Likelihood in Quantum Random Walks

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Stochastic Modelling, Hobart, Nov 15

In 1925 the physicist Max Born worked out the correct way to make predictions about physical systems from their quantum wave functions -- solutions of Schrödinger's equation -- using complex probability amplitudes. Apart from some well-publicised 'thought experiment' discussions by the founding figures, a deeper understanding lay dormant for 40 years (while physicists 'shut up and calculated'), until Bell formulated his famous theorem about correlated measurements. These beginnings have led to the field of quantum information, and potentially a sweeping revision of the mathematics and physics of probability.

The last few years have seen the first commercial products exploiting quantum science and its technological possibilities, like secure key distribution encryption systems. As contradictory as it seems, there may be possibilities ahead for the 'quantum simulation of stochastic systems', which will go faster, further, better than conventional computation can -- a game changer in the making. Against this backdrop, this talk will investigate a standard tool of probability and inference -- the likelihood function -- in the context of a toy model of a quantum random walk on the line.

1. Introduction
2. Complex probability
3. Quantum random walks
4. Likelihood in QRW – a toy model
5. Results

Quantum protocols

- Shor's factoring algorithm
  [prime factorization in polynomial time rather than exponential time classically]
- Grover's algorithm
  [unsorted database search in $O(\sqrt{n})$ steps rather than $O(n)$ classically]
- Quantum random walk
  [achieves depth $O(n)$ after n steps, rather than $O(\sqrt{n})$ classically]
- The *data box* issue.
- Quantum walks galore
  - There are general results on target(s) hitting time, return time, asymptotics and all that;
  - Grover's algorithm can be seen as a special case;
  - Generically there is always a '$\sqrt{\cdots}$' speedup;
  - You can do quantum walks on a network, on Cayley graphs, in higher dimensions, and lots more $\cdots$
  - See for example
    Mario Szegedy, *Quantum speed-up of Markov Chain based algorithms*, DOI: 10.1109/FOCS.2004.53 (IEEE transactions);
    Salvador Elías Venegas-Andraca, *Quantum walks: a comprehensive review* Quantum Information Processing archive Vol 11 #5, Oct 2012 pp 1015-1106

Complex probability

- **Classical description** of probability and stochastic evolution:
  – a probability distribution (for a system with discrete states) is a column vector in some convex (real) space, for example in molecular phylogenetics

$$p = \begin{pmatrix} p_A \\ p_C \\ p_G \\ p_T \end{pmatrix} \quad \longrightarrow \qquad p' = \begin{pmatrix} p'_A \\ p'_C \\ p'_G \\ p'_T \end{pmatrix} = \begin{pmatrix} a & b & c & d \\ e & f & g & h \\ h & g & f & e \\ d & c & b & a \end{pmatrix} \begin{pmatrix} p_A \\ p_C \\ p_G \\ p_T \end{pmatrix}$$

  – that is, $p' = Mp$ under some model of time evolution (for example a Markov process) or an equivalent continuous time version.

- **Quantal description**:
  – probability is represented via a complex matrix ρ – the 'classical' vector is the real diagonal, and the whole matrix ρ undergoes some two-sided change process

$$\rho \quad \longrightarrow \quad \sum\nolimits_{U,V} U \begin{pmatrix} p_A & 0 & 0 & 0 \\ 0 & p_C & 0 & 0 \\ 0 & 0 & p_G & 0 \\ 0 & 0 & 0 & p_T \end{pmatrix} V^* \equiv \begin{pmatrix} p'_A & ? & ? & ? \\ ? & p'_C & ? & ? \\ ? & ? & p'_G & ? \\ ? & ? & ? & p'_T \end{pmatrix}$$

  – that is, $\rho' = \sum_{U,V} U\rho V^*$ under some appropriate transformation rules.

Complex probability – II

This works, but we need a few rules ...

- The **density matrix** ρ is hermitean positive semidefinite with unit trace;
- Given ρ, **the** probability of measuring the system in state i is $p_i = Tr(\rho\mathbb{P}_i)$, where $\mathbb{P}_i$ is the projector on to the i'th subspace.
- Dirac notation: this is usually denoted $\mathbb{P}_i = |i\rangle\langle i|$, $i \in [K] = \{0, 1, \cdots, K-1\}$. $\{|i\rangle, i \in [K]\}$ is the corresponding orthonormal basis (column vectors) and $\{\langle i|, i \in [K]\}$ is the dual basis (transposes, row vectors).
- There are certain admissible time evolutions[1]

$$\rho^{(n+1)} = \mathscr{E}(\rho^{(n)})$$

  best illustrated by examples$\cdots$

[1]Competely positive trace preserving maps, CPTPM

Examples of $\mathscr{E}(\rho)$.

- **Diagonalization map**
  - Let $\omega = e^{2\pi i/K}$ and define the cyclic matrix $\Omega_{i,i+1} = \omega^i\,, 0 \leq i \leq K-1\,.$ Consider

$$\rho' := \mathscr{E}_{diag}(\rho) := \frac{1}{K}\sum_{i=0}^{K-1} \Omega^i \rho \Omega^{-i}$$

  Result: $\rho' = Diag(\rho_{00}, \rho_{11}, \cdots, \rho_{K-1,K-1})$ – the 'classical' diagonal part of ρ.

- **Unistochastic evolution map**
  - Let $\rho = Diag(p_0, p_1, \cdots, p_{K-1})$ be classical, and U a $K \times K$ unitary. Then define

$$\rho' = \mathscr{E}_U(\rho) := \mathscr{E}_{diag}(U\rho U^\dagger)\,.$$

  Result: $\rho' = Diag(p'_0, p'_1, \cdots, p'_{K-1})$ is given by $p' = Mp$, where $M = U \circ U^*$ is the Hadamard (component-wise) product of U and U^* (M is a doubly stochastic matrix)[2].

[2] A.W. Marshall and I. Olkin, *Inequalities: Theory of Majorization and its Applications*, (Academic, NY, 1979).

Quantum random walks for pedestrians

- Classically the state space for a CRW on the line is the Cartesian product $\mathbb{Z} \times \mathbb{Z}_2$ – that is, we have states (m, c) where $m \in \mathbb{Z}$ is the walker location, and $c \in \mathbb{Z}_2$ is the coin state $(\{\mathtt{H}, \mathtt{T}\} \Leftrightarrow \{\underline{0}, \underline{1}\}$ respectively).

- We can set up a quantum analogue of the walker as follows:
    - The corresponding quantal state space is the tensor product

      $$\mathscr{H}_w \otimes \mathscr{H}_c \cong \ell^2(\mathbb{Z}) \otimes \ell^2(\mathbb{Z}_2)$$

      with basis $|m, c\rangle \equiv |m\rangle \otimes |c\rangle$.
    - The state of the system is described by some total density matrix ρ. We have to specify the evolution

      $$\rho^{(n+1)} = \mathscr{E}(\rho^{(n)})$$

      and then measure $\rho^{(n)}$ to find the probability distribution of occupation of different sites m.
    - Initially ρ is decomposable, $\rho = \rho_w \otimes \rho_c$, but at intermediate times may not be so expressible.

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Quantum random walks – II

- **Special case:** classical Bernoulli process as a QRW
  - Define the 2×2 coin projection operators on to the heads and tails subspaces as $\mathbb{P}_{\mathtt{H}}, \mathbb{P}_{\mathtt{T}}$ as usual. Introduce the one step right/left translation operators

$$\mathbb{E}_+ = \sum_{m \in \mathbb{Z}} |m+1\rangle\langle m| \,, \qquad \mathbb{E}_- = \sum_{m \in \mathbb{Z}} |m-1\rangle\langle m| \,.$$

  - Let $V_{cl} = \mathbb{E}_+ \otimes \mathbb{P}_{\mathtt{H}} + \mathbb{E}_- \otimes \mathbb{P}_{\mathtt{T}}$ (unitary!). Assume the system evolves as

$$\rho^{(n+1)} = \mathscr{E}_{cl}(\rho^{(n)}) := V_{cl}\rho^{(n)}V_{cl}^{\dagger} \,.$$

  - Take the walker initially at the origin, with density matrix $\rho_w = |0\rangle\langle 0|$.
  - Let the coin be in the mixed state

$$\rho_c = p|\mathtt{H}\rangle\langle\mathtt{H}| + (1-p)|\mathtt{T}\rangle\langle\mathtt{T}| \,.$$

  - The walker state after each step is defined by marginalization (tracing out the coin):

$$\rho_w^{(n)} = Tr_c(\rho^{(n)}) \,.$$

- After n steps, the p.d.f. P^n_m for the location of the walker at position m is

$$P^n_m = Tr\big(\rho_w^{(n)}\mathbb{P}_m\big) \,, \quad \text{where} \quad \mathbb{P}_m = |m\rangle\langle m| \,.$$

- It is not hard to establish the following:

> **Result: P^n_m – the probability for locating the walker at position m – is the same as in the classical Bernoulli process (with a biassed coin if $p \neq \frac{1}{2}$), based on the binomial distribution.** In particular, the mean distance from the origin $\cong O(\sqrt{n})$.

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Quantum random walks – III

- The interpretation of V_{cl} is as in the standard CRW – if the coin measurement (associated with the $Tr_c(\mathbb{P}_{\mathtt{H}} \cdots)$, $Tr_c(\mathbb{P}_{\mathtt{T}} \cdots)$ part of the evolution) turns up H or T, then the walker is translated to the right or left, respectively.

Q: **what if the coin were able to evolve independently?**

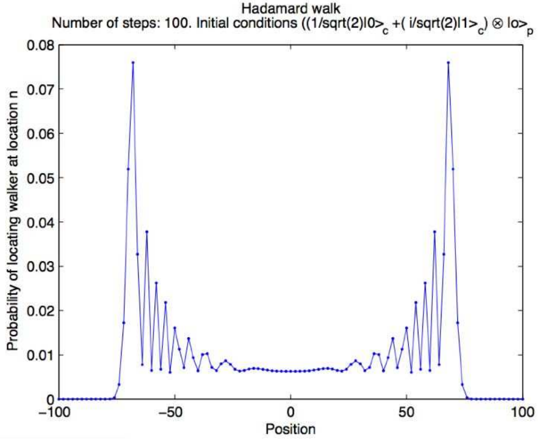
- **General case:** quantum (non-classical), QRW
  - Introduce a coin operator U_c (a 2×2 unitary). The time evolution is now

$$\rho^{(n+1)} = \mathscr{E}_{qu}(\rho^{(n)}) = V_{qu}\rho^{(n)}V_{qu}^{\dagger}, \qquad V_{qu} = V_{cl} \cdot \big(\mathrm{Id} \otimes U_c\big)$$

  - We work with a variant allowing k evolution **cycles** between measurement steps, $V_{qu} \to (V_{qu})^k$.

Quantum random walks – IV

Theorem: for certain classes[3] of U_c the walk is non-classical, and the mean distance from the origin is not $O(\sqrt{n})$ as usual, but now[3] $O(n)$.



[3]Obviously not $U_c = \mathrm{Id}$! [3] Source:`http://dx.doi.org/10.1007/s11128-012-0432-5`

Likelihood!!

- Consider the behaviour of the system in a toy model QRW on the line. We take a quantum model of the coin evolution operator, for example 'orthogonal' type[4] depending on some external parameter θ:

$$U_c^O(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}; \quad \text{e.g.} \quad U_c^O(\tfrac{1}{2}\pi) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

- Consider the probabilities of the walker being at location m, $p_m^{(k)}(\theta)$, after a single step, but in the k-cycle implementation of the QRW, assuming the walker starts at the origin, $\rho_w = |0\rangle\langle 0|$.
- We study the likelihood function $L(\theta)$ for N successive observations of the walker, at walker positions $m_1, m_2, \cdots, m_N$:

$$L(\theta; m_1, m_2, \cdots, m_N) = p_{m_1}^{(k)}(\theta) p_{m_2}^{(k)}(\theta) \cdots p_{m_N}^{(k)}(\theta)$$

- How does this behave under different possible measurement scenarios?

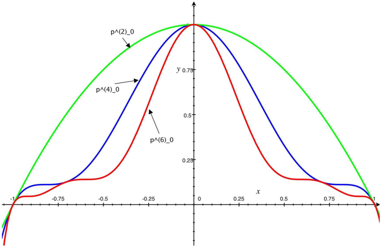
[4] Or of 'unitary' type $U_c^U(\theta) = 1/\sqrt{2}\begin{pmatrix} e^{i\theta} & e^{i\theta} \\ -e^{-i\theta} & e^{-i\theta} \end{pmatrix}$ including the 'Hadamard' walk (the special case $\theta = 0$).

The **reluctant quantum walker** scenario

- What happens to this QRW if we take a completely biassed coin, $\rho_c = |\mathtt{H}\rangle\langle\mathtt{H}|$ but nonetheless assume that we have made N successive measurements with the coin back at the origin? – i.e. the likelihood becomes $L(\theta) = \left(p_0^{(2k)}(\theta)\right)^N$.

The **reluctant quantum walker** scenario

- Here is the likelihood function (actually just $p_0^{(2k)}$) for the first few (even) numbers of cycles $2k = 2, 4, 6$ (plotted against $-1 \leq \cos\theta \leq +1$):



- **Conclusion:** given that the walker remains at the origin, and despite the biassed coin, the likelihood function acquires an ever sharpening maximum with increasing evolution cycles, implying that the coin shuffling evolution can only be driven by the 'bit flip' operator with $\theta = \frac{1}{2}\pi$.

Demosthenes Ellinas & PDJ :
J Phys A (Mathematical & Theoretical):
Biological Modelling (*in preparation*)

http://iopscience.iop.org/1751-8121/page/ biological-modelling

NIKOLAS GEORGIOU/DEMOTIX/CORBIS

NEWS IN FOCUS

Nature Vol 517 (Jan 2015)

University students in Athens protest against the government's plan for education and research reform.

POLITICS

Greek science haunted by hydra of problems

Leading researchers hang on despite austerity, but their Herculean efforts m

BY ALISON ABBOTT

For chemical engineer Athanasios Konstandopoulos, it is as if all the myths of ancient Greece have come to life at once. The task of keeping up top-performing Greek labs such as his Aerosol and Particle Technology Laboratory (APTL) in Thessaloniki requires the strength of Hercules, he says, as well as the dogged persistence of Sisyphus, who was condemned for eternity to repeatedly roll a boulder up a hill and watch it roll down again.

Mortal power has so far maintained the

measures imposed in the wake of the nation's debt crisis in 2010. But five years on, with prolonged austerity pushing Greece into yet another political crisis, scientists are wondering how long that output can be kept up.

In 2014, budgets for research centres and universities in Greece were just one-quarter of their 2009 levels, and take-home salaries had been sliced by around one-third. This year begins with yet more cuts — even as the country implements a long-awaited law meant to reform the research landscape and make it more competitive. Qualified young professionals are leaving the country in unprecedented

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Nektarios Taver
FORTH Institute
Biotechnology (I
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Commission, the
the International
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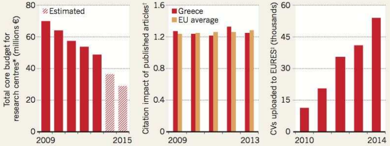
measures. However, it insisted that cuts be coupled to reforms aimed at rejuvenating the country's generally lacklustre research and uni-

HEALTH OF GREEK SCIENCE IN NUMBERS

Goverment funding for research has plummeted (left) but scientists have maintained the quality of their research (middle). Still, qualified young people increasingly seek to leave (right).



*Does not include universities †Weighted by field and relative to global average ‡The European Job Mobility Portal

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