On Quantum Simulation of Phylogenetic Prosesses

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Character set $\Sigma = \{0, 1, ..., N\} = \{0\} \cup \Sigma^*$. (0 "null", no character)
Hilbert space of character states $H \approx l_2(\Sigma) = span(|i\rangle\, ; i \in \Sigma)$,
$dimH = |\Sigma|$. **Linear operators** $Lin(H)$ on H
E.g. **projector** $\widehat{P}_i = |i\rangle \langle i|$
Shift operator $h\,|i\rangle = |i +_N 1\rangle$, ($+_N$ addition modulo N; so $h^N = 1$)
Density matrices $\mathcal{D}(H) = \{\rho \in Lin(H), \rho^\dagger = \rho, \rho \geq 0, Tr\rho = 1\}$.
Discrete prob.d. $(p_0, p_1, p_2, ...p_{N-1}) \rightarrow$ diagonal dm

$$\rho = \sum_{i \in \Sigma^*} p_i \widehat{P}_i$$

(in practice $p_0 = 0$, summation $i \in \Sigma^*$).
Control-shift(not) (unitary) $U_{cn} \in Lin(H \otimes H)$, $U_{cn} = \sum_{k \in \Sigma} \widehat{P}_k \otimes h^k$,
action $U_{cn}\,|i\rangle \otimes |j\rangle = |i\rangle \otimes |j +_N i\rangle$

Splitting map Δ

1-taxon density matrix $\rho = \sum_{i\in\Sigma^*} p_i \widehat{P}_i \longrightarrow \Delta\rho$ 2-taxon density matrix

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

where $p_{ij} = p_i\delta_{ij}$.

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

Let s-taxon density matrix

$$\rho = \sum_{i_1,\ldots,i_s\in\Sigma^*} p_{i_1\ldots.i_s}\widehat{P}_{i_1} \otimes \ldots \otimes \widehat{P}_{i_s}$$

Speciation-Phyletic evolution 2/2

Phyletic evolution map

$$\rho \to \widetilde{\rho} \equiv \mathcal{E}_d^{\otimes s}(U \rho U^\dagger) = \mathcal{E}_d^{\otimes s} \circ Ad\, U(\rho)$$

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

$$\begin{aligned} \widetilde{\rho} &= \sum_{i_1, \dots, i_s \in \Sigma^*} \widetilde{p}_{i_1 \dots i_s} \widehat{P}_{i_1} \otimes \dots \otimes \widehat{P}_{i_s}, \\ \widetilde{p}_{i_1 \dots i_s} &= \sum_{j_1, \dots, j_s \in \Sigma^*} p_{j_1 \dots j_s} (M_1 \otimes \dots \otimes M_s)_{i_1 j_1; \dots; i_s j_s}. \end{aligned}$$

(Notation: **adjoint action** $Ad\, S(\cdot) \equiv S(\cdot) S^\dagger$; **Hadamard** or **entry-wise product** of matrices $(A \circ B)_{ij} = A_{ij} B_{ij}$). Phylectic 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 ρ (**decoherent map**)

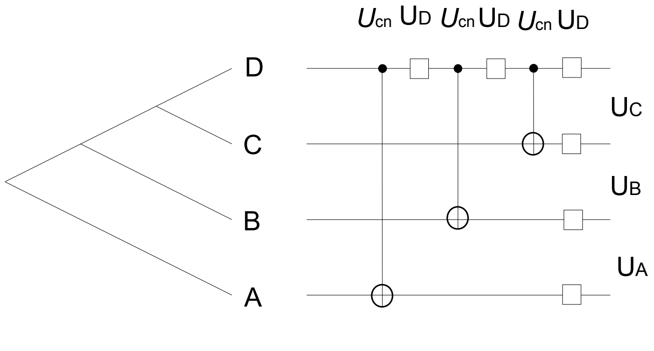
U_{cn} U_D U_{cn} U_D U_{cn} U_D
D
C
B
A
U_C
U_B
U_A

Fig.1a

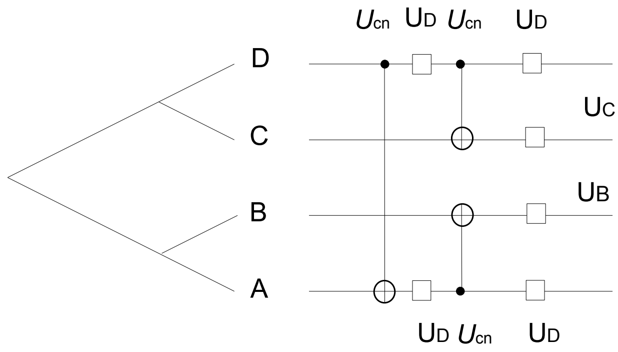
U_{cn} U_D U_{cn} U_D
D
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Fig.1b

Phyletic evolution and quantum walks 1/3

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 $H_c \approx l_2(C) = span(|+\rangle, |-\rangle)$ (at each vertex of phylogenetic tree)
Projectors $P_\pm \in Lin(H_c)$
Coin reshuffling unitary matrix U
Coin-walker states $\rho_c \otimes \rho \quad (\rho_c = |c\rangle \langle c|)$
Conditional unitary $V = (P_+ \otimes h + P_- \otimes h^\dagger) U \otimes \mathbf{1}$ on $H_c \otimes H$

Phyletic evolution and quantum walks 2/3

1-step QW $\mathcal{E} : \mathcal{D}(H) \to \mathcal{D}(H)$ CPTP map
$(\mathcal{E} > 0, id_M \otimes \mathcal{E} > 0, Tr\mathcal{E} = Tr)$

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

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

– **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 $\mathcal{E}_d(\rho) = \sum_{k\in\Sigma^*} \widehat{P}_k \rho \widehat{P}_k$
For s taxa

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

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

$$E_{V^2}(\rho) = \sum_{mn} \widetilde{p}_{mn} \widehat{P}_m \otimes \widehat{P}_n$$

probability tensor

$$\widetilde{p}_{mn} = \sum_{ab} p_{m-a,n-b} q_a^{(c)} q_b^{(c)}$$

discrete pd $q_a^{(c)} := \sum_\gamma M_{j,a-j} M_{j-a,c} \geq 0$
uni-stochastic matrix $M = U \circ U^*$

Hamiltonian implementaions of diagonalizing map

Proposition Diagonalizing map $\mathcal{E}_d$ cast in the form of CPTP map with unitary Kraus generators

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

with $q_k = 1/|\Sigma^*|$. Unitaries U_k related to projectors via discrete Fourier transform, $U_k = \sum_l \omega^{kl} \widehat{P}_l$ and $\omega = \exp(i2\pi/|\Sigma|)$. A unitary dialation of $\mathcal{E}_d$ reads $\mathcal{E}_d(\rho) = Tr_c V_d(\rho_c \otimes \rho) V_d^\dagger$, $V_q = e^{iH}(U_c \otimes \mathbf{1})$, with Hamiltonian $H_{cl} = \sum_{k,l\in\Sigma^*} kl \widehat{P}_k \otimes \widehat{P}_l \otimes \widehat{P}_l$,and $\rho_c = |k\rangle\langle k|$ any $|k\rangle$ canonocal 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 $\rho = \sum_{m\in\Sigma^*} p_m \widehat{P}_m$ 1-taxon density matrix
(Notation $X \equiv \sigma_x$, $Z \equiv \sigma_z$ Pauli sigmas)

Phylogenetic evolutionary models and quantum maps (K,JC) 2/6

Proposition (K,JC;OSR): Let $|\Sigma^*| = 4$ and $\tau \in \{K3, K2, JC\}$

$$\begin{aligned} E_\tau(\rho) &= \sum_{k,l} \lambda^{(\tau)}_{kl} U_{kl}(\rho) U^\dagger_{kl} = \sum_{m\in\Sigma^*} (M_\tau p)_m \widehat{P}_m, \\ M_\tau(a,b,c) &= \sum_{kl} \lambda^{(\tau)}_{kl} U_{kl} \circ U^*_{kl} = \sum_{kl} \lambda^{(\tau)}_{kl} X^k \otimes X^l. \end{aligned}$$

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

$$\begin{aligned} \lambda^{(3K)}_{kl} &= \lambda_{kl}(a,b,c),\ M_{3K} \equiv M(a,b,c) \\ \lambda^{(2K)}_{kl} &= \lambda_{kl}(a,b,b),\ M_{2K} \equiv M(a,b,b) \end{aligned}$$

$$\lambda^{(JC)}_{kl} = \lambda_{kl}(a,a,a),\ M_{JC} \equiv M(a,a,a)$$

Phylogenetic evolutionary models and quantum maps (K,JC) 3/6

Proposition (K,JC;UD): The CPTP map E_τ 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

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

which acts on a composite coin-walker space $H_c \otimes H$, with $4D$ ancillary space. Here V_τ 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_τ 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 $\mathcal{H}_{kl} = \frac{1}{2}\pi[-(k+l)\mathbf{1} \otimes \mathbf{1} + kX \otimes \mathbf{1} + l\mathbf{1} \otimes X]$. □

Phylogenetic evolutionary models and quantum maps (B) 4/6

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 $\rho = \sum_{m\in\Sigma^*} p_m \widehat{P}_m \to \sum_{m\in\Sigma^*} (M_B\, p)_m \widehat{P}_m$. □

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 $\rho_c = |1\rangle\langle 1|$, and $V_B = \sqrt{a}\mathbf{1}\otimes\mathbf{1} + \sqrt{1-a} Y \otimes X$, and $Y \equiv ZX$. □

Phylogenetic evolutionary models and quantum maps (F) 5/6

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

Proposition (F,OSR): Quantum map $\rho \to E_F(\rho) = \sum_{m\in\Sigma^*}(M_F\,p)_m \widehat{P}_m$ 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 : $E_F(\mathbf{1}) \neq \mathbf{1}$
Row-stochastic matrix $M_F = (1-a)\sum_{i,j} F_{ij} \circ F_{ij} + a\mathbf{1}$

Measuring probability $p_\pi = Tr(\sum_{i,j} F_{ij}^\dagger F_{ij}\rho) = Tr(\frac{1}{4}\mathbf{1}_\pi\rho)$

Phylogenetic evolutionary models and quantum maps (F) 6/6

Framework of quantum measurement theory
Two observables: $\mathbf{1}_\pi$ as above, and $\mathbf{1}_\pi^\# = \mathbf{1}_H - \mathbf{1}_\pi$ complementary pd $(\pi_1^\#, \pi_2^\#, \pi_3^\#, \pi_4^\#)$
Non-orthogonal decomposition of unity $\mathbf{1}_H = \mathbf{1}_\pi + \mathbf{1}_\pi^\#$
Observables $\mathbf{1}_\pi, \mathbf{1}_\pi^\#$ measured by means of the so called *instruments* : families of Kraus g. $\{F_{ij}\}_{i,j=0}^1$, $\{F_{ij}^\#\}_{i,j=0}^1$

Measurement probabilities: $p_\pi^\# = Tr(\mathbf{1}_\pi^\# \rho)$, $p_\pi = Tr(\mathbf{1}_\pi \rho)$
Quantum map E_F : $E_F(\rho)$ post-measurement density matrix
Complementary measurement of $\mathbf{1}_\pi^\#$ is not used
Uniform limit $\pi_j = \frac{1}{4}$ then $\mathbf{1}_\pi = \mathbf{1}$, $\mathbf{1}_\pi^\# = \mathbf{0}$ and $p_\pi = 1$
F model $\Longrightarrow$ JC model

Classical likelihood estimation 1/2

Likelihood evaluation NP-hard problem!

Classical likelihood
Recursive pruning at all cherries:
Map $\mu : \mathcal{L} \times \mathcal{L} \to \mathcal{L}$; 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 $M^{B,C}(t_{B,C})$ (branch lengths $t_{B,C}$)

$$L_i^A = (\sum_{j \in \Sigma^*} M_{ij}^B(t_B) L_j^B)(\sum_{k \in \Sigma^*} M_{ik}^C(t_C) L_k^C)$$

Next: **alignment** of s taxa over Λ sites
Characters at site l of alignment: $i_1^{(l)} i_2^{(l)} \ldots i_s^{(l)}$,
Leaf nodes likelihood initialized $L_k^{(l)} = \delta(k, i_k^{(l)})$

Classical likelihood 2/2

Tree likelihood $L_{tr}^{(l)} = (L_{tr\ k}^{(l)})_{k=1}^{s}$ averaged on stationary dist. (π_i) :

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

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

Quantum likelihood 1/3

Quantum simulation
Likelihoods as quantum observables $\widehat{L} \in Lin(H)$
(dual to density operators under the trace inner product)

Likelihood operator at node A : $\widehat{L}_i^A \equiv L^A(t|i) = \mathbb{P}(i|t)$;
$\mathbb{P}(i|t)$ 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 $\widehat{L} \in Lin(H)$ diagonal in vector basis of characters i.e.
$\widehat{L} = \sum_i L_i \left| i \right\rangle \left\langle i \right| =: diag(L)$

Classical to Quantum quantization map for likelihood
Map $diag : \mathcal{L} \rightarrow Lin(H) : L \rightarrow \widehat{L}$

Classical to Quantum quantization map for pruning
Classical pruning $\mu : \mathcal{L} \times \mathcal{L} \rightarrow \mathcal{L}$
Quantum pruning map $\widehat{\mu} : Lin(H) \otimes Lin(H) \rightarrow Lin(H)$
$\widehat{\mu}$ should simulated μ **(and not only!)**

$$
\begin{array}{ccccc}
 & \mathcal{L} \times \mathcal{L} & \stackrel{\mu}{\rightarrow} & \mathcal{L} & \\
diag \times diag & \downarrow & & \downarrow & diag \\
 & Lin(H) \otimes Lin(H) & \underset{\widehat{\mu}}{\rightarrow} & Lin(H) &
\end{array}
$$

$\widehat{\mu}$ induces μ in likelihood vectors

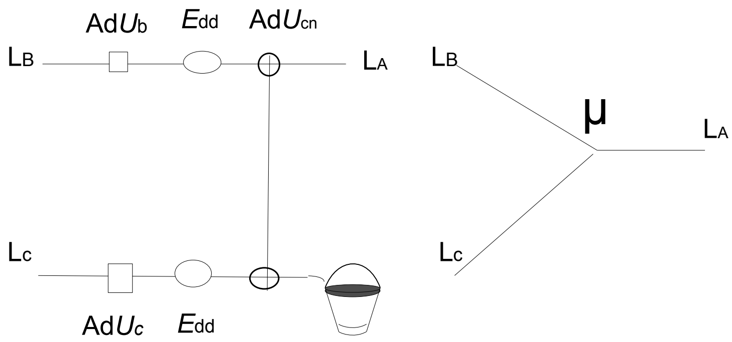
$$
\begin{aligned}
\widehat{\mu} &= diag \circ \mu \circ (diag^{-1} \otimes diag^{-1}) \\
\widehat{\mu}(\widehat{L}^B \otimes \widehat{L}^C) &= diag \circ \mu(L^B \times L^C) = diag(L^A) = \widehat{L}^A
\end{aligned}
$$

Quantum likelihood 3/3

Quantum implementation of pruning map $\widehat{\mu}$

$$\widehat{\mu} = Tr_B \circ Ad\, U_{cn}^{\dagger} \circ \mathcal{E}_{dd} \circ Ad(U_B \otimes U_C)$$

Unistochastic matrices $M^x(t_x) = U_x \circ U_x^*$, (branch lengths t_x) $x = A, B$
Collective CPTP *diagonalizing map* $\mathcal{E}_{dd}(\cdot) = \sum_k \widehat{P}_k \otimes \widehat{P}_k(\cdot)\widehat{P}_k \otimes \widehat{P}_k$



AdUb
Edd
AdUcn
LB
LA
LC
AdUc
Edd
LB
μ
LA
LC

Tree likelihood quantum simulation

Embedding $\widehat{\mu}_{r,r+1} = id^{\otimes r-1} \otimes \widehat{\mu} \otimes id^{\otimes s-r}$ according to tree topology
Tree likelihood operator $\widehat{L}_{tr}^{(l)}$ for site l
Stationary density matrix (sdm) $\rho^{\pi} = diag(\pi) = \sum_i \pi_i \widehat{P}_i$
Tree likelihood for alignment's site l (averaged with sdm)

$$L^{(l)} = Tr(\widehat{L}_{tr}^{(l)} \rho^{\pi}) \equiv \left\langle \widehat{L}_{tr}^{(l)}, \rho^{\pi} \right\rangle$$

Entire alignment (log) likelihood (c.f. the identity $Tr(AB)\,Tr(CD) = Tr(A \otimes C)(B \otimes D)$)

$$L = \max_{w} \log \prod_{l=1}^{\Lambda} \left\langle \widehat{L}_{tr}^{(l)}, \rho^{\pi} \right\rangle = \max_{w} \log Tr(\otimes_{l=1}^{\Lambda} \widehat{L}_{tr}^{(l)}) \rho_{\Lambda}),$$

Stationary density matrices $\rho_{\Lambda} \equiv (\rho^{\pi})^{\otimes \Lambda}$

Entanglement invariants - Phylogenetic invariants 1/3

Two fully separable mixed states ρ, $\widetilde{\rho}$ each describing s taxa are locally equivalent, $\rho \sim \widetilde{\rho}$
if there are unitaries $U = \bigotimes_{i=1}^{s} U_i$ such that $\widetilde{\rho} = U \rho U^{\dagger}$.
Local equivalence implies $E_d^{\otimes s}(\widetilde{\rho}) = E_d^{\otimes s}(\rho)$; denoted $p \sim \widetilde{p}$.
Case of $s = 3$ taxa
Proposition A necessary and sufficient condition for the existence of local equivalence, is that the quantities

$$\begin{aligned} I_i^m &\equiv Tr(\rho_i)^m \\ I_i^{km} &\equiv Tr(\xi_i^k)^m \\ I^t &\equiv Tr(\rho^t) \qquad m = 1, 2, ..., |\Sigma|\,, t = 1, 2, ..., |\Sigma|^2\,, \end{aligned}$$

obtain the same value for ρ and $\widetilde{\rho}$.

Entanglement invariants - Phylogenetic invariants 2/3

Reduced dm $\rho_i = Tr_i \rho$, with $\rho_1 = \sum_{jk}(\sum_i p_{ijk})\widehat{P}_j \otimes \widehat{P}_k$ etc
Also if $\rho_i = \sum_s \lambda_s^i \left|\mu_s^i\right\rangle \left\langle\mu_s^i\right|$ the spectral decomposition of ρ_i, then

$\xi_s^i = Tr_3 \left|\mu_s^i\right\rangle \left\langle\mu_s^i\right|$
E.g. separable mixed states of 3 taxa: **entanglement invariants** (**Markov invariants**) families in the simplex of probability tensor

$$\begin{aligned} I^t &= \sum_{ijk} p_{ijk}^t,\ t = 1, 2, ..., |\Sigma^*|^2 \\ I_i^m &= \sum_{jk}(\sum_i p_{ijk})^m, m = 1, 2, ..., |\Sigma^*| \\ I_i^{km} &= 1 \end{aligned}$$

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 $I^t(z)$, $I_i^m(z)$ **phylogenetic invariants**