Quantum speedup of Monte Carlo methods

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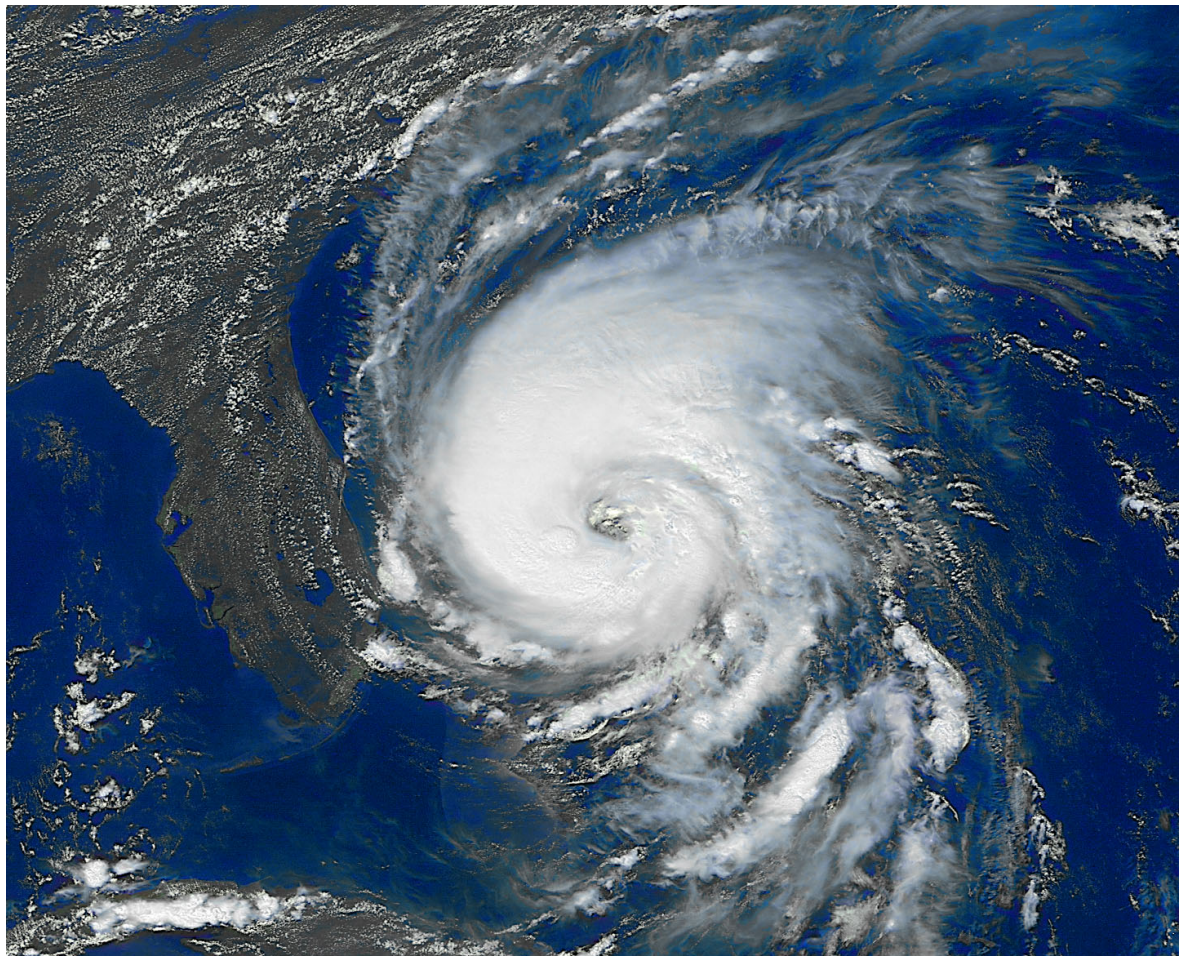
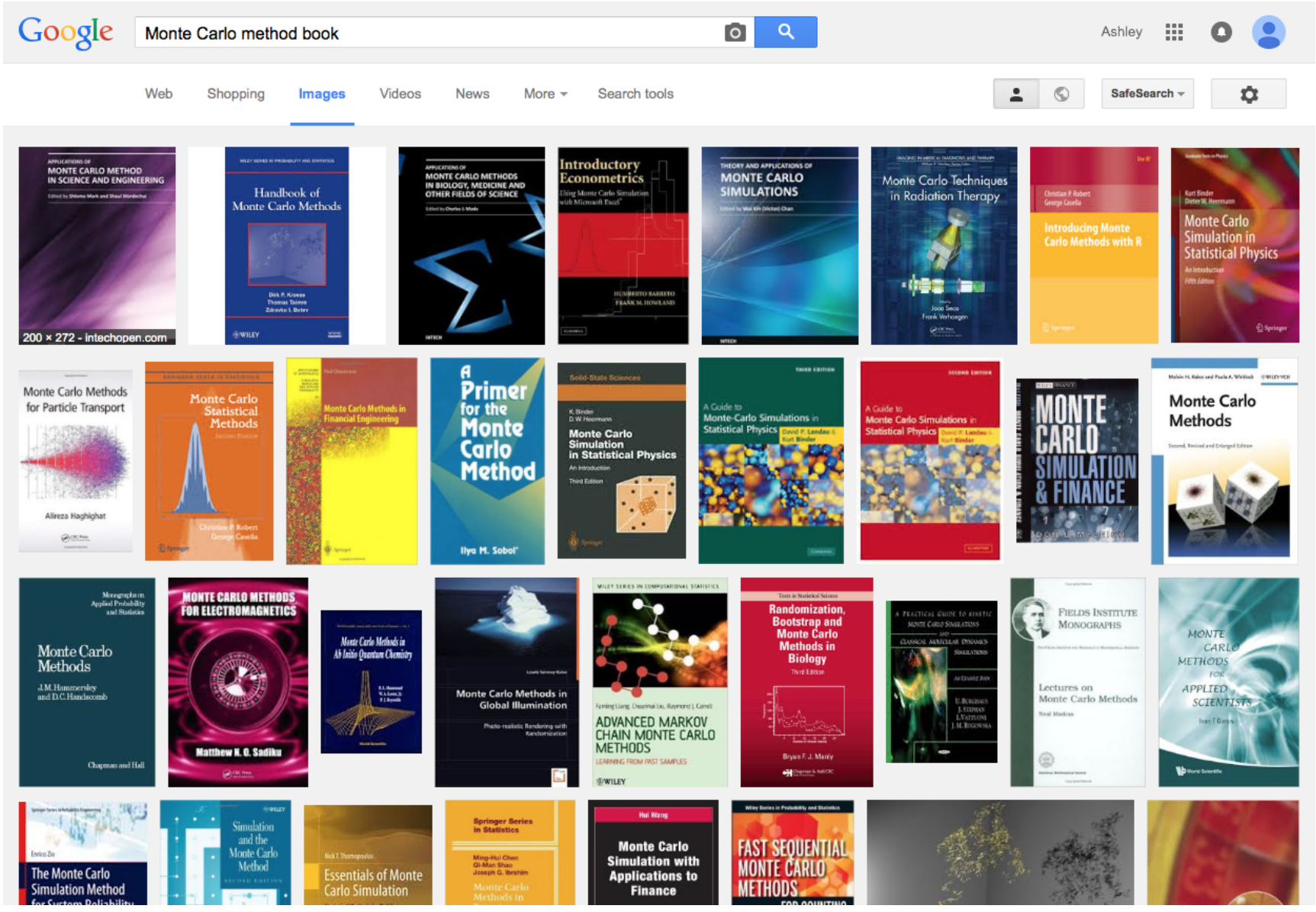
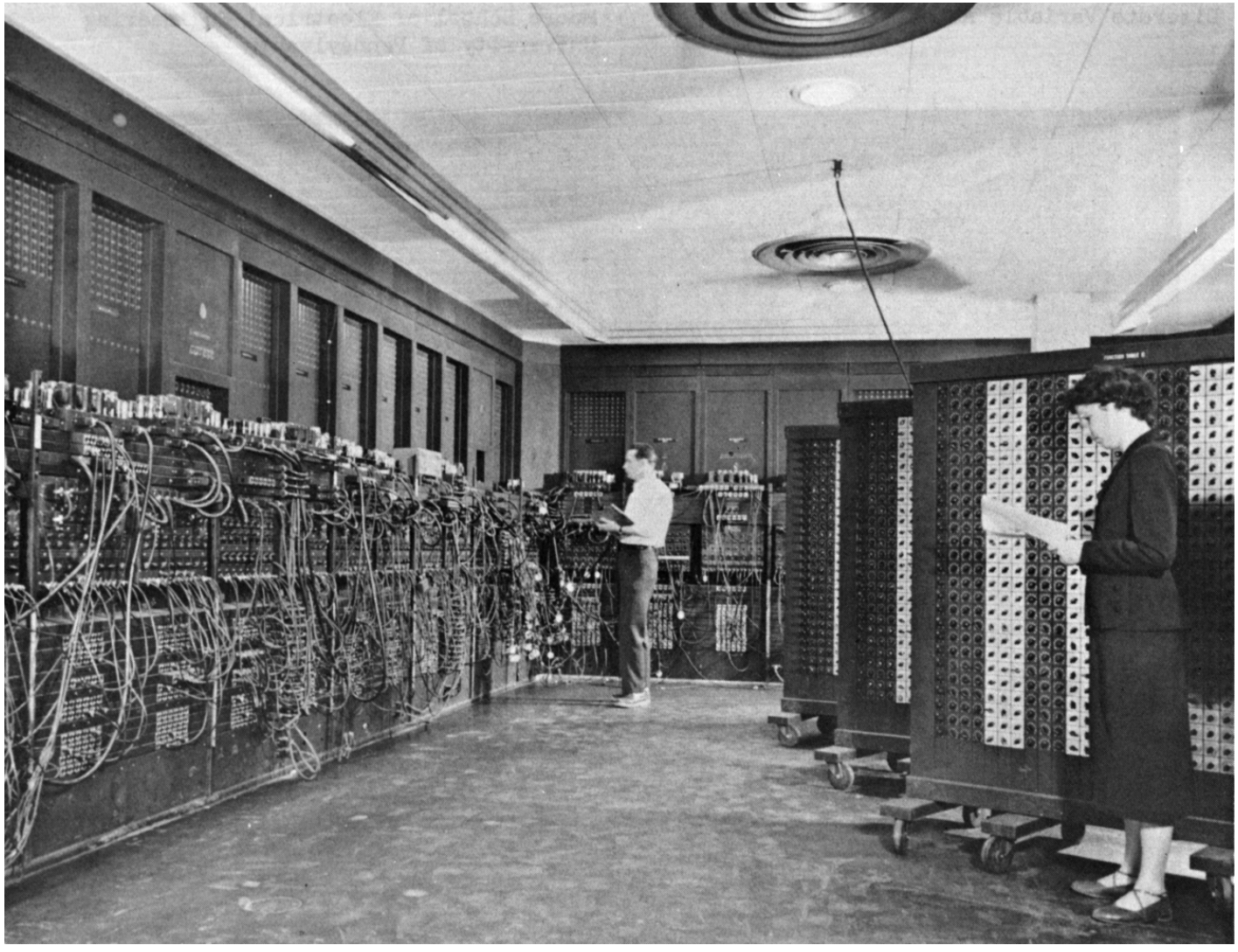


Pic: Wikipedia

These methods are used throughout science and engineering:



. . . and were an application of the first electronic computers:



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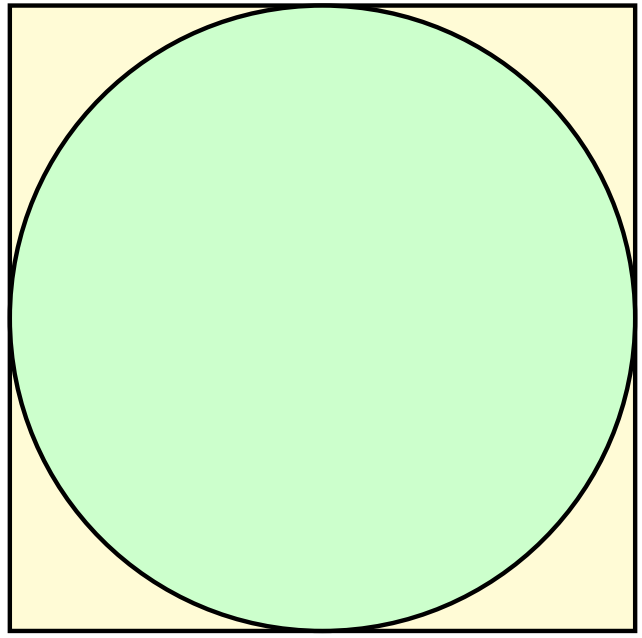
Monte Carlo methods

One very simple example of a Monte Carlo method: approximate π by throwing darts at a dartboard (choosing random points within a square).



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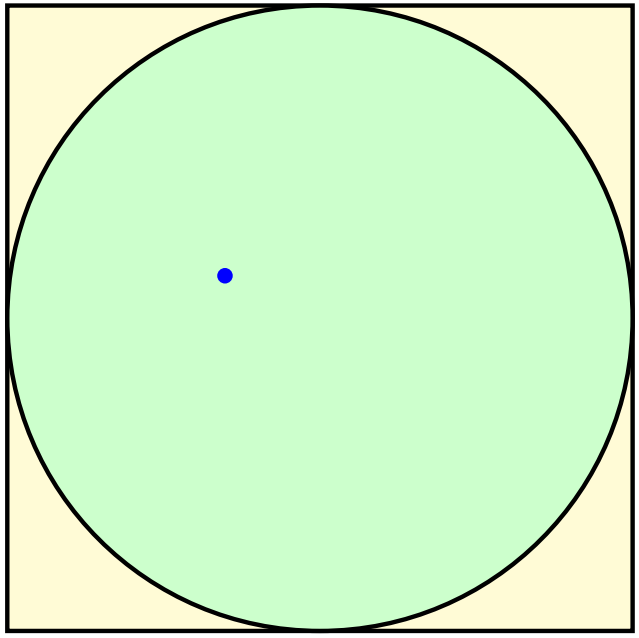
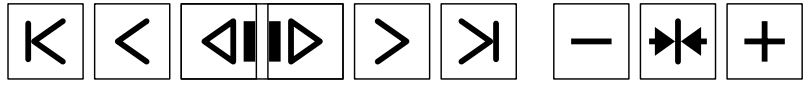
A randomised algorithm for approximating π



Points landed in circle: 1/1.

Approximation to π: 4.0.



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This talk

Today I will discuss a quantum algorithm to speed up Monte Carlo methods in a quite general setting.

And also some applications of the algorithm:

1. Partition function problems in statistical physics
2. Approximate counting problems in combinatorics
3. Approximating the distance between probability distributions

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General problem

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- The output value $v(\mathcal{A})$ is a real-valued random variable.

We assume that we know an upper bound on the variance of this random variable:

$$\mathsf{Var}(v(\mathcal{A})) \leqslant \sigma^2.$$

Classical algorithm

The following natural algorithm solves this problem for any $\mathcal{A}$:

1. Produce k samples $v_1, \ldots, v_k$, each corresponding to the output of an independent execution of $\mathcal{A}$.
2. Output the average $\widetilde{\mu} = \frac{1}{k} \sum_{i=1}^{k} v_i$ of the samples as an approximation of μ.

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- To estimate π up to 4 decimal places with success probability 0.5, we would need $> 10^9$ trials!

Quantum speedup

With a quantum computer, we can do better:

Theorem [AM '15]

There is a quantum algorithm which estimates μ up to additive error ϵ with 99% success probability and

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The underlying algorithm $\mathcal{A}$ can now be quantum itself.

Related work

This problem connects to several previous works, e.g.:

- Approximating the mean of an arbitrary bounded function (with range $[0, 1]$), with respect to the uniform distribution. Quantum complexity: $O(1/\epsilon)$ [Heinrich '01], [Brassard et al. '11].

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Here we generalise these by approximating the mean output value of arbitrary quantum algorithms, given only a bound on the variance.

Ideas behind the algorithm

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- Now the probability of measuring 1 on the last qubit is precisely μ.
- We can use amplitude estimation to approximate μ up to additive error ϵ, using $\mathcal{A}$ (and $\mathcal{A}^{-1}$) $O(1/\epsilon)$ times.

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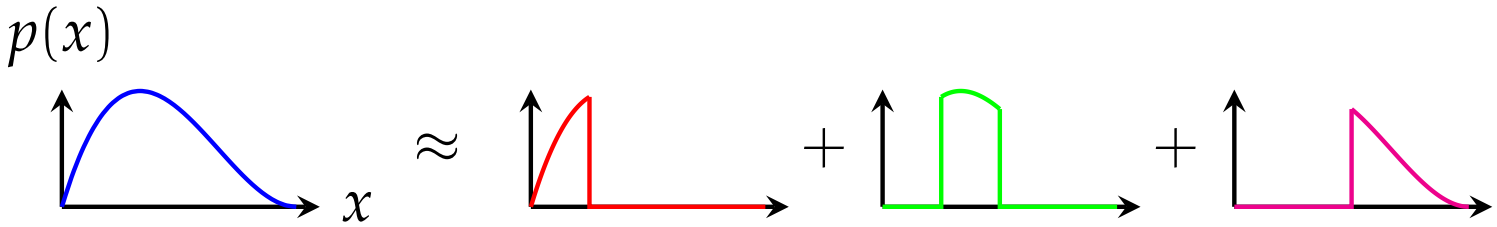
In this case (using ideas of [Heinrich '01]):

- Divide up the output values of $\mathcal{A}$ into blocks, such that in the t'th block $2^{t-1} \leqslant v(\mathcal{A}) \leqslant 2^t$.
- Use $\widetilde{O}(1/\epsilon)$ iterations of the previous algorithm to estimate the average output values in each of the first $O(\log 1/\epsilon)$ blocks, each divided by 2^t.
- Sum up the results (after rescaling them again).



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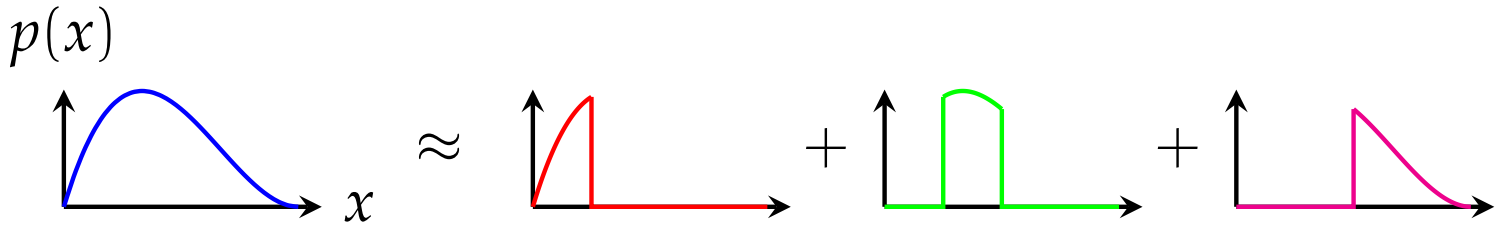

The constraint that $\mathbb{E}[v(\mathcal{A})^2] = O(1)$ implies that the overall error is at most ϵ.

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The final step is to change the dependence on $\mathbb{E}[v(\mathcal{A})^2]$ to a dependence on

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A similar idea works to estimate μ up to relative error ϵ: if $\sigma^2/\mu^2 \leqslant B$, we can estimate μ up to additive error $\epsilon\,\mathbb{E}[v(\mathcal{A})]$ with $\widetilde{O}(B/\epsilon)$ uses of $\mathcal{A}$.

Application: partition functions

Consider a (classical) physical system which has state space Ω, and a Hamiltonian $H : \Omega \to \mathbb{R}$ specifying the energy of each configuration $x \in \Omega$. Assume that H takes integer values in the set $\{0, \ldots, n\}$.

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Encapsulates some interesting problems:

- Physics: The Ising and Potts models
- Computer science: counting k-colourings of graphs, counting matchings (monomer-dimer coverings), ...

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- $A := |\Omega|$ can be exponentially large and $Z(\beta)$ can be hard to compute; e.g. #P-hard. So we resort to randomised methods for approximating $Z(\beta)$.

- We want to approximate $Z(\beta)$ up to relative error ϵ, i.e. output $\widetilde{Z}$ such that

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- One approach: multi-stage Markov chain Monte Carlo (e.g. [Valleau and Card '72, Stefankovič et al. '09]).

Multiple-stage Markov chain Monte Carlo

The basic framework of these methods:

- Let a cooling schedule be a sequence of inverse temperatures $0 = \beta_0 < \beta_1 < \cdots < \beta_\ell = \beta$.
- Express $Z(\beta_\ell)$ as the telescoping product

$$Z(\beta_\ell) = Z(\beta_0) \frac{Z(\beta_1)}{Z(\beta_0)} \frac{Z(\beta_2)}{Z(\beta_1)} \cdots \frac{Z(\beta_\ell)}{Z(\beta_{\ell-1})}.$$

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- Define random variables Y_i where $\mathbb{E}[Y_i] = Z(\beta_{i+1})/Z(\beta_i)$, with respect to the distribution π_i defined by

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  the Gibbs distribution at inverse temperature β_i.
- Estimate $\mathbb{E}[Y_i]$ by sampling from this distribution.

Sampling and estimating

This idea will be efficient if we can satisfy two constraints:

1. The (relative) variance of each random variable Y_i is low: $\mathbb{E}[Y_i^2]/\mathbb{E}[Y_i]^2 = O(1)$ for all i.

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Theorem **[Stefankovič et al. '09]**

For any partition function problem, there exists a cooling schedule satisfying the first constraint with $\ell = \widetilde{O}(\sqrt{\log A})$.

Such a cooling schedule is known as a Chebyshev cooling schedule.

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- In the quantum setting, we can apply our algorithm to accelerate the approximation of $\mathbb{E}[Y_i]$ (scaling goes from $O(1/\epsilon^2)$ to $\widetilde{O}(1/\epsilon)$)...
- ...and we can also replace the classical Markov chains with quantum walks to improve the dependence on τ.

Rapid mixing via quantum walks

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Note 2: The $\widetilde{O}((\log A)\tau)$ part of the bound is the complexity of computing the Chebyshev cooling schedule itself.

Example: The ferromagnetic Ising model

We are given as input a graph $G = (V, E)$ with n vertices. We consider the Ising Hamiltonian

$$H(z) = -\sum_{(u,v)\in E} z_u z_v.$$

for $z \in \{\pm 1\}^n$. We want to approximate

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Then we have the following speedup:

- Best classical runtime known [Stefankovič et al. '09]: $\widetilde{O}(n^2/\epsilon^2)$
- Quantum runtime: $\widetilde{O}(n^{3/2}/\epsilon + n^2)$

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- Best classical runtime known: $\widetilde{O}(n^2/\epsilon^2)$
- Quantum runtime: $\widetilde{O}(n^{3/2}/\epsilon + n^2)$

Counting matchings (monomer-dimer coverings) of a graph with n vertices and m edges:

- Best classical runtime known: $\widetilde{O}(n^2 m/\epsilon^2)$
- Quantum runtime: $\widetilde{O}(n^{3/2} m^{1/2}/\epsilon + n^2 m)$

Application: the total variation distance

- Imagine we can sample from probability distributions p and q on n elements.
- We would like to estimate the total variation distance

$$\|p - q\| = \frac{1}{2} \sum_x |p(x) - q(x)|$$

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- Using quantum mean estimation we improve this to $\widetilde{O}(\sqrt{n}/\epsilon^{3/2})$.

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- We can write $\|p - q\| = \mathbb{E}_x[R(x)]$, where

$$R(x) = \frac{|p(x) - q(x)|}{p(x) + q(x)},$$

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- Wrapping this within $O(1/\epsilon)$ iterations of the mean-estimation algorithm, we obtain an overall algorithm running in time $\widetilde{O}(\sqrt{n}/\epsilon^{3/2})$.

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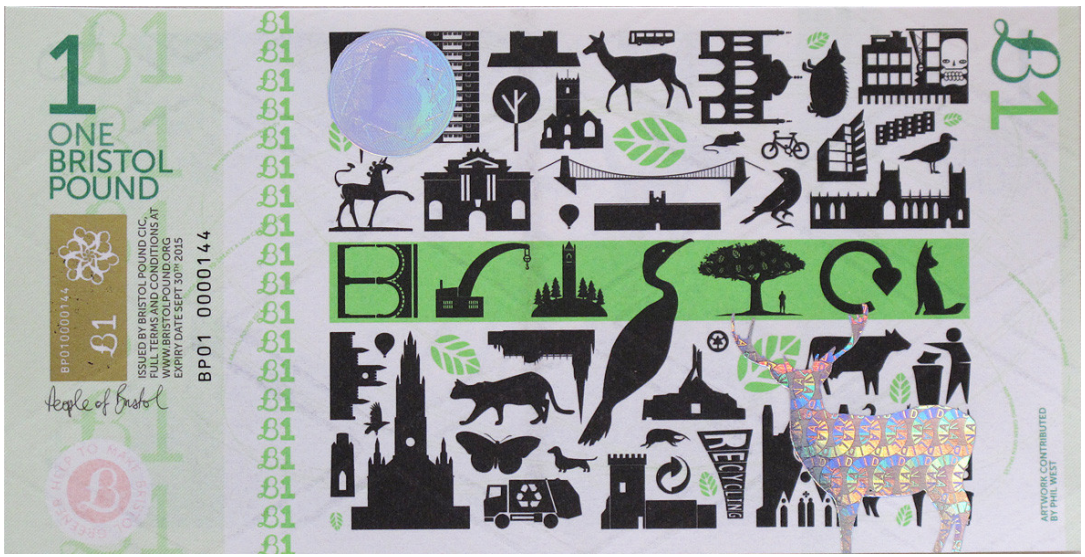

Thanks!