# Phylogenetics as quantum computation

– from quantum random walks to maximum likelihood

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We present a novel application of the discipline of quantum computation-information to the field of evolutionary phylogenetics. The following results will be prefaced by a non-technical review of the idea of how simulation of stochastic models can be achieved by exploiting the behaviour of quantum systems.

A quantum simulation of phylogenetic evolution and inference, is proposed in terms of trace preserving positive maps (quantum channels) operating on quantum density matrices defined on Hilbert spaces encoding states of biological taxa with $K$ characters. Simulation of elementary operations such as speciation (branching of trees, phylogenesis) and phyletic evolution along tree branches (anagenesis), are realized utilizing conditional control-not unitary gates and quantum channels with unitary or complex matrix Kraus generators.

The standard group-based phylogenetic models are implemented via quantum random walks with unitary Kraus generators (random unitary channels), while more general models in the Lie-Markov class, such as the Felsenstein and strand symmetric models, are realized via post-measurement operations. Simulation of iterative cherry-growing and cherry-pruning tree processes is formulated in the quantum setting.

Thus the central problem of phylogenetics -- the statistical estimation of free parameters of stochastic matrices implementing the stochastic evolution of characters along tree branches -- is addressed by formulating an analogous quantum maximum likelihood estimation problem for the free parameters of quantum channels operating along branches.

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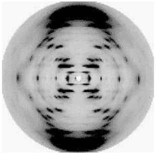

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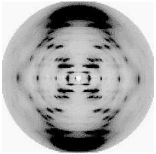

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This progress leads naturally to the question: can quantum mechanics play a role in biology? In many ways it is clear that it already does. Every chemical process relies on quantum mechanics[3].

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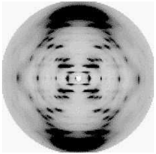

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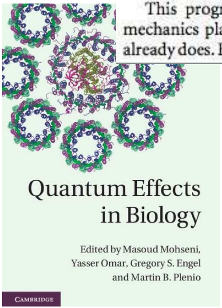


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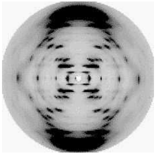

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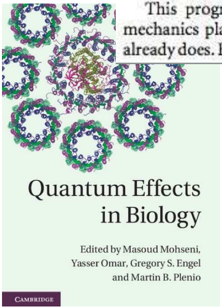


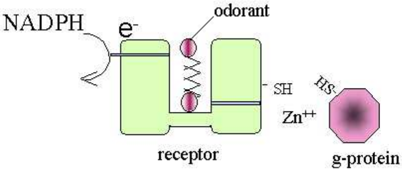


Olfaction = inelastic electron tunnelling?

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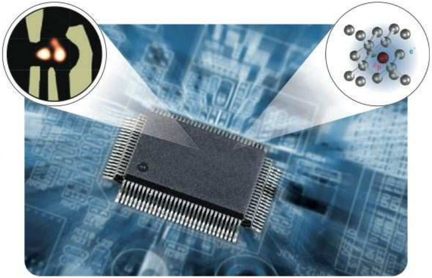

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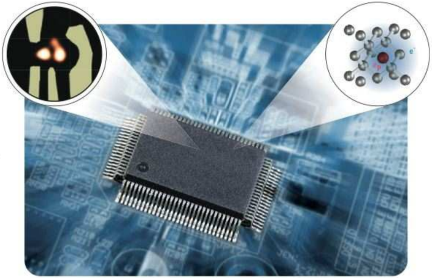

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1. Physics-Biology-Computation – an entangled golden braid?
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   - The complex geometry of stochastic models
   - Schrödinger's bug
   - Probability: 'quantum' vs 'classical'
3. Quantum mechanics 101b
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   - Measurement
   - Density operators
4. Quantum circuit simulations of phylogenetic substitution models
   - Quantum random walks
   - Likelihood
5. Standard phylogenetic models
   - Anagenesis
   - Cladogenesis

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# The complex geometry of stochastic models

- What we usually understand as a classical probability distribution is just the shadow of a complex number construction which is much richer, and worth studying in principle (c.f. Cardano's use of complex numbers in the 16th Century).
- For example, here's a cool way to build stochastic matrices:
  *Lemma: to each $K \times K$ doubly stochastic matrix $M$ can be associated a unitary matrix[1] $U$ such that $M$ is the Hadamard product[2] of $U$ and its complex conjugate, $M = U \circ U^*$ .*
- The construction for the $2 \times 2$ case is:

$$U = \exp \begin{pmatrix} 0 & \eta \\ -\eta^* & 0 \end{pmatrix} = \begin{pmatrix} \sqrt{1-|z|^2} & z \\ -z^* & \sqrt{1-|z|^2} \end{pmatrix}, \quad z = \frac{\sin \eta}{\eta},$$

$$\therefore \quad U \circ U^* \equiv \begin{pmatrix} 1-|z|^2 & |z|^2 \\ |z|^2 & 1-|z|^2 \end{pmatrix},$$

- **The choice of $U$ is non-unique. The geometry underlying the $2 \times 2$ binary symmetric Markov model is the complex projective space $\mathbb{CP}^1$.**

[1] Sums of moduli-squares of elements in each row and column equal unity; different rows and columns complex-orthogonal.

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# Introducing Schrödinger's bug (alive or dead)

- This little critter (bacterium, virus, prion) finds itself in a Petri dish with a radioactive atom. It is small enough to be described by a quantum wavefunction, but its quantum state is correlated to that of the radioactive atom, which has a certain probability to decay:

$$|\psi\rangle = z|\wedge\rangle + z'\,|\vee\rangle$$

- If the atom is undecayed, the bug is 'alive', $|\wedge\rangle$; if decayed, the bug is 'dead', $|\vee\rangle$.
- The probabilities of these events, when the experimenter makes a test, are the modulus-squareds of the complex amplitudes, $|z|^2$ and $|z'|^2$ with $|z|^2 + |z'|^2 = 1$.

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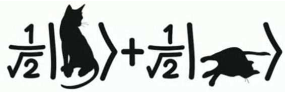
This is usually discussed via a 'thought experiment' known as 'Schrödinger's cat' where the cat state is 50% 'alive or dead',



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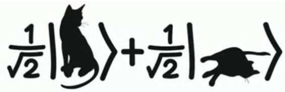

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- A better description is via the density *matrix* (or *density operator*)

$$\rho = |\psi\rangle\langle\psi| = |z|^2 \; |\wedge\rangle\langle\wedge| + zz'^* |\wedge\rangle\langle\vee| + \cdots$$

- A density matrix can be more general than just $|\psi\rangle\langle\psi|$ for some state vector – it is some array of complex numbers with special properties[3] Instead of $|\psi\rangle \to U|\psi\rangle$, time evolution is now $\rho \to U\rho U^\dagger$.
- The resolution of the cat/bug paradox is that there are so-called *decoherent* interactions with the rest of the environment, such as to *remove off-diagonal terms*, leaving simply

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- The bug-in-hand is just an element of a statistical ensemble, each of whose members has probability $|z|^2$, $|z'|^2$ of being found alive or dead, respectively.

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# Quantum operations

- The density operator is subject to time evolution, including dynamics as well as formal measurement processes, according to generalised quantum operations, parametrized by operators $\{U\}$ such that

$$\rho \to \mathscr{E}(\rho) = \sum_U U\rho U^\dagger, \quad \text{where} \quad \sum_U U^\dagger U = I.$$

- Consider in particular the diagonal elements of $\mathscr{E}(\rho)$:

$$\mathscr{E}(\rho)^a{}_a = \sum_b M^a{}_b \rho^b{}_b, \quad \text{and} \quad M^a{}_b = \sum_U U^a{}_b \big(U^a{}_b\big)^* \equiv \big(U \circ U^*\big)^a{}_b$$

Note $\displaystyle \sum_a M^a{}_b \equiv \sum_U \big(U^\dagger U\big)^b{}_b = 1, \quad \text{while} \quad \sum_b M^a{}_b \equiv \sum_U \big(UU^\dagger\big)^a{}_a$

*Prepare a diagonal density operator $\rho = \sum p^a \mathbb{P}_a$, a classical mixed state. Do a general quantum operation (e.g. unitary evolution plus measurement) followed by decoherent diagonal truncation.*
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# Example: diagonal truncation via DFT

- One can implement diagonal truncation via a sum of partial unitaries based on discrete Fourier transforms of the projection operators $\mathbb{P}_a$, $a = 0, 1, \cdots, K-1$ which collapse a general state on to each of the basis states of the selected basis: Firstly define

$$U_a = \sum_{b=0}^{K-1} \omega^{ab} \mathbb{P}_a \,,$$

where $\omega = e^{2\pi i/K}$. Let $q = 1/K$. Then

$$\mathscr{E}_{diag}(\rho) := \sum_{a=0}^{K-1} q\, U_a \rho {U_a}^\dagger \qquad \text{sends} \qquad \rho \to \mathscr{E}_{diag}(\rho) \equiv \sum_{a=0}^{K-1} \rho^a{}_a \mathbb{P}_a$$

– *in precise correspondence with the decoherent maps of Schrödinger's bug.*

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# Example: quantum random walk

*Classical processes like an infinite state Markov chain with forward/backward transition probabilities (birth/death process) can be decomposed into a 'walker' on the line $\mathbb{Z}$, and an auxiliary Bernoulli 'coin' with state space $\mathbb{Z}_2$ which determines whether the state increases or decreases (that is, whether the 'walker' moves forward or backward).*

- The quantum equivalent has product states, $|a\rangle \otimes |m\rangle$, $m \in \mathbb{Z}$, $a \in \mathbb{Z}_2$.
- Start with the 'walker' in state $|m\rangle$ and the 'qubit-coin' in the mixture state $\rho_c = p|+\rangle\langle+| + q|-\rangle\langle-|$ (with $p + q = 1$). Let $\mathbb{P}_\pm$ be the coin projectors, and $E_\pm$ the forward-backward shift operators, taking $|m\rangle$ to $|m \pm 1\rangle$.
- Under the unitary operation $V_{class} = \mathbb{P}_+ \otimes E_+ + \mathbb{P}_- \otimes E_-$, $\rho = \rho_c \otimes |m\rangle\langle m|$ is mapped (marginalizing over the qubit-coin) to

$$\mathscr{E}_{class}(\rho) = Tr_c\big(V_{class}\rho V_{class}^\dagger\big) = p|m+1\rangle\langle m+1| + q|m-1\rangle\langle m-1|$$

*–an ensemble with probability p for moving up, q for moving down.*

- But for a **quantum** random walker we allow the coin to undergo some unitary evolution first, before measuring:

$$\mathscr{E}_{qu}(\rho) = Tr_c\big(V_{qu}\rho V_{qu}^\dagger\big) \qquad \text{where} \qquad V_{qu} = \big(\mathbb{P}_+ \otimes E_+ + \mathbb{P}_- \otimes E_-\big) \cdot U \otimes 1\,.$$

- *Such quantum random walks have the remarkable property that the mean displacement after N steps is typically $O(N)$ (not $O(\sqrt{N})$ ).*

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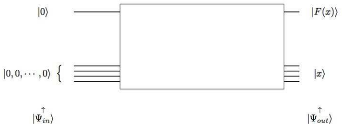
# Quantum simulation of stochastic models?

- *Quantum computing offers potentially huge advantages in terms of parallel processing, memory, AND exponential speed-up. Under the bonnet of the quantum processor is a toolkit of universal gates which can implement any desired unitary up to error bounds, as well as perform measurements. Roughly speaking, truth tables become matrices acting on qubits.*




- For phyletic evolution ($K$ characters, $L$ leaves) we need :
  - $L$ quantum 'wires' carrying qu$K$it systems;
  - Independent dynamics on each 'wire' with decohering maps representing substitutional models (*anagenesis*);
  - A system of entangling interactions between wires representing speciation (*cladogenesis*).

# *Anagenesis* - some standard substitution models

## Doubly stochastic case

> *Birkhoff's theorem: a matrix is doubly stochastic if and only if it can be expressed as a convex sum of permutation matrices.*

- For these, build elementary quantum operations representing arbitrary permutation matrices (the convex sum entails a statistical mixture, whereby the measurement is decided by a classical coin toss). In fact for the permutations themselves, $U_\sigma := \sum |\sigma a\rangle\langle a|$, and a diagonal density operator $\rho = \sum_a p^a |a\rangle\langle a|$, we have under $\rho \to U_\sigma \rho U_\sigma^\dagger$ that

$$p \to p', \qquad p'^a = \sum_b K_{(\sigma)}{}^a{}_b p^b$$

  where $K_{(\sigma)}$ is just the (square of) the matrix of $\sigma$, $K_{(\sigma)}{}^a{}_b = (\langle a|U_\sigma|b\rangle)^2$.

- The Kimura models are *symmetric*, hence doubly stochastic:

$$M_K = aK_{(\mathtt{AG})(\mathtt{CT})} + bK_{(\mathtt{AT})(\mathtt{CG})} + cK_{(\mathtt{AC})(\mathtt{GT})} + (1 - a - b - c)1$$

  where for rates $\alpha$, $\beta$, $\gamma$, we have $a = e^{-\alpha t}$, $b = e^{-\beta t}$, $c = e^{-\gamma t}$.

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## Doubly stochastic case

*Birkhoff's theorem: a matrix is doubly stochastic if and only if it can be expressed as a convex sum of permutation matrices.*

- For these, build elementary quantum operations representing arbitrary permutation matrices (the convex sum entails a statistical mixture, whereby the measurement is decided by a classical coin toss). In fact for the permutations themselves, $U_\sigma := \sum |\sigma a\rangle\langle a|$, and a diagonal density operator $\rho = \sum_a p^a |a\rangle\langle a|$, we have under $\rho \to U_\sigma \rho U_\sigma^\dagger$ that

$$p \to p', \qquad p'^a = \sum_b K_{(\sigma)}{}^a{}_b p^b$$

  where $K_{(\sigma)}$ is just the (square of) the matrix of $\sigma$, $K_{(\sigma)}{}^a{}_b = (\langle a|U_\sigma|b\rangle)^2$.
- The Kimura models are *symmetric*, hence doubly stochastic:

$$M_K = aK_{(\mathtt{AG})(\mathtt{CT})} + bK_{(\mathtt{AT})(\mathtt{CG})} + cK_{(\mathtt{AC})(\mathtt{GT})} + (1-a-b-c)1$$

  where for rates $\alpha$, $\beta$, $\gamma$, we have $a = e^{-\alpha t}$, $b = e^{-\beta t}$, $c = e^{-\gamma t}$.

UTAS

## Felsenstein model

- We need the stationary root frequency distribution, which is by construction (up to scaling): $\pi_{\mathtt{A}} = \alpha$, $\pi_{\mathtt{C}} = \beta$, $\pi_{\mathtt{G}} = \gamma$, $\pi_{\mathtt{T}} = \delta$.
- The corresponding diagonal operators (observables) are

$$\widehat{1}_\pi := \sum\nolimits_a \pi_a |a\rangle\langle a|, \quad \text{and} \quad \widehat{1}_{\pi^\#} := \widehat{1} - \widehat{1}_\pi$$

- As measurements, use $F^\pi_{a,b} = \sqrt{\pi_b}|a\rangle\langle b|$, $F^{\pi^\#}_{ab} = \sqrt{\pi^\#_b}|a\rangle\langle b|$, namely

$$\widehat{1}_\pi = \sum\nolimits_{a,b} F^{\pi\,\dagger}_{ab} F^\pi_{ab}, \qquad \widehat{1}_{\pi^\#} = \sum\nolimits_{a,b} F^{\pi^\#\,\dagger}_{ab} F^{\pi^\#}_{ab}$$

- Finally we need a convex sum of the measurement operation for ($\widehat{1}_\pi$ or $\widehat{1}_{\pi^\#}$) and the trivial measurement $\widehat{1}$ (but discarding $\pi^\#$ outcomes ):

$$\rho \to (1-\lambda) \sum\nolimits_{a,b} F^\pi_{ab} \rho F^{\pi\,\dagger}_{ab} + \lambda\rho$$

which implements the Felsenstein transition matrix

$$M_F = (1-\lambda) \sum\nolimits_{a,b} (F^\pi_{ab})^2 + \lambda 1$$

where $\lambda = e^{-\mu t}$ for some overall rate $\mu$.

# Putting it all together - trees and circuits – *cladogenesis*

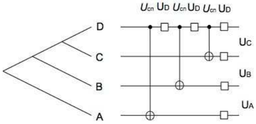
- It turns out that wires are $K+1$-state systems, with basis kets $|0\rangle, |1\rangle, \cdots |K\rangle$ including an additional ancilla or 'reservoir' state $|0\rangle$.
- Prepare neighbouring wires in the mixed (unentangled) state $\rho \otimes |0\rangle\langle 0|$ where $\rho$ is diagonal as usual.
- The 'control shift' operator $U_{\mathtt{CS}}$ acts *across* wires,

$$U_{\mathtt{CS}}|c\rangle|t\rangle := |c\rangle|(t+c)_{\mathtt{mod}_{K+1}}\rangle,$$

$$\therefore \qquad U_{\mathtt{CS}}\Big(\sum\nolimits_a p^a|a\rangle\langle a|\otimes|0\rangle\langle 0|\Big)U_{\mathtt{CS}}^{\dagger} = \sum\nolimits_a p^a|a,a\rangle\langle a,a|$$

After entanglement via $\mathtt{CS}$, a diagonal $\rho$ representing an edge character distribution produces a two-way probability array (GHZ state)

$$P^{a,b} = \begin{cases} p^a, & b=a\,; \\ 0, & b\neq a\,. \end{cases}$$



# Conclusions

- The probability distributions for standard parametrized phylogenetic models on trees can be simulated in a quantum circuit setting using appropriate quantum channels with suitable quantum operations (including generalized measurements). The model parameters are mapped to either coupling strengths or interaction times between entangled qubits, or probabilities of random meaasurement steps determined by suitably biassed classical coin tosses.
- The circuit presentation identifies the quantum protocols required, but is not necessarily the best for implementation, for which *networks* may be superior.
- These models can also be realized in a pure quantum random walk formalism, for a quantum walker on a suitably structured finite state space.
- For such quantum simulations of stochastic models, a likelihood measurement operator formalism also exists ($\Delta E$ & PDJ, in preparation).
- It remains to be seen if the full power of quantum algorithms is available for computation in this setting.

"My problem is that I know too much to tackle that. I'm a strong believer that ignorance is important in science. If you know too much, you start seeing why things won't work. That's why it's important to change your field to collect more ignorance."

Sydney Brenner, biologist.