On Quantum Simulation of Phylogenetic Processes

Demosthenes Ellinas

Technical University of Crete
Phylomania 2011
(collaborator P Jarvis)

U Tasmania
Hobart 10 Nov. 2011
Characters-Spaces-Operators

Character set $\Sigma = \{0, 1, \ldots, N\} = \{0\} \cup \Sigma^*$. (0 “null”, no character)
Hilbert space of character states $H \approx l_2(\Sigma) = \text{span}(|i\rangle; i \in \Sigma)$, $\text{dim}H = |\Sigma|$. Linear operators $\text{Lin}(H)$ on $H$
E.g. projector $\hat{P}_i = |i\rangle \langle i|$
Shift operator $h |i\rangle = |i + N 1\rangle$, ( $+ N$ addition modulo $N$; so $h^N = 1$)
Density matrices $\mathcal{D}(H) = \{\rho \in \text{Lin}(H), \rho^\dagger = \rho, \rho \geq 0, \text{Tr} \rho = 1\}$
Discrete prob.d. $(p_0, p_1, p_2, \ldots p_{N-1}) \rightarrow$ diagonal dm
$$\rho = \sum_{i \in \Sigma^*} p_i \hat{P}_i$$
(in practice $p_0 = 0$, summation $i \in \Sigma^*$).
Control-shift(not) (unitary) $U_{cn} \in \text{Lin}(H \otimes H)$, $U_{cn} = \sum_{k \in \Sigma} \hat{P}_k \otimes h^k$,
action $U_{cn} |i\rangle \otimes |j\rangle = |i\rangle \otimes |j + N i\rangle$
**Splitting map** \( \Delta \)

1-taxon density matrix \( \rho = \sum_{i \in \Sigma^*} p_i \hat{P}_i \rightarrow \Delta \rho \)

2-taxon density matrix

\[
\Delta \rho = U_{cn} (\rho \otimes \hat{P}_0) U_{cn}^\dagger = \sum_{i,j \in \Sigma^*} p_{ij} \hat{P}_i \otimes \hat{P}_j,
\]

where \( p_{ij} = p_i \delta_{ij} \).

Embedding in \( s \)-fold products e.g. \( 1 \otimes^{k-1} \otimes U_{cn} \otimes 1 \otimes^{s-k-1} \), provides \( s \)-taxon phylogenetic trees of various topologies.

Let \( s \)-taxon density matrix

\[
\rho = \sum_{i_1,\ldots,i_s \in \Sigma^*} p_{i_1\ldots i_s} \hat{P}_{i_1} \otimes \ldots \otimes \hat{P}_{i_s}
\]
Phyletic evolution map

$$\rho \rightarrow \tilde{\rho} \equiv \mathcal{E}_d \otimes^s (U \rho U^\dagger) = \mathcal{E}_d \otimes^s \circ \text{Ad} \ U(\rho)$$

local unitary \( U = \bigotimes_{i=1}^s U_i \in \text{Lin}(H) \otimes^s \) local diagonalizing map \( \mathcal{E}_d \otimes^s \), where \( \mathcal{E}_d(\cdot) = \sum_{k \in \Sigma} \hat{P}_k(\cdot) \hat{P}_k \).

\[
\tilde{\rho} = \sum_{i_1, \ldots, i_s \in \Sigma^*} \tilde{p}_{i_1 \ldots i_s} \hat{P}_{i_1} \otimes \ldots \otimes \hat{P}_{i_s}, \\
\tilde{p}_{i_1 \ldots i_s} = \sum_{j_1, \ldots, j_s \in \Sigma^*} p_{j_1 \ldots j_s} (M_1 \otimes \ldots \otimes M_s)_{i_1 j_1; \ldots; i_s j_s}.
\]

(Notation: adjoint action \( \text{Ad} \ S(\cdot) \equiv S(\cdot) S^\dagger \); Hadamard or entry-wise product of matrices \( (A \circ B)_{ij} = A_{ij} B_{ij} \)). Phyletic evolution map induces a doubly-stochastic transformation in the probability tensor via Markov unistochastic matrices \( M_i = U_i \circ U_i^* \); completely positive trace preserving (CPTP) map projecting out the diagonal part of \( \rho \) (decoherent map).
Motivating QW: "...Brownian motion is a poor model, and so is Ornstein-Uhlenbeck", Felsenstein, R-sig-phylo mailing list, 2008

**Quantum walker** space $\equiv$ character Hilbert space $H$

**Quantum coin** Hilbert $H_c \approx l_2(C) = \text{span}(|+\rangle, |-\rangle)$ (at each vertex of phylogenetic tree)

**Projectors** $P_{\pm} \in \text{Lin}(H_c)$

**Coin reshuffling** unitary matrix $U$

**Coin-walker states** $\rho_c \otimes \rho$ ($\rho_c = |c\rangle \langle c|$)

**Conditional unitary** $V = (P_+ \otimes h + P_- \otimes h^\dagger)U \otimes 1$ on $H_c \otimes H$
1-step QW $\mathcal{E} : \mathcal{D}(H) \to \mathcal{D}(H)$ CPTP map
$(\mathcal{E} > 0, \text{id}_M \otimes \mathcal{E} > 0, Tr\mathcal{E} = Tr)$

Representation theory of CPTP maps (non unique!)
– unitary dilation representation of $\mathcal{E}$ (Naimark’s extension thm)

$$\rho \to \mathcal{E}_{V^k}(\rho) = Tr_c V^k (\rho_c \otimes \rho) V^{+k}$$

– operator sum representation of $\mathcal{E}$

$$\rho \to \mathcal{E}_{V^k}(\rho) = \sum_{i \in \Sigma^*} A_i \rho A_i^\dagger$$

Kraus generators $A_i = \langle i | V^k | c \rangle$
Diagonalization map $\mathcal{E}_d(\rho) = \sum_{k \in \Sigma^*} \hat{P}_k \rho \hat{P}_k$

For $s$ taxa

$E_{V^k} \equiv (\mathcal{E}_d \circ \mathcal{E}_{V^k}^{\otimes s})$

E.g. 2-taxa, $k = 2$, $\rho_c = P_\pm$

$E_{V^2}(\rho) = \sum_{mn} \tilde{\rho}_{mn} \hat{P}_m \otimes \hat{P}_n$

probability tensor

$\tilde{\rho}_{mn} = \sum_{ab} \rho_{m-a,n-b} q_a^{(c)} q_b^{(c)}$

discrete pd $q_a^{(c)} := \sum_\gamma M_{j,a-j} M_{j-a,c} \geq 0$

uni-stochastic matrix $M = U \circ U^*$
Proposition  Diagonalizing map $\mathcal{E}_d$ cast in the form of CPTP map with unitary Kraus generators

$$\mathcal{E}_d(\rho) = \sum_{k \in \Sigma^*} \hat{P}_k \rho \hat{P}_k = \sum_{k \in \Sigma^*} q_k U_k \rho U_k^\dagger$$

with $q_k = 1/|\Sigma^*|$. Unitaries $U_k$ related to projectors via discrete Fourier transform, $U_k = \sum_l \omega^{kl} \hat{P}_l$ and $\omega = \exp(i2\pi/|\Sigma|)$. A unitary dilation of $\mathcal{E}_d$ reads $\mathcal{E}_d(\rho) = \text{Tr}_c V_d (\rho_c \otimes \rho) V_d^\dagger$, $V_q = e^{iH}(U_c \otimes 1)$, with Hamiltonian $H_{cl} = \sum_{k,l \in \Sigma^*} k l \hat{P}_k \otimes \hat{P}_l \otimes \hat{P}_l$, and $\rho_c = |k\rangle \langle k|$ any $|k\rangle$ canonical state vector in $H_c \approx l_2(\mathbb{Z}|\Sigma^*|)$, and a choice for reshuffling matrix $U_c = \frac{1}{\sqrt{|\Sigma^*|}} \sum_{k,l \in \Sigma^*} \beta^{kl} |k\rangle \langle l|$, $\beta \in \mathbb{C}$, $|\beta| = 1$. 
Group models:
- Jukes-Cantor (JC)
- Kimura (K2)
- Kimura (K3)
- Binary symmetric model (B)

and

Felsenstein model (F)

CPTP quantum map

\[ E_\tau \equiv \mathcal{E}_d \circ \mathcal{E}_\tau \]

\( \tau \in \{K3, K2, JC\} \) and B model

Initial state \( \rho = \sum_{m \in \Sigma^*} p_m \hat{P}_m \) 1-taxon density matrix

(Notation \( X \equiv \sigma_x, \ Z \equiv \sigma_z \) Pauli sigmas)
Proposition $(K,JC;OSR)$: Let $|\Sigma^*| = 4$ and $\tau \in \{K3, K2, JC\}$

\[
E_\tau(\rho) = \sum_{k,l} \lambda_{kl}^{(\tau)} U_{kl}(\rho) U_{kl}^\dagger = \sum_{m \in \Sigma^*} (M_\tau p)_m \hat{P}_m,
\]

\[
M_\tau(a, b, c) = \sum_{kl} \lambda_{kl}^{(\tau)} U_{kl} \circ U_{kl}^* = \sum_{kl} \lambda_{kl}^{(\tau)} X^k \otimes X^l.
\]

Weights $\lambda_{kl}^{\tau}$ of Markov bi-stochastic matrices $M_\tau$: define weights $\lambda_{kl}(a, b, c)$ as $\lambda_{00} = 1-a-b-c$, $\lambda_{10} = a$, $\lambda_{01} = b$, $\lambda_{11} = c$, then

\[
\lambda_{kl}^{(3K)} = \lambda_{kl}(a, b, c), \quad M_{3K} \equiv M(a, b, c)
\]

\[
\lambda_{kl}^{(2K)} = \lambda_{kl}(a, b, b), \quad M_{2K} \equiv M(a, b, b)
\]

\[
\lambda_{kl}^{(JC)} = \lambda_{kl}(a, a, a), \quad M_{JC} \equiv M(a, a, a)
\]
Proposition (K,JC;UD): The CPTP map $E_\tau$ has, in addition to the operator sum representation above, also a QW like representation $E_\tau(\rho) = Tr_c V_\tau(\rho_c \otimes \rho) V_\tau^\dagger$, in terms of a unitary dilation

$$V_\tau = \left( \sum_{kl} P_k \otimes P_l \otimes U_{kl} \right) U_\tau \otimes \mathbf{1}$$

which acts on a composite coin-walker space $H_c \otimes H$, with 4D ancillary space. Here $V_\tau$ is a control-control-$U_{kl}$ operator. For a coin density matrix with spectral decomposition $\rho_c = \sum_{kl} \mu_{kl} |c_{kl}\rangle \langle c_{kl}|$, the coin-tossing unitary $U_\tau$ should satisfy $\langle kl | U_\tau \circ U_\tau^* | c \rangle = \lambda_{kl}^{(\tau)}$, with $|c\rangle = \sum_{kl} \mu_k |c_{kl}\rangle$ a stochastic vector.

Also $U_{kl} = e^{i\mathcal{H}_{kl}}$ where Hamiltonian operator

$$\mathcal{H}_{kl} = \frac{1}{2} \pi \left[ -(k + l) \mathbf{1} \otimes \mathbf{1} + kX \otimes \mathbf{1} + l\mathbf{1} \otimes X \right].$$
Proposition (B;OSR): Let $|\Sigma^*| = 2$. Let the map $\mathcal{E}_d \circ E_B$ where $E_B(\rho) = (1 - a)\rho + aX\rho X^\dagger$, simulates the binary symmetric model $M_B(a) = (1 - a)\mathbf{1} + aX$ acting as $\rho = \sum_{m \in \Sigma^*} \rho_m \hat{P}_m \rightarrow \sum_{m \in \Sigma^*} (M_B \rho)_m \hat{P}_m$.  

Proposition (B;UD): The “control flip” map $E_B$ is unitarized in composite coin-walker space with a 2D ancillary coin-space as, $E_B(\rho) = Tr_c V_B(\rho_c \otimes \rho) V_B^\dagger$, with the starting coin state $\rho_c = \ket{1}\bra{1}$, and $V_B = \sqrt{a} \mathbf{1} \otimes \mathbf{1} + \sqrt{1-a} Y \otimes X$, and $Y \equiv ZX$.  

Model’s stationary distribution \((\pi_1, \pi_2, \pi_3, \pi_4)\)
Introduce observable \(1_\pi := 4 \sum_i \pi_i \hat{P}_i\)
Kraus operators \(F_{ij} = \sqrt{\pi_j} |i\rangle \langle j|, i, j \in \Sigma = \{1, 2, 3, 4\}\)
Resolution relation \(\sum_{ij} F_{ij}^\dagger F_{ij} = \frac{1}{4} 1_\pi\)

**Proposition (F,OSR):** Quantum map \(\rho \rightarrow E_F(\rho) = \sum_{m \in \Sigma^*} (M_F p)_m \hat{P}_m\) is given by
\[
E_F(\rho) = (1 - a) \frac{1}{p_\pi} \sum_{i,j} F_{ij} \rho F_{ij}^\dagger + a \rho,
\]

Non unital map : \(E_F(1) \neq 1\)
**Row-stochastic** matrix \(M_F = (1 - a) \sum_{i,j} F_{ij} \circ F_{ij} + a 1\)

Measuring probability \(p_\pi = Tr(\sum_{i,j} F_{ij}^\dagger F_{ij} \rho) = Tr(\frac{1}{4} 1_\pi \rho)\)
Framework of quantum measurement theory

Two observables: $1_\pi$ as above, and $1_\pi^\# = 1_H - 1_\pi$ complementary pd $(\pi_1^\#, \pi_2^\#, \pi_3^\#, \pi_4^\#)$

Non-orthogonal decomposition of unity $1_H = 1_\pi + 1_\pi^\#$

Observables $1_\pi, 1_\pi^\#$ measured by means of the so called instruments: families of Kraus $g_{Fij}$

Measurement probabilities: $p_\pi^\# = Tr(1_\pi^\# \rho), p_\pi = Tr(1_\pi \rho)$

Quantum map $E_F: E_F(\rho)$ post-measurement density matrix

Complementary measurement of $1_\pi^\#$ is not used

Uniform limit $\pi_j = \frac{1}{4}$ then $1_\pi = 1, 1_\pi^\# = 0$ and $p_\pi = 1$

F model $\rightarrow$ JC model
Likelihood evaluation NP-hard problem!

Classical likelihood
Recursive pruning at all cherries:
Map $\mu : \mathcal{L} \times \mathcal{L} \rightarrow \mathcal{L}$; daughter n. l. $(L_B, L_C) \Rightarrow$ parent n. l.

$$L_A = \mu(L_B, L_C) = (M^B L^B) \circ (M^C L^C) = L^A$$

Stochastic matrices $M^{B,C}(t_B, t_C)$ (branch lengths $t_{B,C}$)

$$L^A_i = (\sum_{j \in \Sigma^*} M^B_{ij}(t_B)L^B_j)(\sum_{k \in \Sigma^*} M^C_{ik}(t_C)L^C_k)$$

Next: alignment of $s$ taxa over $\Lambda$ sites
Characters at site $l$ of alignment: $i_1^{(l)}, i_2^{(l)}, \ldots, i_s^{(l)}$,
Leaf nodes likelihood initialized $L_k^{(l)} = \delta(k, i_k^{(l)})$
Tree likelihood $L_{tr}^{(l)} = (L_{tr}^{(l)} k)_{k=1}^s$ averaged on stationary dist. ($\pi_i$):

$$L^{(l)} = \sum_k \pi_i L_{tr}^{(l)}$$

Entire alignment: **tree (log) likelihood** $L(T; w^*) = \max_w \log \prod_{l=1}^{\Lambda} L^{(l)}$; $T$ tree topology, $w^*$ optimal model weight parameters
Quantum simulation

Likelihoods as quantum observables \( \hat{L} \in \text{Lin}(H) \)
(dual to density operators under the trace inner product)

Likelihood operator at node \( A \): \( \hat{L}^A_i \equiv L^A(t|i) = \mathbb{P}(i|t) \);
\( \mathbb{P}(i|t) \) conditional prob. of character \( i \in \Sigma^* \), parameters \( t = (T, w) \)
Leaf nodes \( A = 1, 2, ..., s \) internal (ancestral) nodes \( A = s + 1, ..., 2s - 2 \)
Likelihood matrix \( \hat{L} \in \text{Lin}(H) \) diagonal in vector basis of characters i.e.
\( \hat{L} = \sum_i L_i \langle i | i \rangle =: \text{diag}(L) \)

Classical to Quantum quantization map for likelihood

Map \( \text{diag} : \mathcal{L} \rightarrow \text{Lin}(H) : L \rightarrow \hat{L} \)
Quantum likelihood 2/3

Classical to Quantum quantization map for pruning

Classical pruning $\mu : \mathcal{L} \times \mathcal{L} \rightarrow \mathcal{L}$
Quantum pruning map $\hat{\mu} : \text{Lin}(H) \otimes \text{Lin}(H) \rightarrow \text{Lin}(H)$

$\hat{\mu}$ should simulate $\mu$ (and not only!)

\[
\begin{array}{c c c}
\mathcal{L} \times \mathcal{L} & \xrightarrow{\mu} & \mathcal{L} \\
\text{diag} \times \text{diag} & \downarrow & \text{diag} \\
\text{Lin}(H) \otimes \text{Lin}(H) & \xrightarrow{\hat{\mu}} & \text{Lin}(H)
\end{array}
\]

$\hat{\mu}$ induces $\mu$ in likelihood vectors

\[
\hat{\mu} = \text{diag} \circ \mu \circ (\text{diag}^{-1} \otimes \text{diag}^{-1})
\]

\[
\hat{\mu}(\hat{L}^B \otimes \hat{L}^C) = \text{diag} \circ \mu(L^B \times L^C) = \text{diag}(L^A) = \hat{L}^A
\]
Quantum implementation of pruning map $\hat{\mu}$

$$\hat{\mu} = Tr_B \circ Ad \ U_{cn}^\dagger \circ \mathcal{E}_{dd} \circ Ad(UB \otimes UC)$$

Unistochastic matrices $M^x(t_x) = U_x \circ U_x^*$, (branch lengths $t_x$) $x = A, B$

Collective CPTP diagonalizing map $\mathcal{E}_{dd}(\cdot) = \sum_k \hat{P}_k \otimes \hat{P}_k(\cdot) \hat{P}_k \otimes \hat{P}_k$
**Tree likelihood quantum simulation**

**Embedding** \( \hat{\mu}_{r,r+1} = id^\otimes r^{-1} \otimes \hat{\mu} \otimes id^\otimes s^{-r} \) according to tree topology

Tree likelihood operator \( \hat{L}^{(l)}_{tr} \) for site \( l \)

Stationary density matrix (sdm) \( \rho^\pi = diag(\pi) = \sum_i \pi_i \hat{P}_i \)

Tree likelihood for alignment’s site \( l \) (averaged with sdm)

\[
L^{(l)} = Tr(\hat{L}^{(l)}_{tr} \rho^\pi) \equiv \langle \hat{L}^{(l)}_{tr}, \rho^\pi \rangle
\]

Entire alignment (log) likelihood (c.f. the identity

\[
Tr(AB) Tr(CD) = Tr(A \otimes C)(B \otimes D)
\]

\[
L = \max_w \log \prod_{l=1}^{\Lambda} \langle \hat{L}^{(l)}_{tr}, \rho^\pi \rangle = \max_w \log Tr(\otimes_{l=1}^{\Lambda} \hat{L}^{(l)}_{tr}) \rho_\Lambda,
\]

Stationary density matrices \( \rho_\Lambda \equiv (\rho^\pi)^\otimes \Lambda \)
Entanglement invariants - Phylogenetic invariants 1/3

Two fully separable mixed states $\rho, \tilde{\rho}$ each describing $s$ taxa are locally equivalent, $\rho \sim \tilde{\rho}$ if there are unitaries $U = \bigotimes_{i=1}^{s} U_i$ such that $\tilde{\rho} = U \rho U^\dagger$.

Local equivalence implies $E_{d}^{\otimes s}(\tilde{\rho}) = E_{d}^{\otimes s}(\rho)$; denoted $p \sim \tilde{p}$.

Case of $s = 3$ taxa

**Proposition** A necessary and sufficient condition for the existence of local equivalence, is that the quantities

$$
I_i^m \equiv \text{Tr}(\rho_i)^m \\
I_i^{km} \equiv \text{Tr}(\xi_i^k)^m \\
I^t \equiv \text{Tr}(\rho^t) \quad m = 1, 2, ..., |\Sigma|, t = 1, 2, ..., |\Sigma|^2,
$$

obtain the same value for $\rho$ and $\tilde{\rho}$. 
Reduced dm $\rho_i = Tr_i \rho$, with $\rho_1 = \sum_{jk} (\sum_i p_{ijk}) \hat{P}_j \otimes \hat{P}_k$ etc
Also if $\rho_i = \sum_s \lambda_s^i |\mu_s^i\rangle \langle \mu_s^i|$ the spectral decomposition of $\rho_i$, then

$\zeta_s^i = Tr_3 |\mu_s^i\rangle \langle \mu_s^i|$

E.g. separable mixed states of 3 taxa: **entanglement invariants** (**Markov invariants**) families in the simplex of probability tensor

$$I^t = \sum_{ijk} p_{ijk}^t, \ t = 1, 2, ..., |\Sigma^*|^2$$

$$I_i^m = \sum_{jk}(\sum_i p_{ijk})^m, \ m = 1, 2, ..., |\Sigma^*|$$

$$I_{ikm} = 1$$
If resuffling matrices in QW chosen e.g. to be equal to
\[ U(z) = \frac{1}{\sqrt{1-|z|^2}} \begin{pmatrix} 1 & z \\ -z^* & 1 \end{pmatrix} \in SU(2)/U(1), z \in CP \]
Probability tensor depends on \( z \in CP : p_{ijk}(z) \) then entanglement invariants \( I^t(z), I^m_i(z) \) **phylogenetic invariants**