Quantum field theory and phylogenetic branching

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A calculational framework is proposed for phylogenetics, using nonlocal quantum field theories in hypercubic geometry. Quadratic terms in the Hamiltonian give the underlying Markov dynamics, while higher degree terms represent branching events. The spatial dimension $L$ is the number of leaves of the evolutionary tree under consideration. Momentum conservation modulo $\mathbb{Z}_2^L$ in $L \leftarrow 1$ scattering corresponds to tree edge labelling using binary $L$-vectors. The bilocal quadratic term allows for momentum-dependent rate constants – only the tree or trees compatible with selected nonzero edge rates contribute to the branching probability distribution. Applications to models of evolutionary branching processes are discussed.
Evolutionary processes are frequently represented as discrete or continuous time stationary Markov dynamics on some relevant set of system characters. Divergence events correspond to the initiation of two or more sibling processes, which each inherit the character probability distribution of the progenitor and then continue to evolve. It is the task of phylogenetic inference to deduce ancestral interrelationships given observed character probability distributions.

Although the individual ingredients for modelling such branching trees are quite well understood (see for example [1, 2]), to date there is no overall dynamical picture for phylogenetics. In this note we point out that existing tools from physics – namely, quantum field theory and quantum many body theory when suitably interpreted in a stochastic context [3, 4, 5] – can provide both a theoretical perspective and a calculational framework. Below we sketch a general outline of our proposed model; details will be published in a separate paper.

Consider a theory with Hamiltonian of the general form

$$\mathcal{H}(t) = \mathcal{H}_0 + \mathcal{H}_1(t),$$

with

$$\mathcal{H}_0 = \sum_{x,y} \sum_{\alpha,\beta} \Psi_{\alpha}^\dagger(x) M_{\alpha \beta}(x-y) \Psi_{\beta}(y),$$

$$\mathcal{H}_1(t) = \sum_{x,I} \delta(t - t_I) \left( \sum_\alpha W_{\alpha I}^t \Psi_{\alpha}^\dagger(x) \Psi_{\alpha}(x) - \sum_{\alpha,\beta,\gamma} V_{\alpha \beta \gamma I}^t \Psi_{\alpha}^\dagger(x) \Psi_{\beta}^\dagger(x) \Psi_{\gamma}(x) \right),$$

for quantised fields $\Psi_{\alpha}(x)$ of type $\alpha = 1, \ldots, K$. The sum is taken over vertices of a unit hypercube $x, y \in \mathbb{Z}_2^L$, and the theory is manifestly translation invariant under $x \rightarrow x + a$, for $a \in \mathbb{Z}_2^L$. The interaction times $t_I$ are temporally ordered as $0 = t_0 < t_1 < t_2 < \ldots < t_M < t_{M+1} = T$ where $T$ is the total time for the evolution. As will be seen below, cubic interaction terms generate branching events, with the additional quadratic terms necessary to ensure that the theory is overall probability conserving [3].

Quantisation is imposed in such a way that the time evolution generated by the quadratic Hamiltonian $\mathcal{H}_0$ reproduces the standard Markov dynamics on each mode of the field. Consider the following expansions in momentum space $\mathbb{Z}_2^L$:

$$M_{\alpha \beta}(x-y) = \lambda(x-y) M_{\alpha \beta}, \quad \lambda(z) = \sum_k \lambda(k) e^{i\pi k \cdot z},$$

$$\Psi_{\alpha}(x) = \sum_k e^{i\pi k \cdot x} c_{\alpha}(k).$$

Basis states of the system are Fock states of the form

$$|\alpha_1 k_1, \alpha_2 k_2, \ldots, \alpha_N k_N\rangle = c_{\alpha_1}^\dagger(k_1) c_{\alpha_2}^\dagger(k_2) \cdots c_{\alpha_N}^\dagger(k_N) |0\rangle,$$

where the vacuum is defined as usual by the property of being annihilated by the modes $c_{\alpha}(k)$. For the evolution of states $|P(t)\rangle$ under the time independent Hamiltonian $\mathcal{H}_0$, the solution of Schrödinger’s equation

$$\frac{d}{dt} |P(t)\rangle = -\mathcal{H}_0 |P(t)\rangle$$

for evolution after time $T$, namely

$$|P(T)\rangle = e^{-\mathcal{H}_0 T} |P(0)\rangle,$$
must be computed with the help of the canonical commutation relations of the field. At this stage it is only necessary to impose the trilinear condition:

$$\sum_k [c^\dagger_\alpha(k)c_\beta(k), c_\gamma(\ell)] = \delta^\alpha_\gamma c_\beta(\ell). \quad (6)$$

Consider for example separable states such as

$$|p(k_1, t)\rangle \otimes |p(k_2, t)\rangle \otimes \ldots \otimes |p(k_N, t)\rangle \quad (7)$$

representing a number of processes evolving in parallel, with each $|p(k, t)\rangle$ a single-particle state corresponding to a probability distribution for characters of an individual process,

$$|p(k, t)\rangle = \sum_\alpha p_\alpha(k, t)|\alpha k\rangle. \quad (8)$$

With (3), (6), either fermionic or bosonic quantisation lead to the time evolution of (7) such that the probability distribution of each individual mode is given by the solution of the appropriate classical master equation,

$$p_\alpha(k, T) = (e^{-\lambda(k)T \cdot M})_\alpha^\beta p_\beta(k, 0) \equiv U(k)_\alpha^\beta p_\beta(k, 0). \quad (9)$$

Turning to the full, time-dependent Hamiltonian $\mathcal{H}(t) = \mathcal{H}_0 + \mathcal{H}_1(t)$, (3) must be replaced by the time ordered exponential

$$|P(T)\rangle = \mathbb{T}e^{-\int_0^T dt \mathcal{H}(t)}|P(0)\rangle, \quad (10)$$

which in turn is expressible in the usual way as sums of multiple integrals of time-ordered products $\ldots \mathcal{H}(t')\mathcal{H}(t'') \ldots$. Consider in particular the $L \leftarrow 1$ process, and its evolution kernel representing the corresponding probability distribution of characters. Choose the distinct outgoing momenta in some ordering to be the simple binary vectors $(0, 0, \ldots, 1), (0, \ldots, 1, 0), \ldots$, and $(1, 0, \ldots, 0)$ respectively. Since momentum conservation modulo $\mathbb{Z}_2^L$ must hold by translation invariance, this fixes the incoming momentum to be the maximal value $(1, 1, \ldots, 1)$. The probability distribution is then a sum over all terms generated by the expansion of the time ordered exponential. Contributions from admissible tree diagrams are enumerated by labelling edges with momenta $k$, with vertices for interaction times $t_I$ having one incoming and two outgoing momenta $k, k', k''$. Along edges, the probability distribution $p_\alpha(k, t)$ evolves via (3) for the appropriate time intervals $\Delta_{IJ} = (t_J - t_I)$ for $I < J$, so that the effective rate constant is $\kappa(k) \equiv \lambda(k)\Delta_{IJ}$. At vertices, momentum conservation ensures that a particular character type splits with appropriate sharing of the probability and type between the two subsequent edges (with momenta such that $k = k' + k''$). A plausible description of the divergence event is $V_{\alpha\beta}^{\gamma\delta} \equiv \delta^\gamma_\alpha \delta^\delta_\beta$, which means that the two sibling processes commence evolution on their respective edges with characters distributed identically to that of their progenitor. Clearly, the model admits further generalisation to nondiagonal or even trilocal or time-smeared interaction terms. Note that the additional diagonal quadratic terms in $\mathcal{H}_1(t)$ are necessary to ensure that the theory is overall probability conserving but do not contribute to the tree diagrams.
under consideration. The question of which tree or trees contribute to $L \leftarrow 1$ scattering is encoded in the bilocal form of $\mathcal{H}_0$ (see (1)). Only momenta $k$ corresponding to nonzero rate constants $\lambda(k)$ are allowed. For computation based on a given tree, it is thus possible to choose nonzero rate constants $\lambda(k)$ for selected momenta corresponding to the binary edge labelling unique to that tree’s topology [2].

As an illustration, consider the case $L = 3$, $M = 2$. Nonzero rate constants for the model [2] are chosen for the root and leaf momenta $\vec{7} = (111)$, $\vec{1} = (001)$, $\vec{2} = (010)$ and $\vec{4} = (100)$ respectively, together with a single additional momentum $\vec{6} = (110)$ (see figure 4). Write $\mathcal{H}_1(t) = \mathcal{V}_1^1 \delta(t-t_1) + \mathcal{V}_2^2 \delta(t-t_2)$. The time ordered exponential in (10) may be written as a product,

$$\mathcal{T} e^{-\int_0^T dt \mathcal{H}(t)} = \mathcal{T} e^{-\int_{t_1}^T dt \mathcal{H}(t)} V_2 \mathcal{T} e^{-\int_{t_1}^{t_2} dt \mathcal{H}(t)} V_1 \mathcal{T} e^{-\int_0^{t_1} dt \mathcal{H}(t)},$$

(11)

where $V_I$ are time ordered exponentials for small intervals $\delta_I$ covering $t_I$. These have the form $1 - \mathcal{H}_0 \delta_I - \mathcal{V}_I + \cdots$, the higher order terms being ordered monomials in $\mathcal{H}_0$ and $\mathcal{V}_I$ multiplied by nested $\delta$-function integrals. In the limit $\delta_I \to 0$, 

$$\mathcal{T} e^{-\int_0^T dt \mathcal{H}(t)} = e^{-\mathcal{H}_0(T-t_2)}(1 - \mathcal{V}_2^2 + \cdots) e^{-\mathcal{H}_0(t_2-t_1)}(1 - \mathcal{V}_1^1 + \cdots) e^{-\mathcal{H}_0 t_1}.$$  

(12)

Clearly the contribution to the $3 \leftarrow 1$ scattering probability associated with the tree of figure 4 is, as required, the unique nonzero term arising from inserting intermediate states in the above with the correct intermediate edge momenta, giving finally

$$\langle \alpha_1 \beta_1 \gamma_1 \delta_1^2 \alpha_2 \beta_2 \delta_2^2 | e^{-\mathcal{H}_0(T-t_2)} \mathcal{V}_2^2 e^{-\mathcal{H}_0(t_2-t_1)} \mathcal{V}_1^1 e^{-\mathcal{H}_0 t_1} | p(\vec{7}, 0) \rangle =$$

$$\sum U(\kappa_2) \alpha_2^{\beta_2} U(\kappa_4) \alpha_4^{\beta_4} \gamma_6 \cdot U(\kappa_6) \beta_6^\gamma U(\kappa_1) \alpha_1^{\beta_1} \mathcal{V}_1^1 \beta_7^\gamma \cdot U(\kappa_7) \beta_7^\alpha \alpha_1^\gamma p_0(\vec{7}, 0).$$

In phylogenetics, the probability distributions or dispersion tensors of characters of interest are given directly from observations. Whether these are compatible with calculations for a specific tree remains a question of statistics. Our model [2] relates phylogenetic inference for evolutionary processes to a scattering problem for the associated quantum field theory. Recent work using Fourier-Hadamard inversion techniques for phylogenetic reconstruction in molecular phylogenetics [4, 8] can be interpreted in our model as working with position states rather than in the momentum representation.

The overall calculational framework provided by giving a definite dynamical model for the branching process has potentially wide applicability. The picture can be extended in practice by embellishment of various features. As already mentioned, these include for example vertex decorations. A further possibility is a perturbative expansion of the quadratic term to compute the modulation of systematic substitution frequency types by the effects of Poissonian background rates. Details of the model, and prospects for such extensions, will be published in a separate paper.

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Figure 1: Binary labelling scheme for a tree on 3 leaves ($L = 3$) with branching events at intermediate times $t_1, t_2$. Nonzero rate constants for the model (1) are chosen for the root and leaf momenta $\vec{7} = (111)$, $\vec{1} = (001)$, $\vec{2} = (010)$ and $\vec{4} = (100)$ respectively, together with a single additional momentum $\vec{6} = (110)$. 