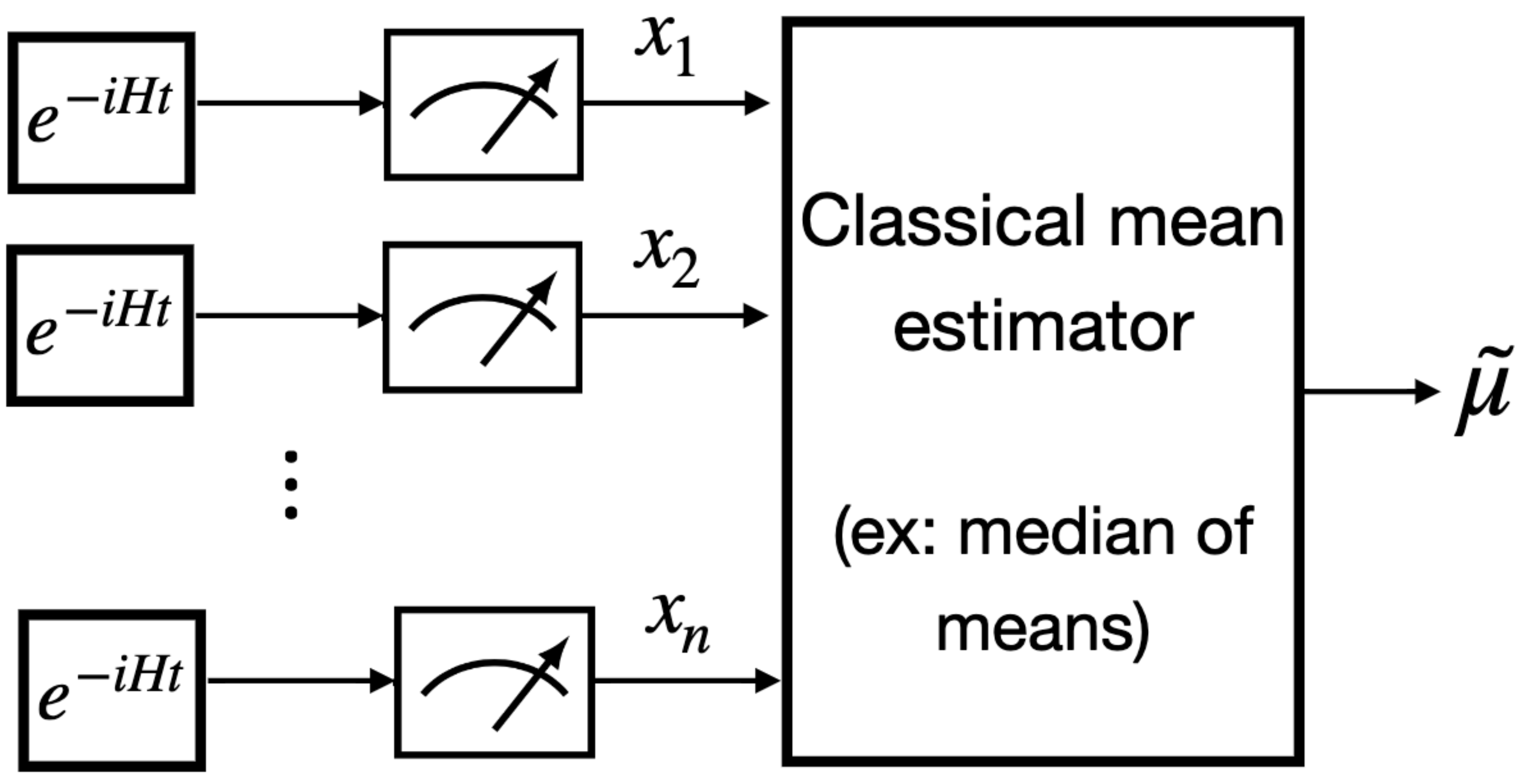


$$\mu = \langle \psi | O | \psi \rangle$$

$$\sigma^2 = \langle \psi | (O - \mu)^2 | \psi \rangle$$

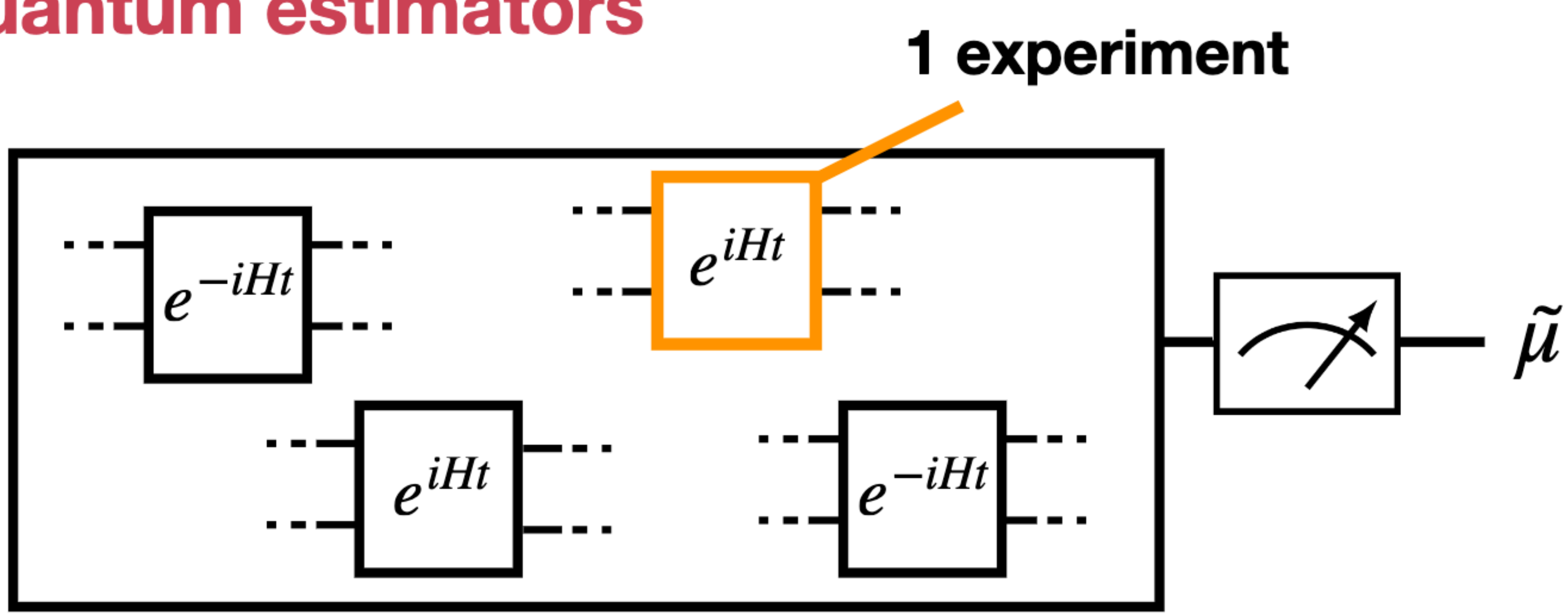
Objective: minimize the deviation $\varepsilon(n)$ for n experiments

Classical estimators



$$\varepsilon(n) \approx \frac{\sigma}{\sqrt{n}}$$

Quantum estimators



Previous work:

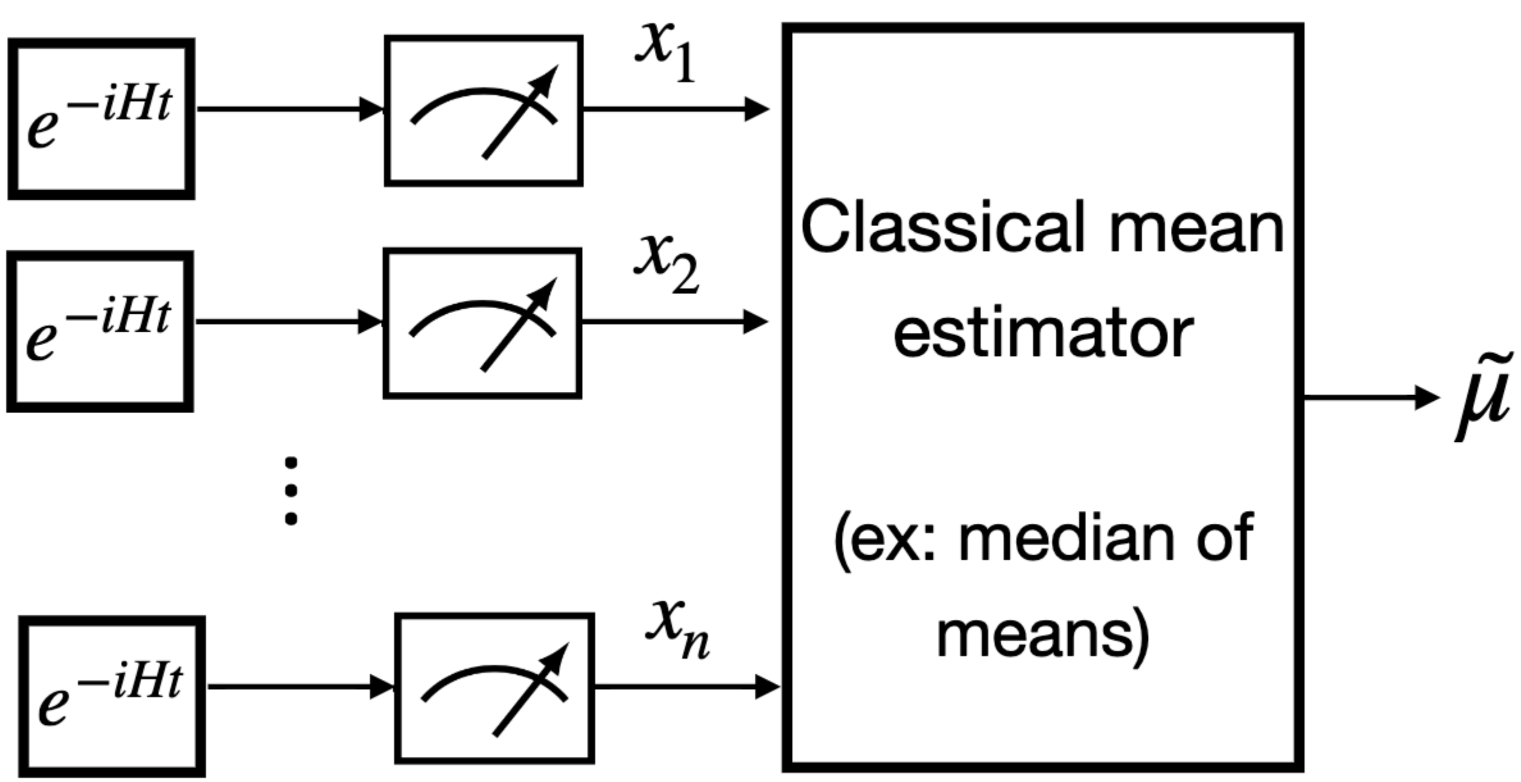
- Suboptimal in σ

  [Gro98,Ter99,AW99,BDGT11]

- Parametrized by σ

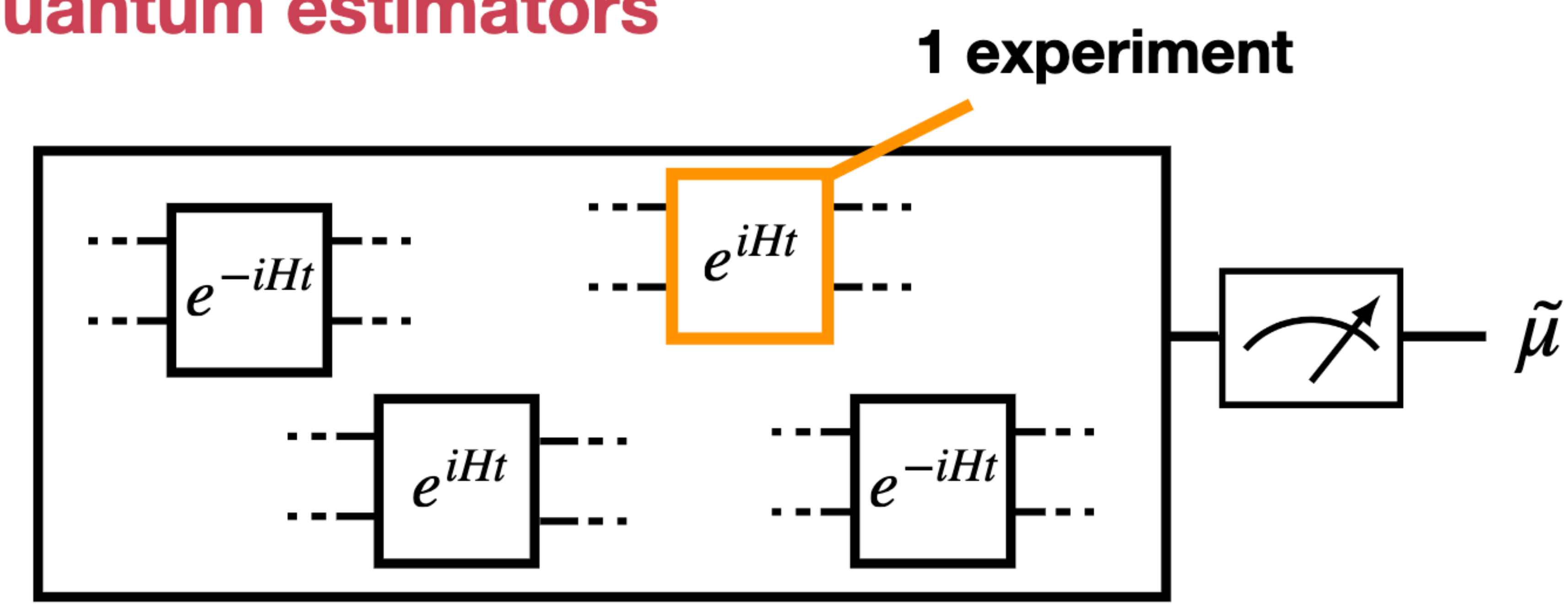
  [Hei02,Mon15,HM19]

Classical estimators



$$\varepsilon(n) \approx \frac{\sigma}{\sqrt{n}}$$

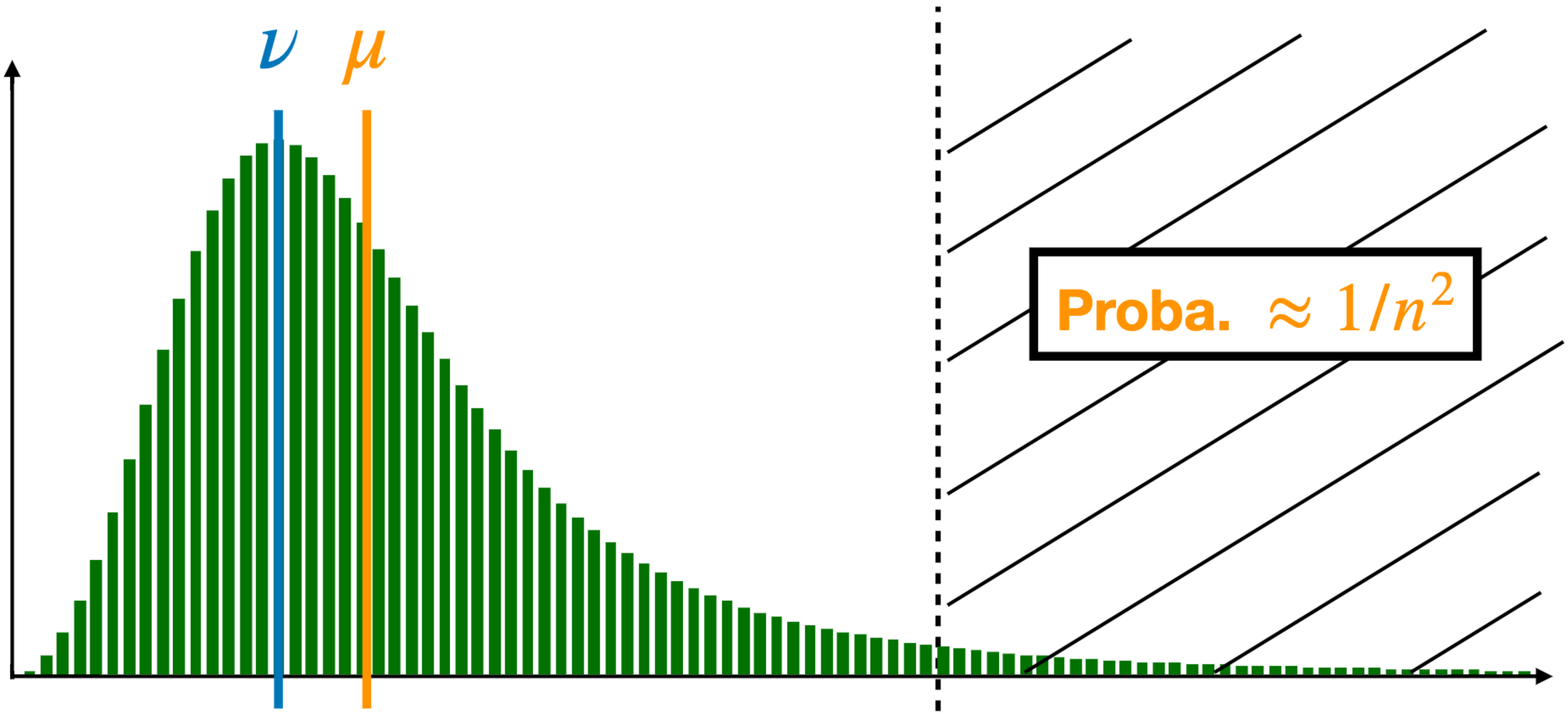
Quantum estimators



$$\varepsilon(n) \approx \frac{\sigma}{n}$$

Techniques

Truncated Mean Estimation:



Truncated mean

Estimated by $\log n$ instances of Phase Estimation

Truncation level

Estimated by Amplitude Amplification

Random Sampling

Goal: generate random samples given the **description** of a distribution p

$$x_1, x_2, \ldots \sim p$$

Distribution p

A quantum approach: Prepare-and-measure a quantum state encoding the target distribution

$$|p\rangle = \sum_x \sqrt{p_x}\,|x\rangle \qquad \textit{\textbf{(q-sample)}}$$

→ Time to prepare $|p\rangle$ with a quantum computer can be **smaller** than time to sample p with a classical computer.

→ Q-samples are important for quantum linear algebra, quantum walks, …

Black-box state preparation

$x \in \{1,\ldots,N\}$

p_x

Each probability can be generated quickly

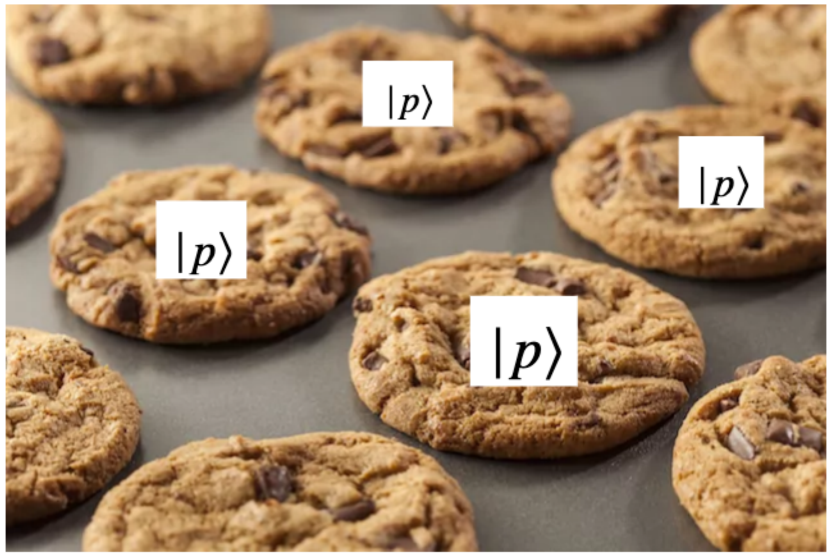
(oracle $x \mapsto p_x$)

How much **time** do we need to prepare $|p\rangle$?

Cost for 1 copy

[Gro00]

$$\Theta(\sqrt{N})$$



Cost for K copies

$$O(K\sqrt{N})\ ?$$

$$\Theta(\sqrt{KN})$$

Techniques

Quantum Rejection Sampling method:

$$|q\rangle \xrightarrow[\text{[Gro00, ORR13, …]}]{\text{Amplitude Amplification}} |p\rangle$$

Easy to prepare

(ex: uniform distribution)

Objective state

Select $|q\rangle$ with larger $|\langle q|p\rangle|$

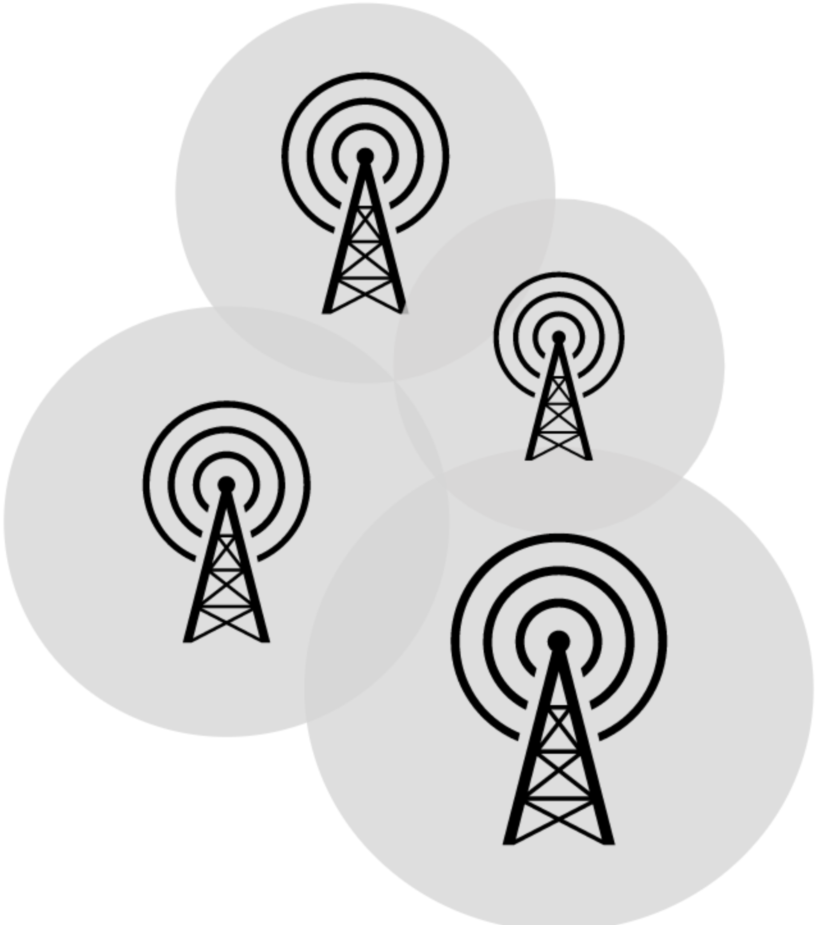
Precompute the K largest entries in p

Energy stocks

Day 1	10%	45%	25%	20%
Day 2	5%	35%	30%	30%
Day 3	?	?	?	?

Online prediction with expert advice

Radio tower placement

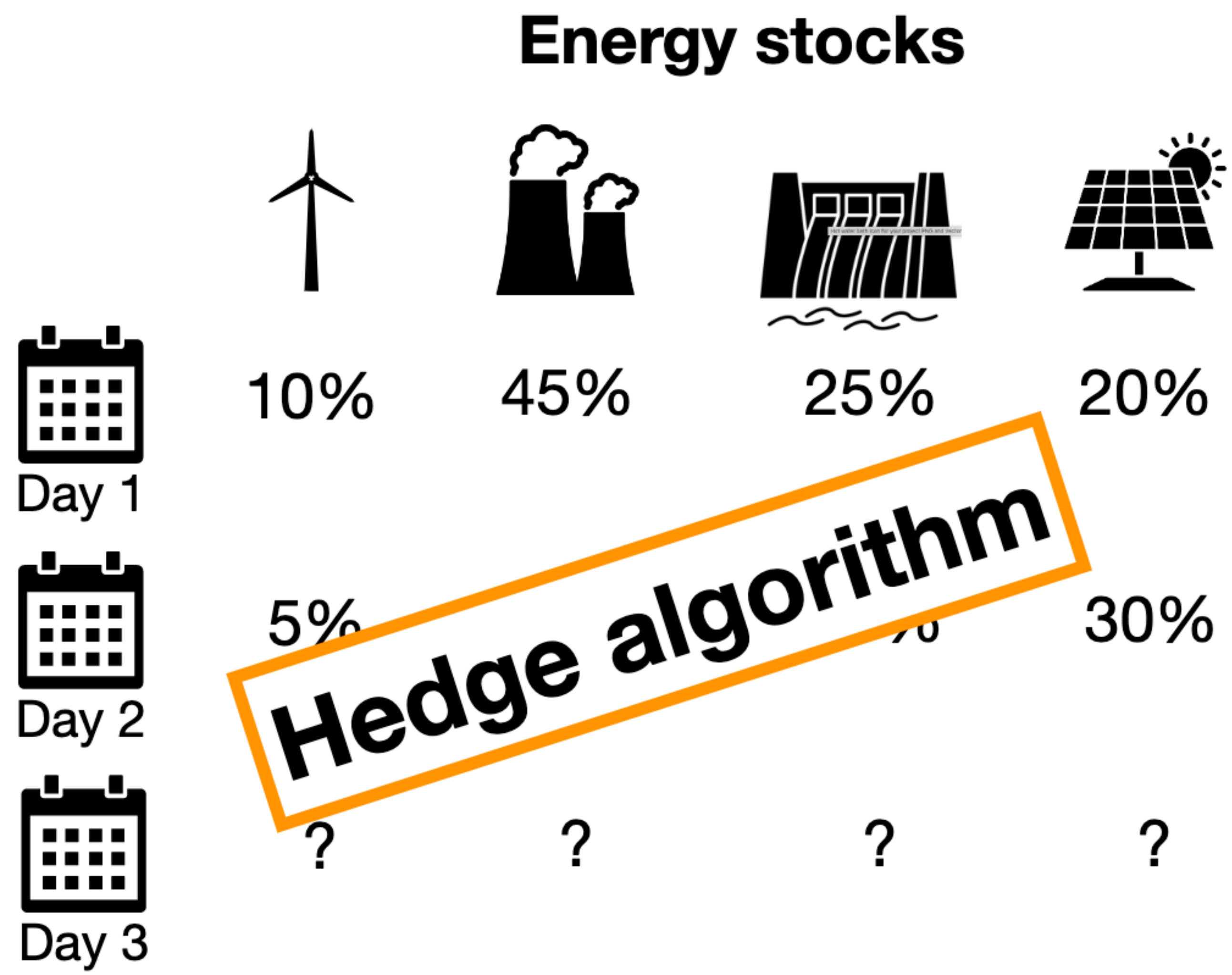


Submodular function minimization

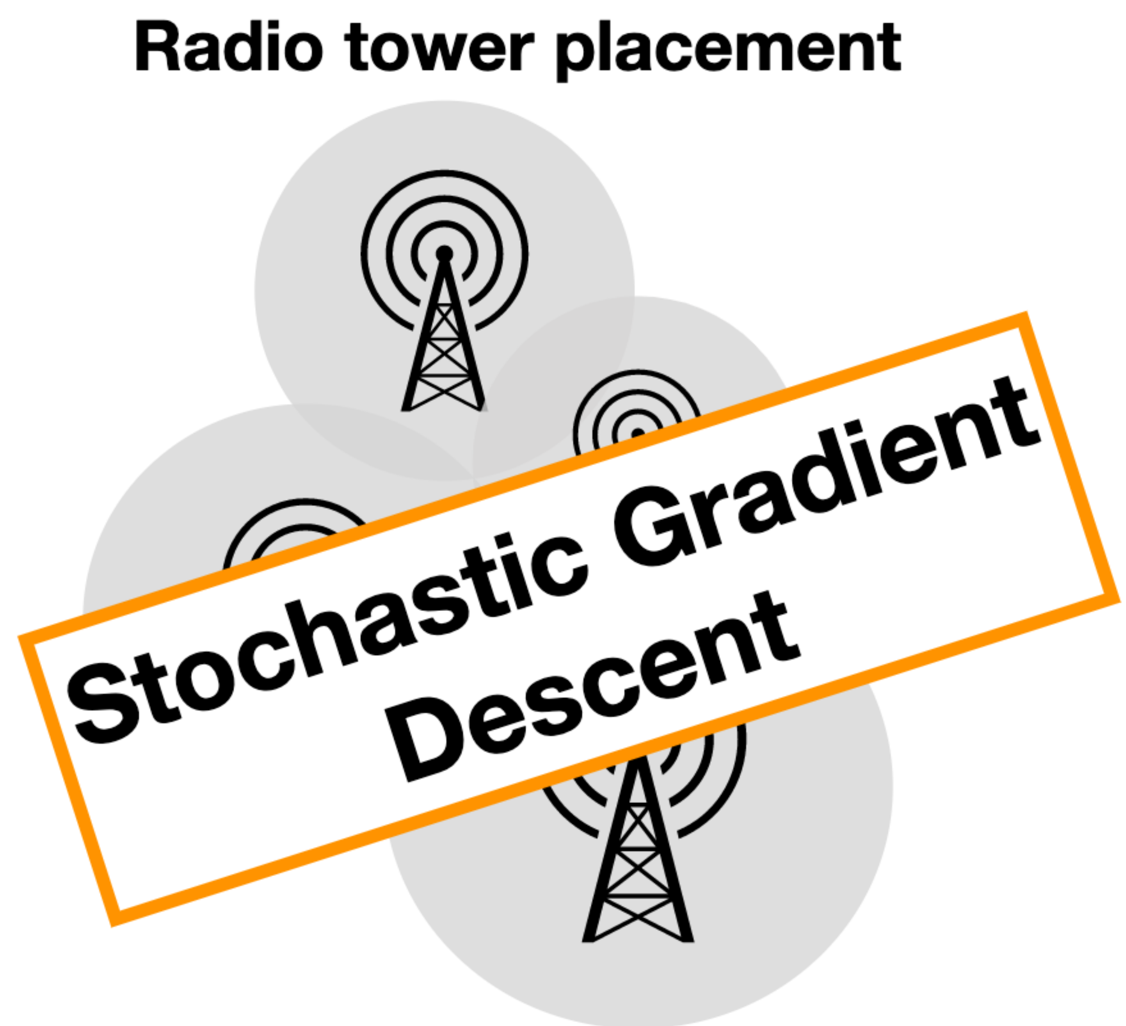
Iterative updates: $x^{(1)} \longrightarrow x^{(2)} \longrightarrow \ldots \longrightarrow x^{(t)}$

Random update by **sampling** from a distribution $p^{(t)}$

Quantum speedup



Online prediction with expert advice



Submodular function minimization

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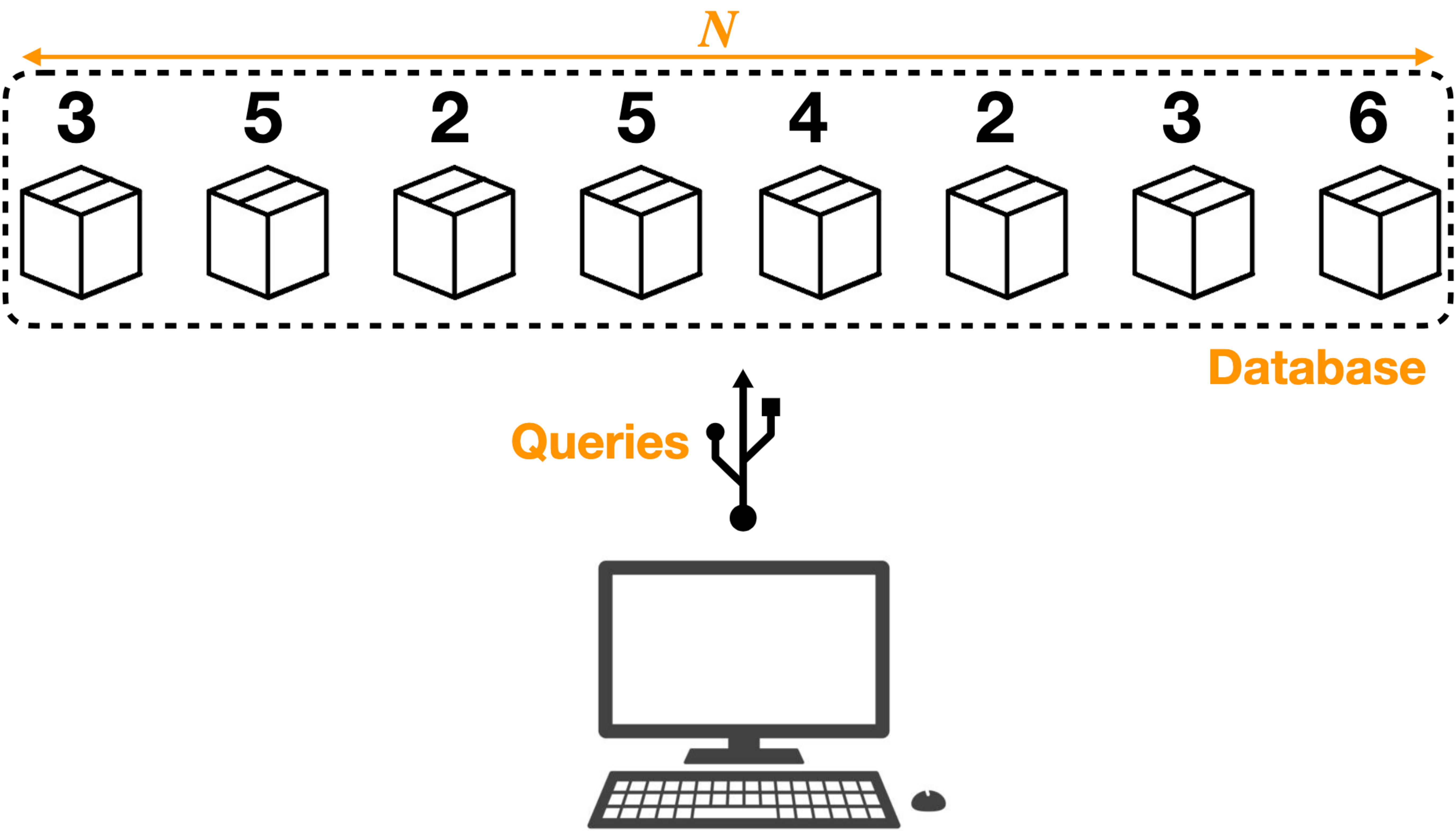
Random update by **sampling** from a distribution $p^{(t)}$

Quantum speedup

Small-Memory Algorithms

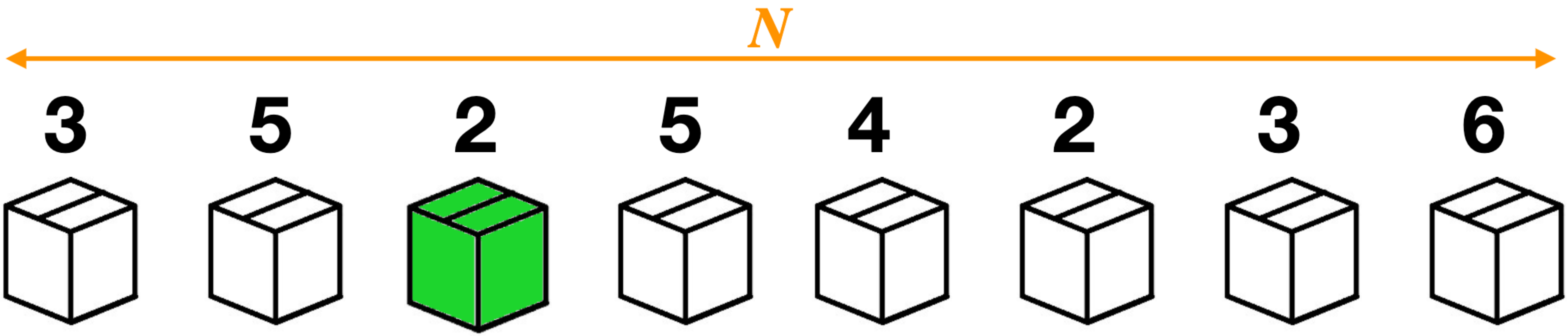
Memory: most critical computational resource?

- Size of datasets keeps increasing (network traffic, particle physics experiments,…)
- Processor-memory bottleneck: bandwidth/latency improve at a slower rate than processor speed
- Near-term quantum computers will have small and error-prone memories



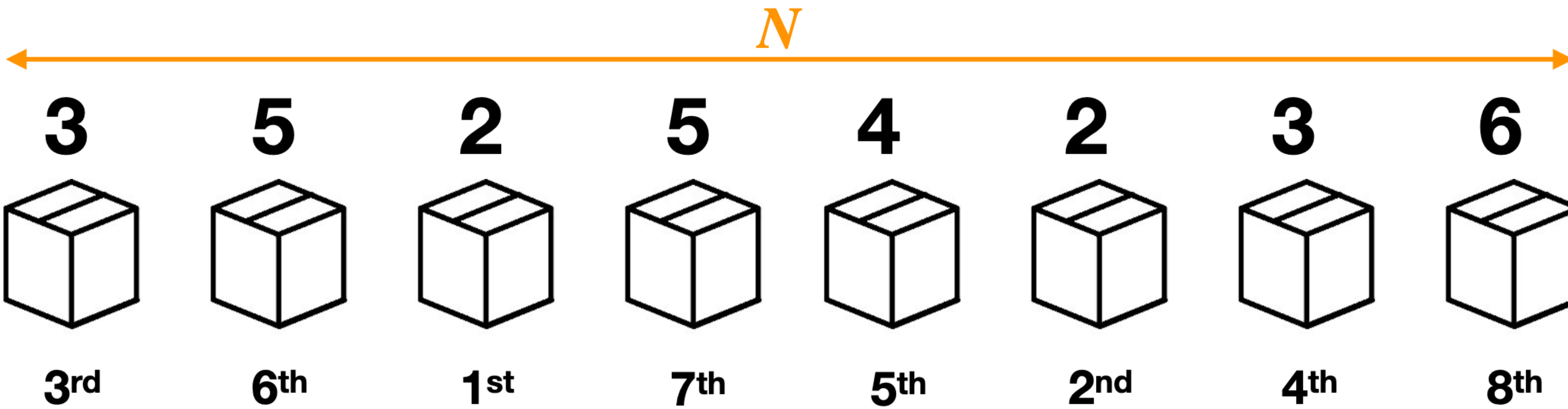
Small computer

with memory of size $\Theta(\log N)$



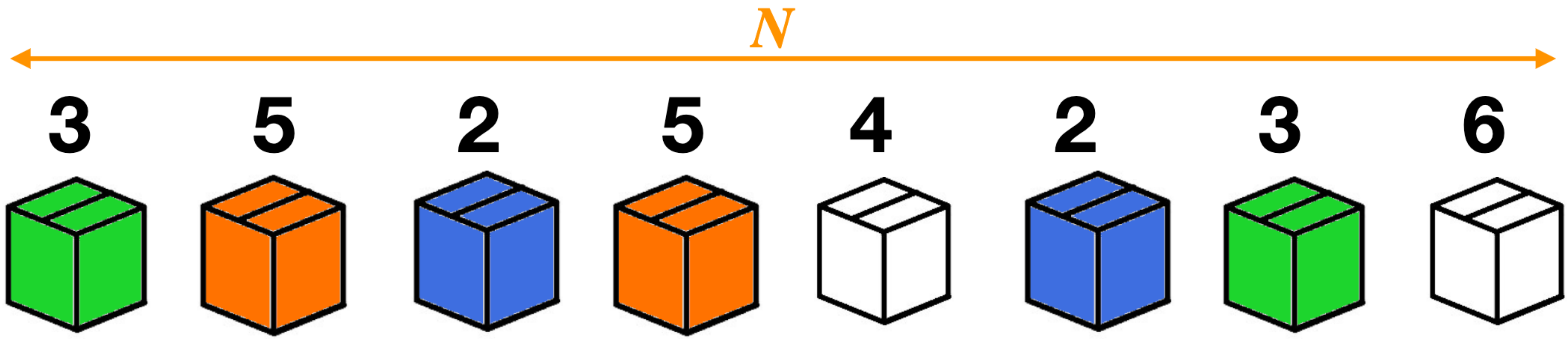
How many **queries** when the memory is limited to $\Theta(\log N)$ (qu)bits?

	Classical	**Quantum**
Minimum Finding	$\Theta(N)$	$\Theta(\sqrt{N})$
		[DH96,BBBV97]



How many **queries** when the memory is limited to $\Theta(\log N)$ (qu)bits?

	Classical	**Quantum**
Minimum Finding	$\Theta(N)$	$\Theta(\sqrt{N})$
Sorting	$\tilde{\Theta}(N^2)$	$\tilde{\Theta}(N^{3/2})$
	[BC82]	[KŠdW07]



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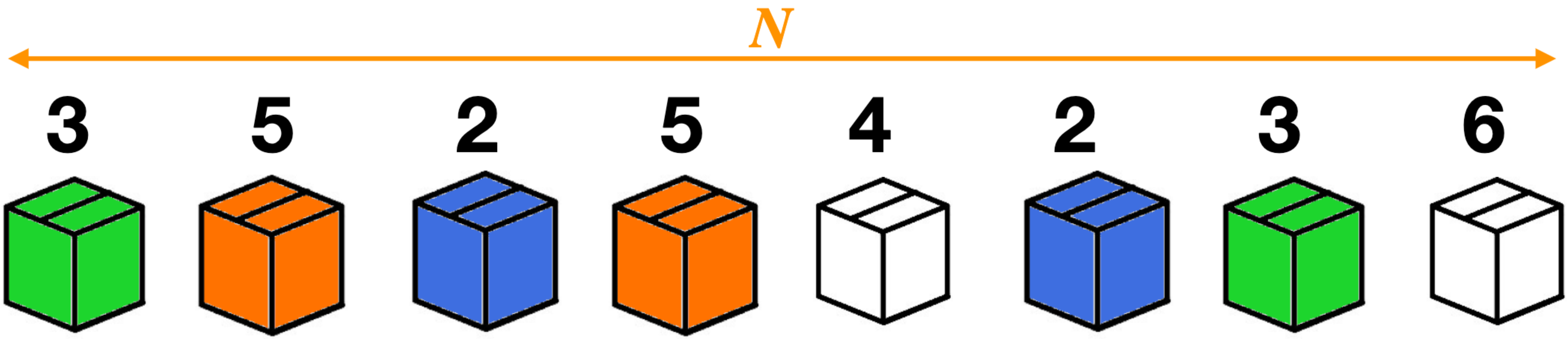
	Classical	**Quantum**
Minimum Finding	$\Theta(N)$	$\Theta(\sqrt{N})$
Sorting	$\tilde{\Theta}(N^2)$	$\tilde{\Theta}(N^{3/2})$
Collision Pairs Finding (random $f : [N] \to [N]$)	$\tilde{\Theta}(N^{3/2})$ [vOW99,Din20]	**?**



How many **queries** when the memory is limited to $\Theta(\log N)$ (qu)bits?

	Classical	**Quantum**
Minimum Finding	$\Theta(N)$	$\Theta(\sqrt{N})$
Sorting	$\tilde{\Theta}(N^2)$	$\tilde{\Theta}(N^{3/2})$ Simpler proof
Collision Pairs Finding (random $f : [N] \to [N]$)	$\tilde{\Theta}(N^{3/2})$	$\tilde{\Omega}(N^{4/3})$

Techniques

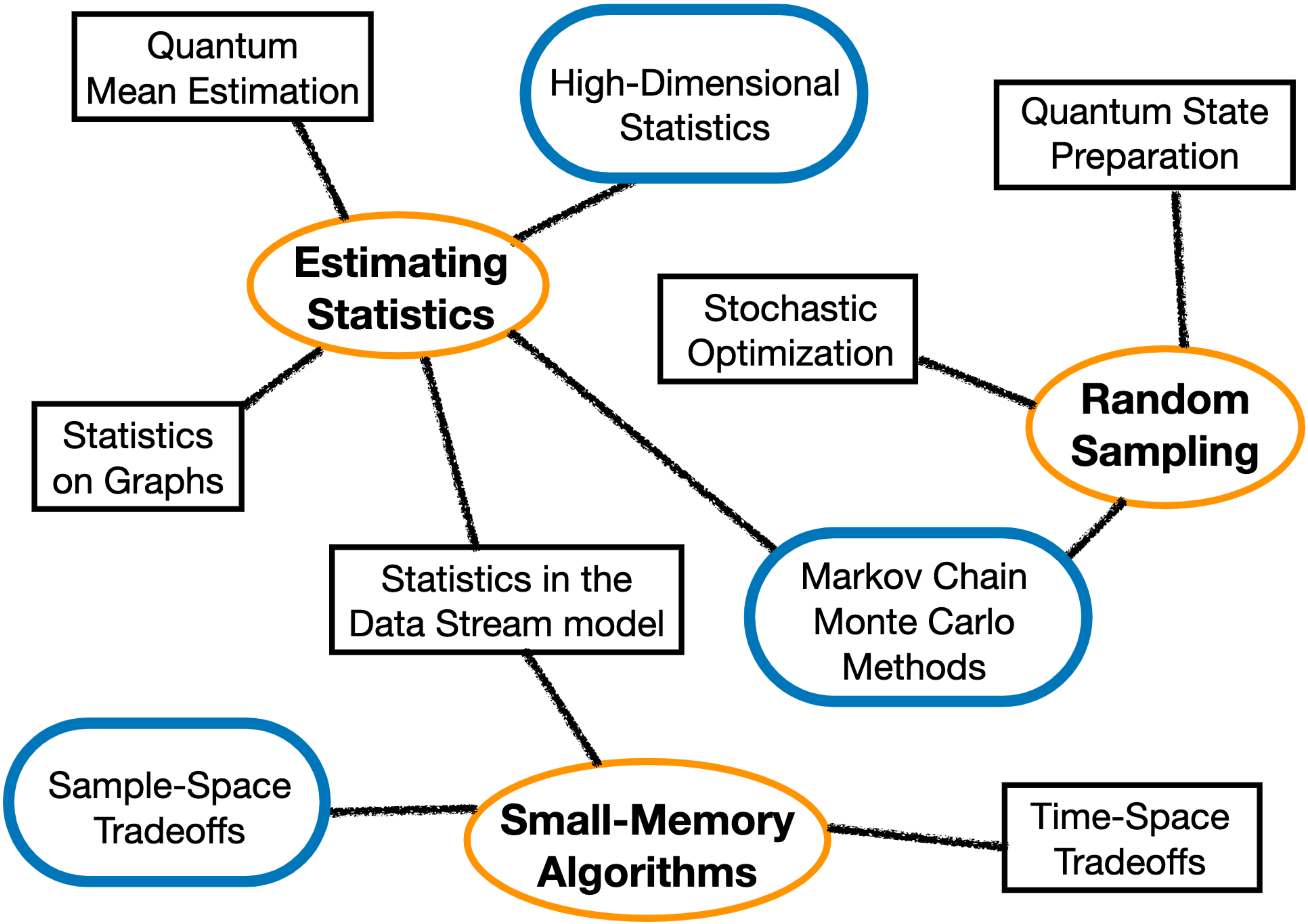
Small success probability regime:

Any algorithm that finds $\approx \log(N)$ collisions with success probability $\geq 1/N$ must use $\tilde{\Omega}\left(N^{1/3}\right)$ quantum queries.

Even if the memory is unlimited

Lower bound method based on a simpler and generalized version of the **recording query technique** of [Zhandry'19].

Conclusion


Quantum
Mean Estimation
High-Dimensional
Statistics
Quantum State
Preparation
Estimating
Statistics
Stochastic
Optimization
Random
Sampling
Statistics
on Graphs
Statistics in the
Data Stream model
Markov Chain
Monte Carlo
Methods
Sample-Space
Tradeoffs
Small-Memory
Algorithms
Time-Space
Tradeoffs