Quantum vs. Classical – Implications for numerics

Using quantum methods to study classical stochastic dynamics

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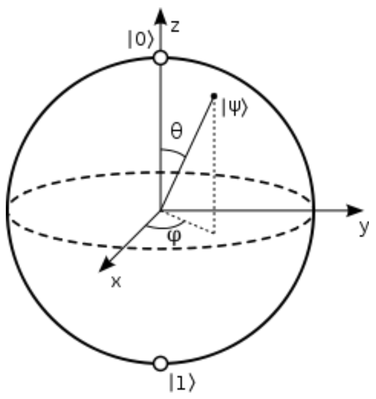
Example: Pure qubit



Configuration $\mathbf{i}$ represented by $|\,\mathbf{i}\rangle$.

Vectors $\{|\,\mathbf{i}\rangle\}$ form an orthonormal basis.

Vector spaces:
Quantum, complex
Classical, real and +ve

Observable O takes value $O_{\mathbf{i}}$ in configuration $\mathbf{i}$.

$\langle O\rangle$ is expectation value.

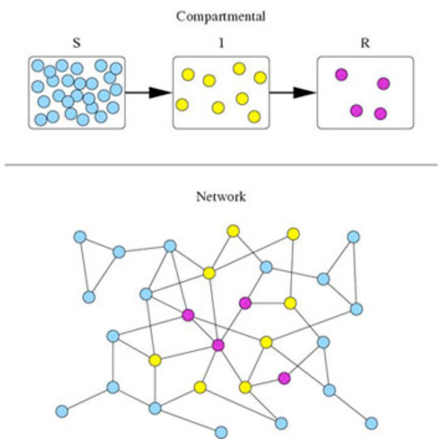
Usually easiest to minimise 2-norm error.

Quantum easier than classical!

Pure quantum vs. classical stochastic

	Quantum	Classical
Source of uncertainty	Fundamental, pure quantum superposition	Classical uncertainty, lack of knowledge
Description	State vector $\|\,\psi\rangle = \sum_{\mathbf{i}} \psi_{\mathbf{i}}\|\,\mathbf{i}\rangle$	Probability vector $\|\,P\rangle = \sum_{\mathbf{i}} P_{\mathbf{i}}\|\,\mathbf{i}\rangle$
Evolution	Schrödinger equation $\mathrm{i}\hbar\frac{\mathrm{d}\|\,\psi\rangle}{\mathrm{d}t} = H\|\,\psi\rangle$	Master equation $\frac{\mathrm{d}\|\,P\rangle}{\mathrm{d}t} = H\|\,P\rangle$
Probabilities	$\|\psi_{\mathbf{i}}\|^2$	$P_{\mathbf{i}}$
Properties	H is Hermitian $U(t) = \mathrm{e}^{-\mathrm{i}Ht/\hbar}$ is unitary	H is infinitesimal stochastic $S(t) = \mathrm{e}^{Ht}$ is stochastic
Error bounds	$\|\langle O\rangle^{\psi} - \langle O\rangle^{\phi}\| \leq \max_{\mathbf{i}}\{O_{\mathbf{i}}\}\|\|\,\psi\rangle - \|\,\phi\rangle\|_2$	$\|\langle O\rangle^{P} - \langle O\rangle^{Q}\| \leq \max_{\mathbf{i}}\{O_{\mathbf{i}}\}\|\|\,P\rangle - \|\,Q\rangle\|_1$

Example: Epidemic flows



Classical rate equation written in Schrödinger form.

"Hamiltonian" H contains **transition rates** between configurations.

Stochastic operators take one probability vector to another.

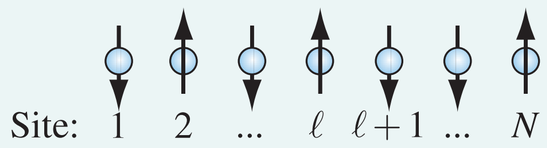
All entries are positive, and columns add to unity.

p-norms:

$$|||\,v\rangle||_p = \left(\sum_{\mathbf{i}} |v_{\mathbf{i}}|^p\right)^{\frac{1}{p}}$$

Matrix product state methods

Motivation. Take a multi-partite system, e.g., a spin chain



Each site has d possible configurations $i_\ell = 1, 2, ..., d$.
This means there are d^N global configurations $\mathbf{i} = (i_1 i_2 \cdots i_N)$.

Curse of dimensionality!

Example: 100 sites with 2 local states
1267650600228229401496703205376 configurations
158456325028528675 terabytes

Matrix product state methods allow us to *efficiently* store, evolve and compute expectation values from the state vector.

Storage. Product state

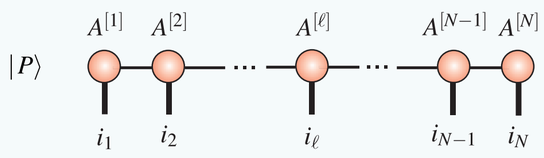
$$P_{\mathbf{i}} = P^{[1]}_{i_1} P^{[2]}_{i_2} \cdots P^{[N]}_{i_N}$$

Efficient but uncorrelated.

Generalisation: matrix product state

$$P_{\mathbf{i}} = A^{[1]}_{i_1} \times A^{[2]}_{i_2} \times \cdots \times A^{[N]}_{i_N}$$

$(1\times\chi)$ $(\chi\times\chi)$ $(\chi\times 1)$



Efficient and describes correlations.

Evolution. Split into time-steps

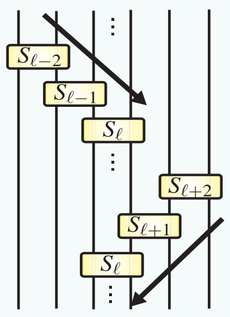
$$S(t) = \mathrm{e}^{Ht} = \mathrm{e}^{H\delta t}\mathrm{e}^{H\delta t}\cdots\mathrm{e}^{H\delta t}$$

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

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

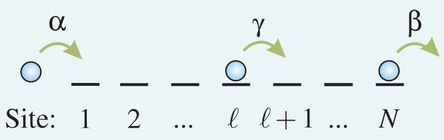
Sequence of two-site gates

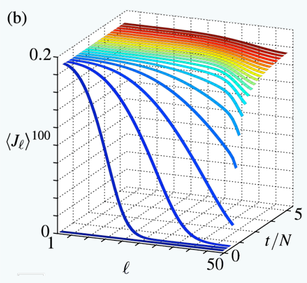
Two-site gates can be implemented approximately and efficiently.



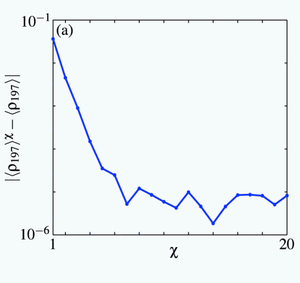
Applied to a classical system

The TASEP. A paradigm for traffic, queues, and protein transport.

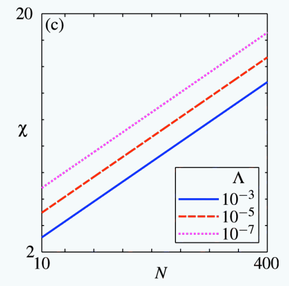




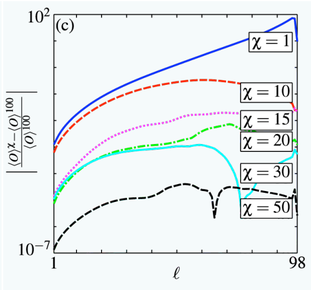
Evolution from an empty state



Observable error drops rapidly with size of matrices



Even for large systems, small matrices shown to be accurate



Convergence of expectation value shows accuracy

Quantum methods simulate this classical model very succesfully

Future questions and references

What physical property ensures simulability for classical systems?

How do these methods compare to Monte Carlo methods?

When does sampling break down, when are these methods needed?

What are the important 1D classical models with local transitions?

Which other quantum-based methods can be made classical?

[1] S.R. White, Phys. Rev. Lett. **69**, 2863 (1992) [2] G. Vidal, Phys. Rev. Lett. **93**, 040502 (2004)
[3] R.A. Blythe *et al*, J. Phys. A **40**, R333 (2007) [4] B. Derrida *et al*, J. Phys. A **26**, 1493 (1993)

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