

CENTRE FOR QUANTUM TECHNOLOGY, SINGAPORE

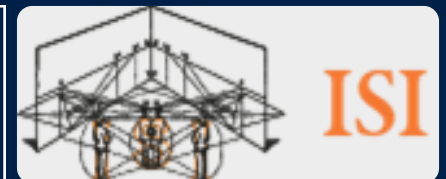
CLARENDON LABORATORY AND KEBLE COLLEGE, UNIVERSITY OF OXFORD

INSTITUTE FOR SCIENTIFIC INTERCHANGE, TURIN

Tensor networks vs. Monte Carlo for stochastic processes

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19th November 2014, UCL



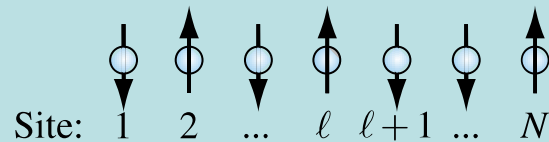
Overview

1. The system – classical stochastic and pure quantum dynamics
2. Our method – Tensor networks
3. Main rival – Dynamical Monte Carlo
4. Comparison for high variance observables

Representing the state of a system

Introducing the basics

Quantum (pure states)



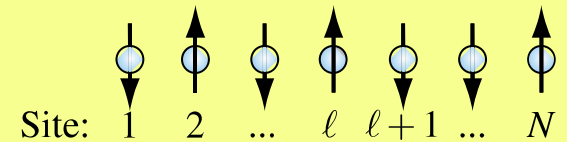
z_ℓ, d values
 $z_\ell = \pm 1, d = 2$

$\mathbf{z} = (z_1, \dots, z_N)$
 $D = d^N$

$$|\psi\rangle = \sum_{\mathbf{z}} \psi(\mathbf{z}) |\mathbf{z}\rangle$$

$$|\psi(\mathbf{z})|^2$$

Stochastic (probabilistic mixtures)



z_ℓ, d values
 $z_\ell = \pm 1, d = 2$

$\mathbf{z} = (z_1, \dots, z_N)$
 $D = d^N$

$$|P\rangle = \sum_{\mathbf{z}} P(\mathbf{z}) |\mathbf{z}\rangle$$

$$P(\mathbf{z})$$

Local configs
 (e.g. spin $\frac{1}{2}$)

Global configs

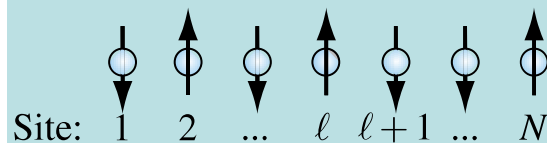
State vector

Probabilities

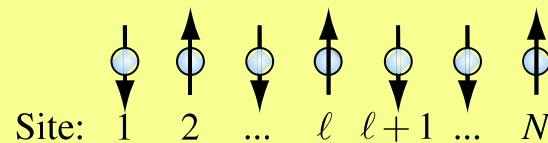
Evolving the state of a system

*Introducing
the basics*

Unitary evolution



Markovian stochastic process



Master equation

$$\frac{\partial P(\mathbf{z}, t)}{\partial t} = \sum_{\mathbf{z}' \neq \mathbf{z}} (P(\mathbf{z}', t) H(\mathbf{z}', \mathbf{z}) - P(\mathbf{z}, t) H(\mathbf{z}, \mathbf{z}'))$$

Rearrangement

$$\langle \mathbf{z} | H | \mathbf{z}' \rangle = H(\mathbf{z}', \mathbf{z}) \text{ for } \mathbf{z}' \neq \mathbf{z},$$

$$\langle \mathbf{z} | H | \mathbf{z} \rangle = - \sum_{\mathbf{z}' \neq \mathbf{z}} H(\mathbf{z}, \mathbf{z}').$$

Evolution equation

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H |\psi(t)\rangle$$

$$\frac{\partial}{\partial t} |P(t)\rangle = H |P(t)\rangle$$

Evolution operator

$$|\psi(t)\rangle = e^{-iHt/\hbar} |\psi(0)\rangle$$

$$|P(t)\rangle = e^{Ht} |P(0)\rangle$$

Solving the representation problem

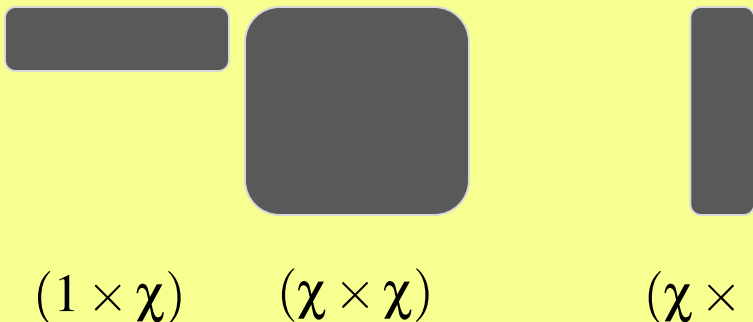
Recall: Dimension explosion

$$D = d^N$$

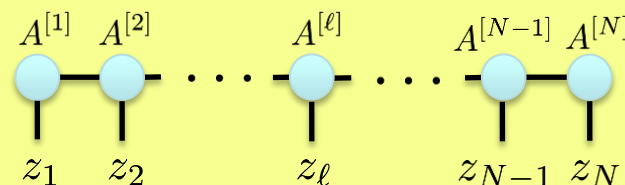
Mean Field $P(\mathbf{z}) = P^{[1]z_1} P^{[2]z_2} \dots P^{[N]z_N}$

Matrix Product State

$$P(\mathbf{z}) = A^{[1]z_1} A^{[2]z_2} \dots A^{[N]z_N}$$



MPS as a tensor network



$$Nd\chi^2$$

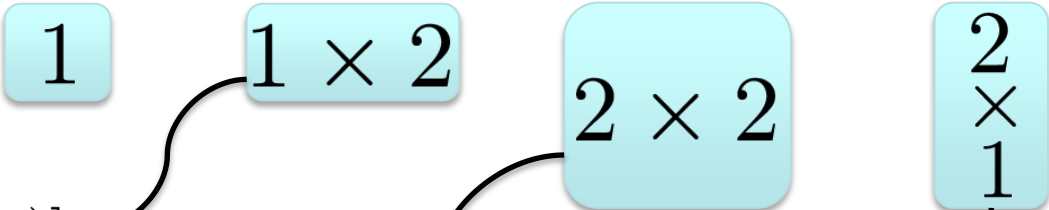
Gibbs distribution compressibility

Gibbs distribution for e.g. the 1D Ising model

$$P(\mathbf{z}) = \exp[-\beta E(\mathbf{z})], \quad E(\mathbf{z}) = -J \sum_{\ell=1}^N z_{\ell} z_{\ell+1} - \lambda \sum_{\ell=1}^N z_{\ell}$$

It factorises

$$P(\mathbf{z}) = A^{[1]z_1} \dots A^{[\ell]z_{\ell}} \dots A^{[N]z_N}$$



$$A_{\mu_1}^{[1]z_1} = \exp[\beta z_1 (J\mu_1/2 + \lambda)]$$

$$A_{\mu_{\ell-1}\mu_{\ell}}^{[\ell]z_{\ell}} = \exp[\beta z_{\ell} (J(\mu_{\ell-1} + \mu_{\ell})/2 + \lambda)]$$

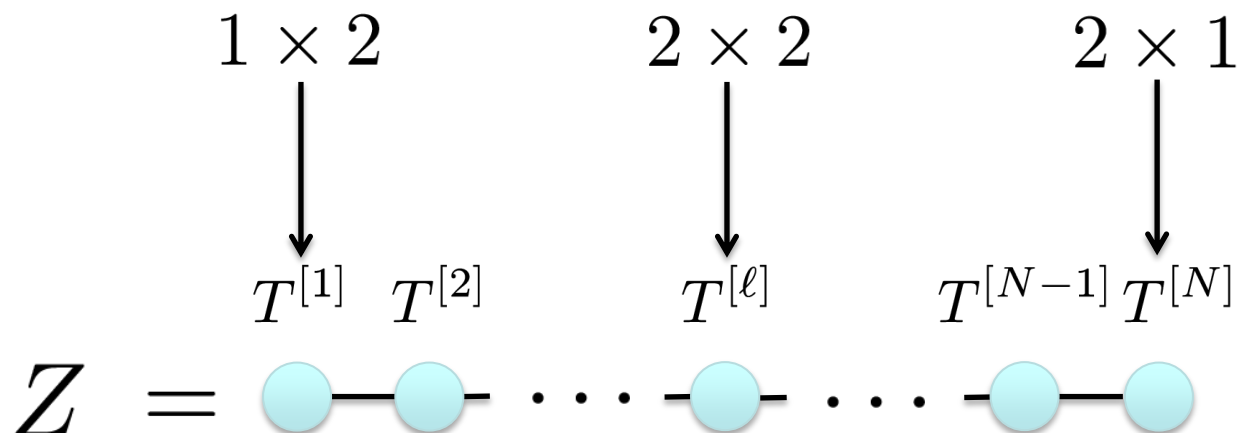
$$A_{\mu_{N-1}}^{[N]z_N} = \exp[\beta z_N (J\mu_{N-1}/2 + \lambda)]$$

$\chi = d = 2$
 $\mu_{\ell} \in \{-1, 1\}$

Transfer matrices

Transfer matrix method

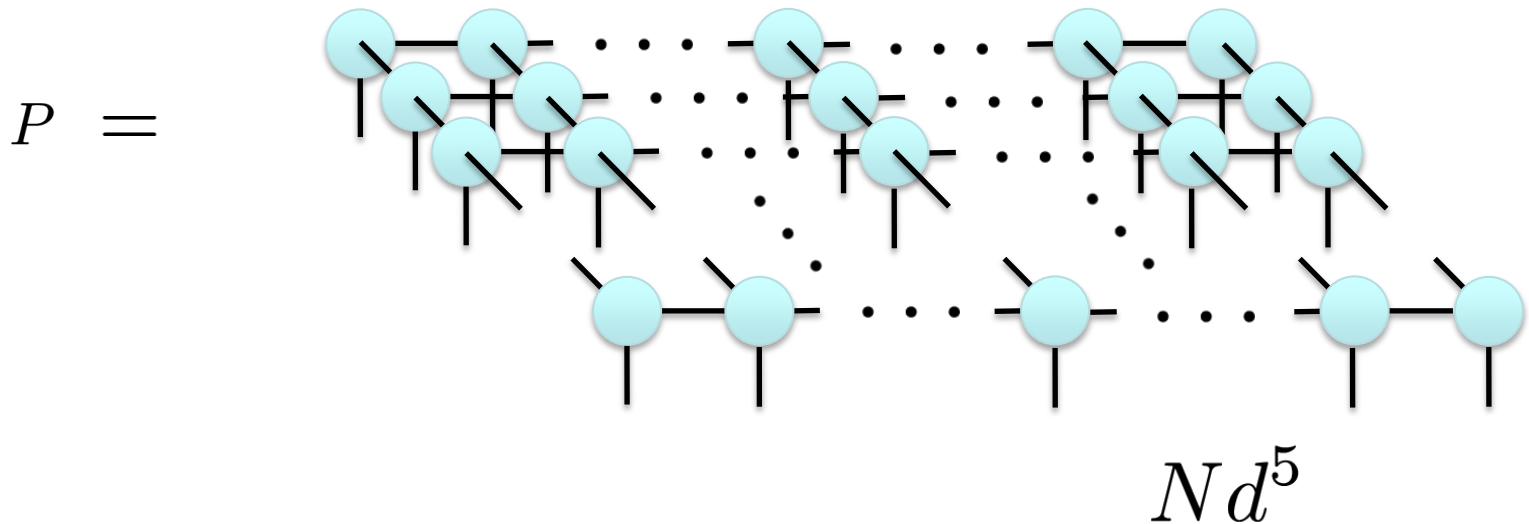
$$Z = \sum_{\mathbf{z}} P(\mathbf{z}) = \left(\sum_{z_1} A^{[1]z_1} \right) \cdots \left(\sum_{z_N} A^{[N]z_N} \right) = T^{[1]} \cdots T^{[N]}$$



2D and beyond

Works with other geometries, e.g. 2D arrangement:

$$E(\mathbf{z}) = -J \sum_{\langle \ell \ell' \rangle} z_{\ell} z_{\ell'} - \lambda \sum_{\ell} z_{\ell}$$



M. Levin and C. P. Nave, Phys. Rev. Lett. **99**, 120601 (2007).

Solving the evolution problem

Recall: Evolution operator

$$|P(t)\rangle = e^{Ht} |P(0)\rangle$$

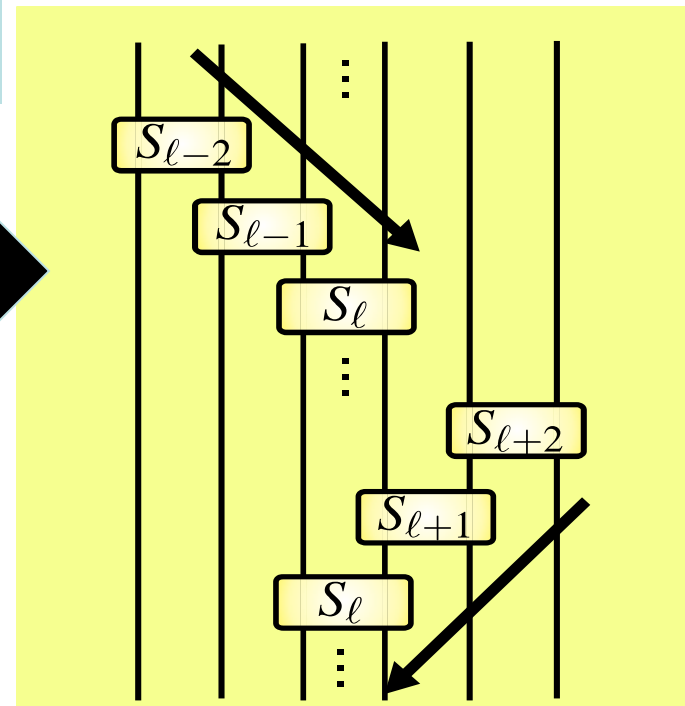
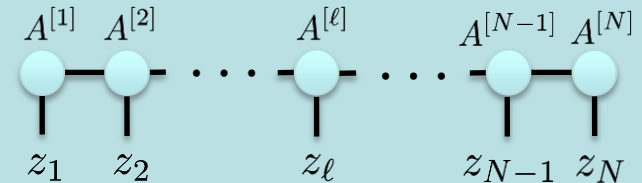
Assume: Nearest-neighbour

$$H = \sum_{\ell=1}^{N-1} h_{\ell,\ell+1},$$

$$e^{Ht} = e^{H\delta t} e^{H\delta t} \dots e^{H\delta t}$$

$$e^{H\delta t} = \underbrace{\left(\prod_{\ell=1}^{N-1} e^{h_{\ell,\ell+1}\delta t/2} \right)}_{S_\ell = \text{two-site gate}} \left(\prod_{\ell=N-1}^1 e^{h_{\ell,\ell+1}\delta t/2} \right) + O(\delta t^3)$$

Recall: Tensor Network



No runaway of correlations in quench

Steady distributions, e.g. Gibbs, have limited correlations and are thus compressible.

A quench begins AND ENDS in a steady distribution.

Correlations can't keep building up as for pure quantum systems.

The competitor – Dynamical Monte Carlo

Expected value

$$\langle O \rangle = \int [Ds] O[s] \mathcal{P}[s]$$

Sample paths

$$s^1, \dots, s^M$$

Average

$$\bar{O}_M = \frac{1}{M} \sum_{m=1}^M O[s^m]$$

Typical error

$$\langle \Delta \bar{O}_M \rangle = \sqrt{\frac{\text{Var}[O]}{M}}$$

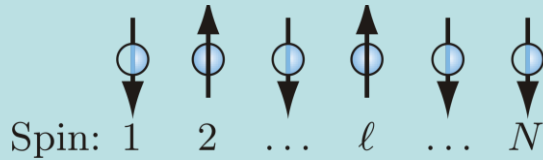
Number of paths needed

$$M = \frac{\text{Var}[O]}{\epsilon \langle O \rangle^2} = \frac{v}{\epsilon}$$

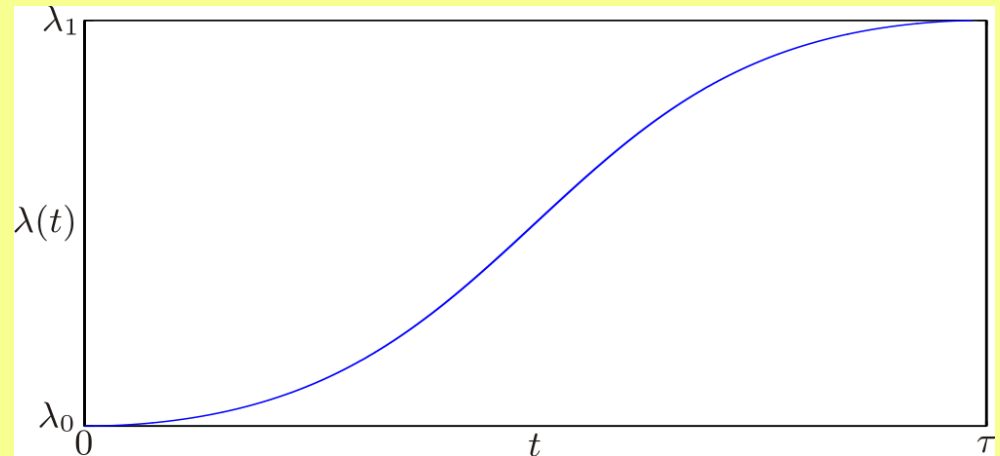
Large variance
=
Difficult

Quench

Recall: Ising chain



Drive away from equilibrium

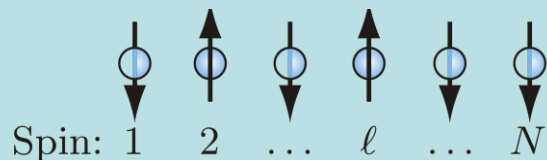


While it also thermalises

$$H(\mathbf{z}, \mathbf{z}') = \frac{h}{1 + \exp[-\beta(E(\mathbf{z}) - E(\mathbf{z}'))]}$$

High variance observables

Recall: Ising chain



Configuration-dependent
(magnetisation)

$$M(t) = \sum_{\ell} z_{\ell}(t)$$

Path-dependent
(work done)

$$W(t) = - \int_0^t ds M(s) \dot{\lambda}(s)$$

High-variance examples
(exponentially scaling with N)

$$v = e^{\mathcal{O}(N)}$$

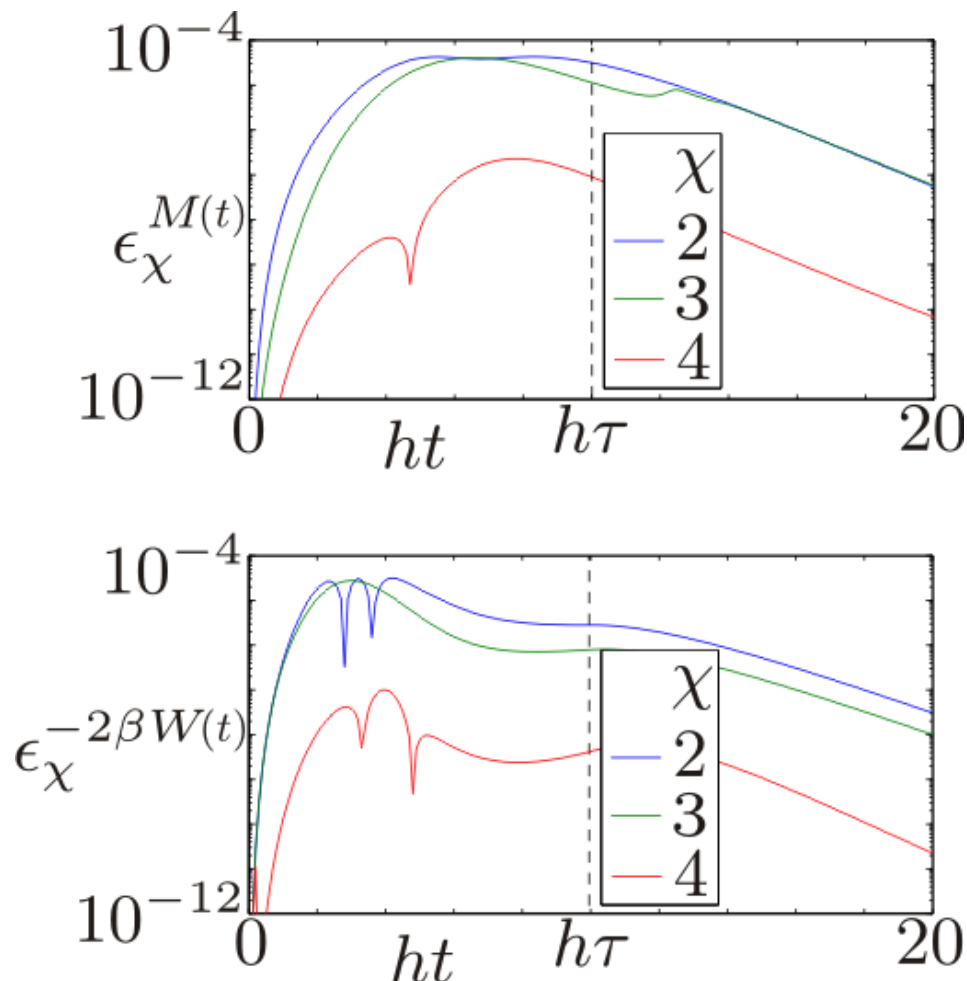
$$e^{M(t)}$$

$$e^{-2\beta W(t)}$$

$$e^{-\beta W(t)}$$

Small system results

Fractional error due to compressibility at a single time, small system



Parameters

$$N = 8$$

$$h\tau = 10$$

$$\beta J = 1$$

$$\beta\lambda_0 = 0$$

$$\beta\lambda_1 = 1$$

Accurate compression

$$\epsilon_\chi^{-\beta W(t)} = 0$$

Exact compression

Large system results

Recall: DMC and variance

$$M = \frac{\text{Var}[O]}{\epsilon \langle O \rangle^2} = \frac{v}{\epsilon}$$

Parameters

$$N = 200$$

$$h\tau = 10$$

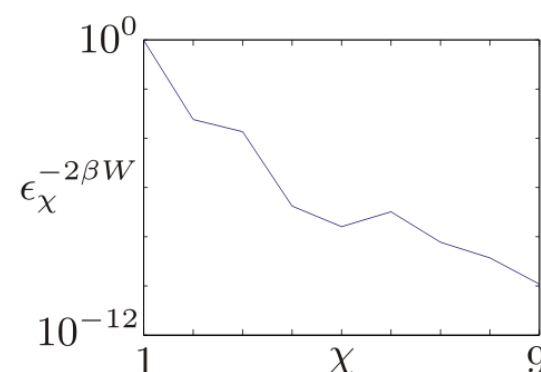
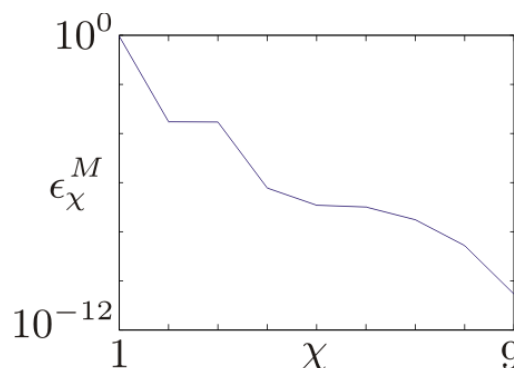
$$ht = 10$$

$$h\delta t = 10^{-3}$$

$$\beta J = 1$$

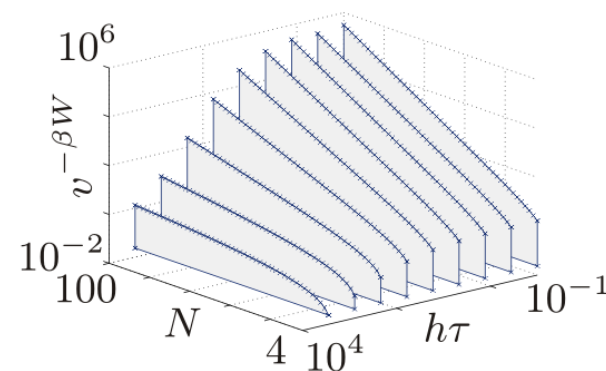
$$\beta \lambda_0 = 0$$

$$\beta \lambda_1 = 1$$



$$\epsilon^{-\beta W} \approx \alpha N (h\delta t)^2$$

$$\alpha = 4.65 \times 10^{-2}$$



Exponentially increasing variance

Exponential samples needed to match tensor networks

Example: 200-spin calculation, taking an hour, but needing $\approx 10^{17}$ samples

Summary and future directions

1. Tensor networks simulate stochastic processes
 2. Is this the way to estimate high variance observables?
 3. Good option for tensor networks in 2D?
-

What else can we do with tensor networks – PDEs?

Thanks for listening



Thomas Elliott



Stephen Clark



Dieter Jaksch

T. H. Johnson, S. R. Clark, and D. Jaksch, Phys. Rev. E **82**, 036702 (2010)

T. H. Johnson, T. J. Elliott, S. R. Clark, and D. Jaksch, arXiv:1410.3319

Tensor Network Library, tensornetworktheory.org

Questions?