Functional solutions of stochastic problems

Juha Honkonen, University of Helsinki

July 23-24, 2023

Outline

Second quantization of master equation

Functional integral, coherent-state construction

Functional integral, perturbation theory

Master equation

Second quantization of master equation
▷ Master equation
Verhulst model (directed percolation)
Fock space for master equation
Liouville operator
Expected values
Initial Poisson distribution
Functional integral, coherent-state construction
Functional integral, perturbation theory

Markov processes of discrete variables are described by master equations.

Consider a *jump process* (birth-death process), whose PDF obey a generic master equation

$$\frac{\partial}{\partial t}P\left(n,t|m,t_0\right) = \sum_l \left[W(n|l,t)P\left(l,t|m,t_0\right) - W(l|n,t)P\left(n,t|m,t_0\right)\right] .$$

Transition probabilities per unit time $W(n|l,t)$ are usually given in the model.

Calculation of expected values in terms of QFT due to Doi.

Verhulst model (directed percolation)

Expected value of individuals obeys the *rate equation*

$$\frac{\mathrm{d}n}{\mathrm{d}t} = -\beta n + \lambda n - \gamma n^2 \,.$$

In the stochastic version (due to Feller) the PDFs obey

$$\begin{aligned}
\frac{\mathrm{d}P(t,N)}{\mathrm{d}t} &= \lambda(N-1)P(t,N-1) - \left(\beta N + \gamma N^2\right) P(t,N)\,,\\
\frac{\mathrm{d}P(t,n)}{\mathrm{d}t} &= [\beta(n+1) + \gamma(n+1)^2]P(t,n+1) + \lambda(n-1)P(t,n-1)\\
&\quad - \left(\beta n + \lambda n + \gamma n^2\right) P(t,n)\,, \quad 0 < n < N\,,\\
\frac{\mathrm{d}P(t,0)}{\mathrm{d}t} &= (\beta+\gamma)P(t,1)\,.
\end{aligned}$$

Reflecting upper and absorbing lower boundary. Percolation: unbounded from above.

Fock space for master equation

Second quantization of master equation
Master equation
Verhulst model (directed percolation)
▷ Fock space for master equation
Liouville operator
Expected values
Initial Poisson distribution
Functional integral, coherent-state construction
Functional integral, perturbation theory

The set of master equations for $P(t,n)$ is reduced to a single equation by "second quantization" of Doi.

Fock space: operators $\hat{a}$, $\hat{a}^+$, $[\hat{a}, \hat{a}^+] = 1$ and basis vectors $|\, n \,\rangle$:

$$\hat{a}|\, 0 \,\rangle = 0\,, \quad \hat{a}^+|\, n \,\rangle = |\, n{+}1 \,\rangle\,, \quad \hat{a}^+\hat{a}|\, n \,\rangle = n|\, n \,\rangle\,, \quad \langle\, n \,|\, m \,\rangle = n!\delta_n$$

Master equations yield kinetic equation for state vector $|\, P_t \,\rangle$:

$$|\, P_t \,\rangle = \sum_{n=0}^{\infty} P(t,n)|\, n \,\rangle\,, \quad \frac{\mathrm{d}|\, P_t \,\rangle}{\mathrm{d}t} = \hat{L}(\hat{a}^+,\, \hat{a})|\, P_t \,\rangle\,.$$

Formal solution is generated by the *Liouville operator* $\hat{L}$:

$$|\, P_t \,\rangle = \exp\left[t\hat{L}(\hat{a}^+,\, \hat{a})\right]|\, P_0 \,\rangle\,,$$

Liouville operator

Second quantization of master equation
Master equation
Verhulst model (directed percolation)
Fock space for master equation
▷ Liouville operator
Expected values
Initial Poisson distribution
Functional integral, coherent-state construction
Functional integral, perturbation theory

Liouville operator $\hat{L}$ is determined by the set of master equations; basic rules of construction:

$$nP(t,n)|\,n\,\rangle = \hat{a}^{+}\hat{a}P(t,n)|\,n\,\rangle,$$
$$nP(t,n)|\,n-1\,\rangle = \hat{a}P(t,n)|\,n\,\rangle\,,$$
$$nP(t,n)|\,n+1\,\rangle = \hat{a}^{+}\hat{a}^{+}\hat{a}P(t,n)|\,n\,\rangle\,.$$

Liouville operator for the Verhulst model:

$$\hat{L}(\hat{a}^{+},\hat{a}) = \beta(I-\hat{a}^{+})\hat{a} + \gamma(I-\hat{a}^{+})\hat{a}\hat{a}^{+}\hat{a} + \lambda(\hat{a}^{+}-I)\hat{a}^{+}\hat{a}\,.$$

Normal form is needed for simple calculation of coherent matrix elements of Liouvillian. In the third term $[\,\hat{a},\hat{a}^{+}] = 1$ yields

$$\hat{L}'(\hat{a}^{+},\hat{a}) = (\beta+\gamma)(I-\hat{a}^{+})\hat{a} + \gamma(I-\hat{a}^{+})\hat{a}^{+}\hat{a}\hat{a} + \lambda(\hat{a}^{+}-I)\hat{a}^{+}\hat{a}\,.$$

Expected values

Expected values obtained with the use of the projection vector $\langle\, P\,|$:

$$\langle\, P\,| = \sum_{n=0}^{\infty} \frac{1}{n!}\,\langle\, n\,| = \sum_{n=0}^{\infty} \frac{1}{n!}\,\langle\, 0\,|\hat{a}^n\,, \quad \langle\, P\,|\,\hat{a}^+ = \langle\, P\,|\,, \quad \langle\, P\,|\,n\,\rangle = 1\,,$$

$$\langle\, P\,|O(\hat{a}^+\hat{a})|\,P_t\,\rangle = \langle\, P\,|\sum_{n=0}^{\infty} O(n)P(t,n)|\,n\,\rangle = \sum_{n=0}^{\infty} O(n)P(t,n)$$

Conservation of probability: the leftmost factor in all monomials of the Liouville operator is $(I-\hat{a}^+)$, thus $\langle\, P\,|\hat{L} = 0\,.$

Doi shift: use $(\exp\hat{a})\,\hat{a}^+ = (\hat{a}^+ + I)\exp\hat{a}$ to move $\exp\hat{a}$ of $\langle\, P\,|$ to the left:

$$\begin{aligned}\langle\, P\,|O(\hat{a}^+\hat{a})\exp\!\left[t\hat{L}(\hat{a}^+,\,\hat{a})\right]|\,P_0\,\rangle \\ = \langle\, 0\,|O((\hat{a}^+ + I)\hat{a})\exp\!\left[t\hat{L}(\hat{a}^+ + I,\,\hat{a})\right]\exp\hat{a}|\,P_0\,\rangle\,.\end{aligned}$$

Initial Poisson distribution

Second quantization of master equation
Master equation
Verhulst model (directed percolation)
Fock space for master equation
Liouville operator
Expected values
▷ Initial Poisson distribution
Functional integral, coherent-state construction
Functional integral, perturbation theory

It is customary to use initial Poisson distribution

$$P(0,n) = \frac{n_0^n e^{-n_0}}{n!} \,.$$

Leftmost factor in expected value assumes convenient form

$$\exp \hat{a} |\, P_0 \,\rangle = \exp \hat{a} \sum_{n=0}^{\infty} P(0,n) |\, n \,\rangle = \exp(n_0 \hat{a}^+) |\, 0 \,\rangle \,.$$

Polynomial distribution obtained by derivatives wrt n_0. Seeding a single particle: $P(0,1) = 1\,; P(0,n) = 0\,, n \neq 0$ corresponds to

$$(\exp \hat{a}) \hat{a}^+ |\, 0 \,\rangle = (\hat{a}^+ + I) |\, 0 \,\rangle = \left[\left(\frac{\partial}{\partial n_0} + I \right) \exp(n_0 \hat{a}^+) |\, 0 \,\rangle \right] \bigg|_{n_0=0} \,.$$

Coherent states

Second quantization of master equation

Functional integral, coherent-state construction

▷ Coherent states

Interpolation procedure for generating function

Expansion in time increment

Approximate functional integral

"Superfluous" terms and ambiguity of functional integral

Functional integral, perturbation theory

Interpolation of functional integral by coherent states ($\phi \in \mathbf{C}$)

$$
|\,\Phi\,\rangle = \sum_{n=0}^{\infty} \frac{1}{n!}\,\phi^n \left(\hat{a}^+\right)^n |\,0\,\rangle = \exp(\phi\hat{a}^+)\,|\,0\,\rangle ; \quad \hat{a}\,|\,\Phi\,\rangle = \phi\,|\,\Phi\,\rangle \,.
$$

Normalization of $|\,\Phi\,\rangle$ varies; here $\langle\,\Phi\,|\,\Phi'\,\rangle = \exp(\phi^*\phi')\,.$

Resolution of the unity

$$
I = \iint \frac{d\phi d\phi^*}{2i\pi} \exp(-\phi^*\phi)|\,\Phi\,\rangle\langle\,\Phi\,|\,.
$$

Coherent-state matrix element of operator in normal form

$$
\langle\,\Phi\,|\hat{L}'(\hat{a}^+,\hat{a})|\,\Phi'\,\rangle = L'(\phi^*,\phi)\exp(\phi^*\phi')\,.
$$

Interpolation procedure for generating function

Generating function of expected values (normal form operators, initial Poisson; A^*, N_0 are coherent state parameters)

$$G(A,A^*) = \langle\, A \,|\, \exp A \exp\big[t\hat{L}'(\hat{a}^+ + I,\, \hat{a})\big] |\, N_0 \,\rangle\,.$$

Introduce coherent-state resolutions of unities to obtain

$$G(A,A^*) = \iint \frac{d\phi_N d\phi_N^*}{2i\pi} \iint \frac{d\phi_0 d\phi_0^*}{2i\pi} \langle\, A \,|\, \exp(A - \phi_N^*\phi_N - \phi_0^*\phi_0) |\, \Phi_N \,\rangle$$
$$\times \langle\, \Phi_n \,|\, \exp\big[t\hat{L}'(\hat{a}^+ + I,\, \hat{a})\big] |\, \Phi_0 \,\rangle \langle\, \Phi_0 \,|\, N_0 \,\rangle = \iint \frac{d\phi_N d\phi_N^*}{2i\pi} \iint \frac{d\phi_0 d\phi_0^*}{2i\pi}$$
$$\times \exp(A^*\phi_N + A - \phi_N^*\phi_N - \phi_0^*\phi_0 + \phi_0^* n_0) \langle\, \Phi_N \,|\, \exp\big[t\hat{L}'(\hat{a}^+ + I,\, \hat{a})\big] |\, \Phi_0 \,\rangle\,.$$

Expansion in time increment

Second quantization of master equation

Functional integral, coherent-state construction

Coherent states

Interpolation procedure for generating function

▷ Expansion in time increment

Approximate functional integral

"Superfluous" terms and ambiguity of functional integral

Functional integral, perturbation theory

Split evolution exponential

$$\exp\Big[t\hat{L}'(\hat{a}^+ + I,\, \hat{a})\Big] = \Big\{\exp\Big[\hat{L}'(\hat{a}^+ + I,\, \hat{a})t/N\Big]\Big\}^N .$$

Introduce resolutions of unities in between. Approximate matrix elements and exponentiate

$$\begin{aligned}
&\langle\, \Phi_i \,|\, \exp\Big[\hat{L}'(\hat{a}^+ + I, \hat{a})t/N\Big] |\, \Phi_{i-1}\,\rangle \\
&\approx \langle\, \Phi_i \,|\Big[1 + \hat{L}'(\hat{a}^+ + I, \hat{a})t/N\Big] |\, \Phi_{i-1}\,\rangle \\
&= [1 + L'(\phi_i^* + 1, \phi_{i-1})t/N] \exp(\phi_i^*\phi_{i-1}) \\
&\qquad\qquad \approx \exp\left[\phi_i^*\phi_{i-1} + L'(\phi_i^* + 1, \phi_{i-1})t/N\right] .
\end{aligned}$$

Approximate functional integral

Second quantization of master equation

Functional integral, coherent-state construction

Coherent states
Interpolation procedure for generating function
Expansion in time increment
▷ Approximate functional integral
"Superfluous" terms and ambiguity of functional integral

Functional integral, perturbation theory

Interpolation through coherent-state unity resolutions yields

$$G(A,A^*) = \iint \frac{d\phi_0 d\phi_0^*}{2i\pi} \prod_{n=1}^{N} \iint \frac{d\phi_n d\phi_n^*}{2i\pi} \exp\Big[A^*\phi_N + A + \phi_0^* n_0 - \phi_0^*\phi_0 - \phi_n^*(\phi_n - \phi_{n-1}) + L'(\phi_n^*+1, \phi_{n-1}) t/N\Big] \,.$$

Integral sum in exponential yields dynamic action

$$\sum_{n=1}^{N} [-\phi_n^*(\phi_n - \phi_{n-1}) + L'(\phi_n^*+1, \phi_{n-1}) t/N]$$

$$= \sum_{n=1}^{N} \left[-\phi_n^* \frac{\phi_n - \phi_{n-1}}{\Delta t} + L'(\phi_n^*+1, \phi_{n-1})\Delta t\right]$$

$$\xrightarrow[\Delta t \to 0]{} \int_0^t \left[-\phi^*(u)\frac{\partial \phi}{\partial u} + L'(\phi^*(u)+1, \phi(u))\right] du \,.$$

"Superfluous" terms and ambiguity of functional integral

Second quantization of master equation

Functional integral, coherent-state construction

Coherent states
Interpolation procedure for generating function
Expansion in time increment
Approximate functional integral
▷ "Superfluous" terms and ambiguity of functional integral

Functional integral, perturbation theory

Derivatives wrt souce terms $A^*\phi(t) + A + n_0\phi^*$ specify the averaged quantity and initial condition.

The term $-\phi(0)^*\phi(0)$ is not included in the time integral. Without the Doi shift we would have had $-\phi(t)^*\phi(t)$.

This term is necessary for perturbation theory. Perturbation theory is important in practical calculations and because "correctly defining the path integral is equivalent to constructing a renormalized perturbation theory" (A. A Slavnov & L. D. Faddeev).

The customary normal ordering of operators has been used. There is no such operator ordering in the classical problem.

Perturbation theory, however, is unambiguous.

Second quantization of master equation

Functional integral, coherent-state construction

Functional integral, perturbation theory

▷ Perturbation theory

Gaussian integral of the discretized problem

Propagator of the repeated integral

Propagator of the functional integral

Perturbative functional integral and Peliti action

Word of warning on the normal form

Correct Peliti action

Perturbation theory is Gaussian integrals. Standard trick:

$$\exp\left[\int_0^t dt L'(\{\phi^* + 1\}, \{\phi\})\right]$$
$$= \exp\left[\int_0^t dt L'\left(\left\{\frac{\delta}{\delta A} + 1\right\}, \left\{\frac{\delta}{\delta A^*}\right\}\right)\right]$$
$$\times \exp\left[\int_0^t dt\,(A\phi^* + A^*\phi)\right]\Bigg|_{A=A^*=0}.$$

yields Gaussian integral

$$G_0(A, A^*) = \iint \mathcal{D}\phi^*\mathcal{D}\phi\,\exp\left[\int_0^t dt\,(-\phi^*\partial_t\phi + A\phi^* + A^*\phi) - \phi(0)^*\phi(0)\right].$$

Gaussian integral of the discretized problem

Triangular matrix of quadratic form in interpolation approximation

$$G_0(A, A^*) \approx \iint \prod_j \frac{d\phi_j^* d\phi_j}{2i\pi} \exp\Big[-\sum_{j=1}^{N} \left(\phi_j^* \phi_j - \phi_j^* \phi_{j-1}\right) - \phi_0^* \phi_0$$

$$+ \sum_{j=0}^{N} \left(A_j \phi_j^* + A_j^* \phi_j\right) \Delta t \Big], \;\; \sum_{j=1}^{N} \left(\phi_j^* \phi_j - \phi_j^* \phi_{j-1}\right) + \phi_0^* \phi_0 = \sum_{i,j=0}^{N} \phi_i^* M_{ij} \phi_j$$

yields retarded propagator (without $\phi_0^* \phi_0$ quadratic form is degenerate)

$$M = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ -1 & 1 & 0 & \cdots & 0 \\ 0 & -1 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{pmatrix}, \qquad M^{-1} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 1 & 1 & 0 & \cdots & 0 \\ 1 & 1 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & \cdots & 1 \end{pmatrix}.$$

Propagator of the repeated integral

Discrete propagator is the matrix of the quadratic form of sources

$$G_0(A, A^*) \approx \exp\left[\sum_{i,j=0}^{N} A_i^* \Delta t M_{ij}^{-1} A_j \Delta t\right] = \exp\left[\sum_{i=0}^{N} A_i^* \Delta t \sum_{j=0}^{i} A_j \Delta t\right].$$

In the normal form interaction terms contain fields with neighbouring subscripts: ϕ_i^* and ϕ_{i-1}^*. Contraction between these vanishes, because $\phi_0^* = 0$ and $\phi_N = 0$ (sum of elements just above main diagonal):

$$\sum_{i,j=0}^{N} \frac{\partial}{\partial \phi_i} M_{ij}^{-1} \frac{\partial}{\partial \phi_j^*} \sum_{n=1}^{N} \phi_n^* \phi_{n-1} = \sum_{n=1}^{N} M_{n-1,n}^{-1} = 0\,.$$

Absence of single propagator loops due to definition of integral sum.

Propagator of the functional integral

Continuum propagator: limit kernel of discrete quadratic form of sources

$$G_0(A, A^*) \approx \exp\left[\sum_{i,j=0}^{N} A_i^* \Delta t M_{ij}^{-1} A_j \Delta t\right] = \exp\left[\sum_{i=0}^{N} A_i^* \Delta t \sum_{j=0}^{i} A_j \Delta t\right]$$

$$\xrightarrow[\Delta t \to 0]{} \exp \int_0^t du \int_0^t du'\, A^*(u)\theta(u-u')A(u')\,.$$

Propagator determines perturbation theory, $\partial_t \theta(t-t') = \delta(t-t')$, therefore

$$G_0(A, A^*) = \exp \int_0^t du \int_0^t du'\, A^*(u)\theta(u-u')A(u')$$

$$= \iint \mathcal{D}\phi^* \mathcal{D}\phi \exp \int_0^t dt \left(-\phi^* \partial_t \phi + A\phi^* + A^*\phi\right)\,.$$

Correct definition of Gaussian absorbed the spurious term $\phi(0)^*\phi(0)$.

Perturbative functional integral and Peliti action

Functional integral for Green functions in perturbation theory

$$G(A,A^*) = \iint \mathcal{D}\phi\mathcal{D}\phi^* \exp\left\{S(\phi,\phi^*) + \int_0^t [\phi(u)A^*(u) + \phi^*(u)A(u)]\right\}$$

with the dynamic Peliti action (initial Poisson)

$$S(\phi,\phi^*) = \int_0^t dt\left[-\phi^*\frac{\partial}{\partial t}\phi + L'(\phi^*+1,\phi)\right] + n_0\phi^*(0)\,.$$

For the Verhulst model the Peliti action is

$$S = \int_0^t dt\left\{\phi^*\left[-\frac{\partial}{\partial t}\phi + (\lambda-\beta-\gamma)\phi\right] - \gamma\phi^*\phi^2 + \lambda{\phi^*}^2\phi - \gamma{\phi^*}^2\phi^2\right\} + n_0\phi^*(0)\,.$$

Coherent-state construction: action in normal form, **no closed loops of single propagator**! The propagator at coinciding arguments is not defined!

Word of warning on the normal form

The stationarity equations of Peliti action should reproduce the rate equation. Check on Verhulst model:

$$\frac{\delta S}{\delta \phi^*} = -\frac{\mathrm{d}\phi}{\mathrm{d}t} + (\lambda - \beta - \gamma)\phi - \gamma\phi^2 + 2\lambda\phi^*\phi - 2\gamma\phi^*\phi^2 = 0\,,$$

$$\frac{\delta S}{\delta \phi} = \frac{\mathrm{d}\phi^*}{\mathrm{d}t} + (\lambda - \beta - \gamma)\phi^* - 2\gamma\phi^*\phi + \lambda{\phi^*}^2 - 2\gamma{\phi^*}^2\phi = 0\,.$$

On the obvious solution of the latter $\phi^* = 0$ the former yields

$$\frac{\mathrm{d}\phi}{\mathrm{d}t} = (\lambda - \beta - \gamma)\phi - \gamma\phi^2\,, \text{ but} \qquad \frac{\mathrm{d}n}{\mathrm{d}t} = -\beta n + \lambda n - \gamma n^2\,.$$

Liouville operators are equal $\hat{L}'(\hat{a}^+, \hat{a}) = \hat{L}(\hat{a}^+, \hat{a})$, Liouville functionals are not $L'(\phi^*, \phi) \neq L(\phi^*, \phi)$.

Correct Peliti action

Dynamic action does not feel original ordering of operators.

Full reduction operator spans propagators on all vertices producing single-propagator loops.

Normal ordering of Liouville operator tantamount to neglecting graphs with single-propagator loops (Wick's theorem).

Practical prescription: replace operators by fields in original Liouville operator and declare absence of single-propgator loops. Result for Verhulst model

$$S = \int_0^t dt \left\{ \phi^* \left[-\frac{\partial}{\partial t}\phi + (\lambda - \beta)\phi \right] - \gamma\phi^*\phi^2 + \lambda{\phi^*}^2\phi - \gamma{\phi^*}^2\phi^2 \right\} + n_0\phi^*(0)\,.$$

This seems to be hand waving, but is corroborated by old-fashioned Green function approach.