Multitimescale method for approximating the path action relevant to non-equilibrium statistical physics.

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Abstract

A path integral formalism has been proposed recently for non-equilibrium statistical physics applications (see [2]). In this contribution we outline an efficient method for its numerical evaluation. The method used is based on the multiscale MCMC method of Ceperley and co-workers in quantum applications. A significant new feature of the method proposed is that the time endpoint is not fixed and indeed the endpoint sample is the principal object of interest.

1 Background

The action proposed in [2] may be written as

\[
S = \Delta t \int \left\{ \left( \dot{\lambda} - \Theta(\lambda) \right)^T g \left( \dot{\lambda} - \Theta(\lambda) \right) + \Psi(\lambda) \right\} dt
\]

where \( \Psi \geq 0 \) and \( g \) is a Riemannian (non-negative definite) tensor often called the Fisher information matrix. \( \Delta t \) is the minimum timescale associated with the slow modes of the system being modelled. A generalized Boltzmann principle then constructs a path measure using \( \exp(-S) \). Quantities of interest for this theory can be obtained by constructing a sample set of paths according to the proposed measure. Such a sample can be obtained using the Markov Chain Monte Carlo methodology pioneered in the context of quantum Bose condensates by Ceperley and co-workers [1]. This uses a multitimescale approach to speed path sampling via a Brownian bridge style interleaving of time nodes. Thus at the coarsest level the midpoint between the assumed fixed endpoints is retained. At the next level the midpoints of all three previously defined nodes are used. This “interleaving” of nodes continues until the finest level desired is
obtained. Ceperley proposes that at each multiscale level (bar the finest) an approximate rapidly computable action $S_k = -\log \pi_k$ be used. This is a function of the variables at level $k$ and below which are denoted by $s_0, s_1, \ldots, s_k$ and abbreviated as $s$.

As is usual in MCMC methods, in order to make a transition at level $k$ of $s_k \rightarrow s'_k$ we require a trial transition probability function at each level for which samples are rapidly obtainable. Note that transitions are made starting at the coarsest level and proceeding to the finest. This is facilitated by the interleaving of multiscale time points. Denote this transition probability for level $k$ by $T_k(s'_k)$ and note that it will not, in our case, depend on the starting state $s_k$.

Ceperley then shows that if we choose the acceptance rule

$$A_k(s'_k) = \min \left\{ 1, \frac{T_k(s_k)\pi_k(s')\pi_{k-1}(s)}{T_k(s'_k)\pi_k(s)\pi_{k-1}(s')} \right\} \quad (2)$$

as well as ensuring that the finest $\pi_m$ is exact (up to time discretization) then a sample will be produced according to $\pi_m$ and the multiscaling will aid in producing a “reasonably rapid” sampling of path space.

Let us suppose we were able to select $\pi_k$ to be the marginal density with respect to the variables $s_0, s_1, \ldots, s_k$ i.e. the variables $s_{k+1}, \ldots, s_m$ are integrated out from $\pi_m$. Then if we select $T^*_k(s_k) = \pi_k/\pi_{k-1}$ it is easily seen firstly that $T^*_k$ is actually a probability density for the $s_k$ (since integrating out the $s_k$ of $\pi_k$ obviously produces $\pi_{k-1}$ so it is normalized correctly) and secondly with such a choice all trial transitions are accepted (see equation (2)) at all levels meaning a very rapid algorithm since in MCMC rejected transitions imply further sampling of the original $s$.

The above strategy is called the heat bath MCMC method. Unfortunately, of course, it is only practical for very special $\pi_m$ i.e. ones which may be integrated analytically. The best known of these are the Gaussian densities. For the application under consideration the actions are never exactly Gaussian so instead we produce a good Gaussian approximation $\pi^a_m$ to the exact $\pi_m$ and use this to produce, by analytical integration, a set of $\pi^a_k$. We then set

$$\pi_k = \pi^a_k \quad k < m$$

$$T_k = \frac{\pi^a_k}{\pi^a_{k-1}} \quad k \leq m$$

With such a choice it is clear that acceptance always occurs at all levels bar the finest when the exact $\pi_m$ is required in the acceptance rule (2). For this level we obtain

$$A_m(s') = \min \left\{ 1, \frac{\pi^a_m(s')\pi_m(s')}{\pi^a_m(s)\pi_m(s)} \right\}$$

This strategy is quite different to that used in Bose condensates by Ceperley. There the molecular interaction term in the action is highly non-quadratic for close approaches of the often densely packed molecules. In our case a quadratic
approximation is responsible for a large part of the irreversible relaxation of the statistical system at least for the examples studied to date (see [3]). The current strategy also has the practical advantage that Gaussian densities for \( T_k \) enable rapid sampling. It is reasonably clear also that the amount of acceptance depends on the accuracy of the quadratic approximation to the last level action.

## 2 Gaussian approximation of action

There are evidently many ways in which a quadratic approximation of the action could be constructed. The optimal strategy would be to ensure that the approximation was most accurate for the most likely paths. Intuitively this might be ensured if linearizations were performed about a path close to the mean trajectory of the statistical system. Since this trajectory is not known a priori, then a judicious guess would seem the best approach. Note that theoretically the accuracy of the approximation only affects the speed of convergence of the MCMC produced sample and not the ultimate accuracy of a reasonably large sample. Thus if convergence (acceptance) is too slow then this may be an indication of a suboptimal action approximation. Let us assume that a trial trajectory \( \lambda(t) \) is specified (see below for possible choices).

We then choose initially to approximate \( g \) and \( \Psi \) as respectively \( g(\lambda = 0) \) and \( \phi_{ij} \lambda_i \lambda_j \). The second on the basis that the irreversible term is minimized at \( \lambda = 0 \) which from numerical studies is often the equilibrium trial density. We linearize \( \Theta \) about \( \lambda(t) \) and write

\[
\Theta \simeq \mathcal{A}(t) + A(t)(\lambda - \bar{\lambda})
\]  

where \( \mathcal{A} \) and \( A \) are computable from \( \Theta \) and \( \bar{\lambda}(t) \). The time discretized approximate action at level \( m \) can then be written as

\[
S(\lambda) \simeq \tau_s \Delta t \sum_{n=1}^{N} \left( \frac{\lambda_{n+1} - \lambda_n}{\Delta t} \right) - \frac{1}{2} \left( A_{ik}^{n+1} \lambda_k^{n+1} + A_{ik}^{n} \lambda_k^{n} \right) - B_{n+0.5}^{i, j} g_{ij} (i \leftrightarrow j)
\]

\[
= \mathcal{A}_i^{n+0.5} - \frac{1}{2} \left( A_{ik}^{n+1} \lambda_k^{n+1} + A_{ik}^{n} \lambda_k^{n} \right)
\]

where the summation of repeated indices convention is being assumed; the second bracket is simply the first with \( j \) replacing \( i \); \( \tau_s \) is notionally equal to the fine time step \( \Delta t \) but could be subjected to tuning given the uncertainty over the precise value of the latter quantity. Finally \( \mathcal{A} \) is evaluated at the midpoint of \( n \) and \( n + 1 \). In order to perform Gaussian marginalizing integrations of various \( \lambda^k \) we need to rewrite \( S \) in terms of quadratic and linear combinations of such variables.

To facilitate notational efficiency in manipulating (4), replace the upper index \( n \) with \( 0 \), \( n + 1 \) with \( + \) and \( n - 1 \) with \( - \). Two summands will produce terms of the form \( \lambda^0 \lambda_j^0 \), \( \lambda^0 \lambda_j^+ \), \( \lambda^0 \lambda_j^- \) and \( \lambda^0 \) which are needed to evaluate an
integration of the variables $\lambda^0_i$. For the first type, from the summand involving $n$ and $n+1$ we obtain the terms

$$\tau_s \lambda^0_i \lambda^0_j \left[ \frac{g_{ij}}{\Delta t} + A^0_{ki} g_{ki} + \frac{\Delta t}{4} A^0_{ki} A^0_{ij} g_{kl} + \frac{\Delta t}{2} \delta_{ij} \right]$$

From the summand involving $n$ and $n-1$ terms of this form will also occur but in that case the second term in the square brackets has a reversed sign so we obtain in total

$$\tau_s \lambda^n_i \lambda^n_j \left[ \frac{2g_{ij}}{\Delta t} + \frac{\Delta t}{2} A^0_{ki} A^0_{ij} g_{kl} + \Delta t \delta_{ij} \right]$$

(6)

The second type of (quadratic) term comes only from the summand involving $n$ and $n+1$:

$$\tau_s \lambda^0_i \lambda^+_j \left[ -\frac{2g_{ij}}{\Delta t} + A^+_{kj} g_{ik} - A^0_{ki} g_{jk} + \frac{\Delta t}{2} A^0_{ki} A^+_0 A^+_l g_{lk} \right]$$

(7)

The third type of term comes analogously to the last but from the summand involving $n$ and $n-1$:

$$\tau_s \lambda^-_i \lambda^0_j \left[ -\frac{2g_{ij}}{\Delta t} + A^0_{kj} g_{ik} - A^-_i g_{jk} + \frac{\Delta t}{2} A^-_i A^0_0 A^+_l g_{lk} \right]$$

(8)

Turning now to the linear term we note that they occur due to the presence of $B$ in the discetized action. We keep track of both the $\lambda^0$ and $\lambda^+$ terms since the latter in the summand $n-1$ and $n$ will contribute to the total $\lambda^0$ piece. The cross terms give

$$\tau_s \left[ 2 \left( \lambda^0_i - \lambda^+_j \right) g_{ij} B^0_j + \Delta t B^0_i \ g_{ij} \right] \left( A^0_{jk} \lambda^0_k + A^+_j \lambda^+_k \right)$$

($B^0 \equiv B^{0^{+0.5}}$) which rearranges to

$$\tau_s \left[ \lambda^0_i \left( 2g_{ij} B^0_j + \Delta t A^0_{jki} g_{kj} B^0_k \right) - \lambda^+_j \left( 2g_{ij} B^0_j - \Delta t A^+_j g_{kj} B^+_k \right) \right]$$

Thus the total contribution from the action to the linear $\lambda^0$ term is

$$\tau_s \lambda^0_i \left[ 2g_{ij} \left( B^0_j - B^-_j \right) + \Delta t A^0_{jki} g_{kj} \left( B^0_k + B^-_k \right) \right]$$

or

$$2\tau_s \lambda^0_i \left[ g_{ij} \left( B^{0^+_j - B^-_j} \right) + \Delta t A^0_{jki} g_{kj} B^0_k \right]$$

(9)

### 3 Determination of general level action

As integration of the variables associated with each level $k$ occurs, a new marginalized action appears which is used to determine the transition probability $T_{k-1}$ for the next coarser level. A matrix recursion scheme is required to
determine the Gaussian densities $\pi_k$. Because of the Brownian bridge construction we may write the part of the level $k$ action involving the $2^{k-1}$ variables to be integrated as

$$S(k) = \sum_{n=1}^{N} \frac{1}{2} \lambda_j^l \lambda_j^l e_j^l(k) + \lambda_j^l (\lambda_j^l H_{ij}^k(k) + \lambda_j^l H_{ij}^k(k) + K^l_i(k))$$  \hspace{1cm} (10)$$

$$l(n, k) \equiv 1 + \Delta(2n - 1)$$

$$N \equiv 2^{k-1}$$

$$\Delta \equiv 2^m - k$$

where the $G$, $H$ and $K$ need to be determined recursively. This structure reflects the interleaving nature of the multiscale construction. There are (excluding endpoints see below) $N - 1$ variables not integrated at this level. They occur at time indices

$$l(r, k) + \Delta \hspace{1cm} r = 1, \ldots, N - 1$$

Each acquires matrix contributions from integrated variables at $l(r, k)$ and $l(r + 1, k) = l(r, k) + 2\Delta$. Using the usual multivariate Gaussian integration formula we can integrate the first of these variables (functional form of the density being the Gaussian $\exp(-S(k))$ obtaining the contributions

$$- \frac{1}{2} [\lambda_j^l + \Delta \lambda_j^l] [\lambda_j^l H_{ij}^k(k) + \lambda_j^l H_{ij}^k(k) + K^l_i(k)] [G^l(k)]^{-1} [i \leftrightarrow k]$$  \hspace{1cm} (11)$$

Another analogous contribution comes from the second integration variable mentioned above. Comparing this with the form of $\lambda^l$ we read off the recursion relations for the matrices $G$

$$G^{l-\Delta}(k-1) = G^{l+\Delta}(k-1) - H^{l+\Delta}(k) G^l(k) - H^{l}(k) - H^{l+\Delta}(k) G^{l+\Delta}(k)$$  \hspace{1cm} (12)$$

Now the only terms of the form $\lambda^l + \Delta \lambda^l$ come from (11). Furthermore at level $k - 1$ only one of the variables with time index $l + \Delta$ and $l - \Delta$ will be an integration variable due to the interleaving construction. This term therefore is assigned entirely to the time index to be integrated and by convention

$$H^{l-\Delta}(k-1) = H^{l-\Delta}(k-1)$$  \hspace{1cm} (13)$$

Comparison of this term’s form with the form of $\lambda^l$ shows that

$$H^{l-\Delta}(k-1) = - (H^{-l}(k))^{t} [G^l(k)]^{-1} H^{l}(k)$$  \hspace{1cm} (14)$$

Note that the required $H^-$ terms are obtainable from (13). Finally the linear term involving $K$ is easily seen to imply for the vectors $K$

$$K^{l+\Delta}(k-1) = K^{l+\Delta}(k) - H^{l+\Delta}(k) [G^l(k)]^{-1} K^l(k) - H^{l-(l+2\Delta)}(k) [G^{l+2\Delta}(k)]^{-1} K^{l+2\Delta}(k)$$  \hspace{1cm} (15)$$
Equations (12), (14) and (15) define the recursion which allows $T_k$ to be constructed since this is simply the multivariate Gaussian $C \exp \left( -S(k) \right)$. The start of this recursive chain is obtained by setting $k = m$ and comparing with the equations (6), (7), (8) and (9) from the last section:

$$G_{ij}(m) = 2\tau_s \left[ \frac{2g_{ij}}{\Delta t} + \frac{\Delta t}{2} A_{ki}^l A_{lj}^i g_{kl} + \Delta t \phi_{ij} \right]$$

$$H_{ij}^{+1}(m) = \tau_s \left[ -\frac{2g_{ij}}{\Delta t} + A_{kj}^{l+1} g_{ik} - A_{kj}^l g_{jk} + \frac{\Delta t}{2} A_{ki}^l A_{lj}^{l+1} g_{kl} \right]$$

$$H_{ij}^{-1}(m) = \tau_s \left[ -\frac{2g_{ij}}{\Delta t} + A_{kj}^l g_{ik} - A_{kj}^{l-1} g_{jk} + \frac{\Delta t}{2} A_{ki}^{l-1} A_{lj}^l g_{kl} \right]$$

$$K_i^l(m) = 2\tau_s \left[ g_{ij} \left( \tilde{B}_j^{l+1/2} - \tilde{B}_j^{l-1/2} \right) + \Delta t A_{ij}^l g_{jk} \tilde{B}_k^l \right]$$

Note that for $k = m$ we have $\Delta = 1$.

4 Temporal boundary points

For the application here, the starting point is fixed but the endpoint is not. We deal with that in the context of the interleaving “Brownian bridge” construction by placing the floating endpoint in the level 0 set of variables and adding the following contribution to the approximate action at every level:

$$S_{\text{end}}(k) = \frac{1}{2} \lambda_i^M \lambda_j^M G_{ij}^M(k) + \lambda_i^M K_i^M(k)$$

$$M \equiv 2^m$$

Note the absence of the cross terms which is caused by truncating the action at the endpoint which omits the forward term and the inclusion already of the backward term in the final interior terms. This modification sets recursion relations for $G^M$ and $K^M$ but note that the cross term coefficients $H$ are not affected since the ones required are already computed in the previous section. We can read off the required relations from the interior relations (12) and (15) in the previous section by dropping the forward terms:

$$G^M(k - 1) = G^M(k) - H^{+(M-\Delta)}(k) G^{M-\Delta}(k)^{-1} H^{+(M-\Delta)}(k)$$

$$K^M(k - 1) = K^M(k) - H^{+(M-\Delta)}(k)^T \left[ G^{M-\Delta}(k) \right]^{-1} K^{M-\Delta}(k)$$

In terms of sampling, the starting point (level zero variables) now occurs with the endpoint random variable which follows a Gaussian described by $G^M(0)$ and $K^M(0)$. Intuitively one expects the mean of this density to vary from close to the initial conditions for short time actions through to values close to that for the mean of the equilibrium consistency distribution when the action time interval is long. Once the endpoint is determined the other random variables are sampled following the interleaving pattern described in the previous section. The interleaving nature ensures that all sampling distributions are independent with respect to their time. If the variables are vectors however this may not be true with respect to the vector index.
5 Linearization trajectory

As mentioned previously, $\lambda(t)$ is required to compute the various linearized terms associated with $A$. Experience with simple turbulence systems suggests the following form as a rough approximation for the evolution of the slow variable co-ordinates of the system:

$$\dot{\lambda} - \Theta(\lambda) = -\frac{1}{2} \nabla \Phi(\lambda)$$  \hfill (16)

To reiterate, this choice is not required to be exact, simply to ensure that the linearization is sufficiently accurate for “most” paths in order to ensure that the acceptance rate of the MCMC method is reasonable. Clearly the “acid test” here is this latter rate and if it is too low for the choice made in (16) then another choice may be indicated.

6 A sample linearization: The truncated Burgers model.

Here we have for various slow variable choices, the complex relation

$$\Theta_{2k-1}(\lambda) + i\Theta_{2k}(\lambda) = -\frac{i}{2} k \sum_{k=k_1+k_2} z_{k_1} z_{k_2}$$  \hfill (17)

where $z_j \equiv \lambda^{2j-1} + i\lambda^{2j} \quad 0 < j < m$

$$z_j^* = z_{-j}$$

$$z_0 = 0$$

$$z_l = 0 \quad |l| > m$$

The index $k$ runs $1, \ldots, 2m$; while $j$, $k_1$ and $k_2$ run from $-m, \ldots, m$. Linearizing as

$$\lambda_l = \lambda_l^0 + \lambda_l'$$

we obtain

$$\Theta_{2k-1}' + i\Theta_{2k}' = C_k = -i k \sum_{k=k_1+k_2} \overline{z}_{k_1} z_{k_2} = -i k \sum_{k_1=-m}^{m} \overline{z}_{k-k_2} z_{k_2}'$$

$$\equiv Z_{kk_2} z_{k_2}'$$

$$Z_{kl} = -ik z_{k-l}$$

where the obvious summation convention is assumed on the second line. Set the following:

$$Z_{kl} = X_{kl} + iY_{kl}$$

$$z_l' = b_l + ic_l$$
so
\[ b_{-|j|} = b_{|j|} \]
\[ c_{-|j|} = -c_{|j|} \]
then it is easily checked that
\[
\Theta'_{2k-1} = X_{kk_2}b_{k_2} - Y_{kk_2}c_{k_2} = \sum_{k_2=1}^{m} (E_{kk_2}b_{k_2} + F_{kk_2}c_{k_2})
\]
\[
\Theta'_{2k} = Y_{kk_2}b_{k_2} + X_{kk_2}c_{k_2} = \sum_{k_2=1}^{m} (E'_{kk_2}b_{k_2} + F'_{kk_2}c_{k_2})
\]
where
\[
E_{kk_2} = X_{kk_2} + X_k(-k_2)
\]
\[
E'_{kk_2} = Y_{kk_2} + Y_k(-k_2)
\]
\[
F_{kk_2} = Y_k(-k_2) - Y_{kk_2}
\]
\[
F'_{kk_2} = X_{kk_2} - X_k(-k_2)
\]
Now since \(\lambda_{2j-1} = b_j\) and \(\lambda_{2j} = c_j\) we can construct the matrix \(A\) for equation (3) i.e. we have
\[
\Theta' = AX'
\]
with
\[
A_{2r(2s-1)} = E'_{rs}
\]
\[
A_{2r(2s)} = F'_{rs}
\]
\[
A_{(2r-1)(2s-1)} = E_{rs}
\]
\[
A_{(2r-1)(2s)} = F_{rs}
\]
where \(0 < r < 2m\) but \(0 < s < m\). Note that the vector \(\Theta'\) is double the length of \(\lambda'\) because the sum in (17) allows values of \(k\) beyond the possible values for \(k_1\) and \(k_2\).

7 The “free particle” case
Set \(A = \phi = 0\) and \(g = I\). We have then
\[
G^l(m) = 2\alpha I
\]
\[
H^{\pm l}(m) = -\alpha I
\]
\[
\alpha = \frac{2\tau_s}{\Delta t}
\]
and so
\[
G^{l+1}(m-1) = G^{l+1}(m) - H^{l+1}(m)^t \left[ G^l(m) \right]^{-1} H^{l+1}(m) - H^{-(l+2)}(m)^t \left[ G^{l+2}(m) \right]^{-1} H^{-(1+2)}(m)
\]
\[
= 2\alpha I - 2\alpha^2 \frac{1}{2\alpha} I = \alpha I
\]
and
\[
H^{\pm(i\pm1)}(m-1) = -H^{-l}(m) \left[ G^l(m) \right]^{-1} H^{+l}(m) = -\alpha^2 \frac{1}{2\alpha} I = -\frac{\alpha}{2} I
\]

Iterating we obtain easily
\[
\begin{align*}
G^i(k) &= \frac{\alpha}{2^{k-m-1}} I \\
H^{\pm i}(k) &= -\frac{1}{2} G^i(k)
\end{align*}
\]

This form for \( T \) is discussed by Ceperley [1]. Effectively it implies increasing the time increment \( \Delta t \) by a factor of two as the timescale level becomes coarser by one.

8 Most accurate quadratic approximation for the action.

In order to increase acceptances in the MCMC method and hence reduce the computational burden, the best quadratic approximation is needed. The algorithm detailed above produces a 100% acceptance rate when the exact action is quadratic since it is a heat bath method. In order to produce a quadratic approximation we linearized \( \Theta(\lambda) \). In the present section we instead construct a second order Taylor expansion for the action using a mean trajectory of the type discussed above.

The most general discretised action may be written as
\[
S = \Delta t \sum_{n=1}^{N} L(n) dt
\]

where the obvious summation convention holds and \( n \) is the time index for which the convention does not hold in what follows. A second order Taylor expansion about the mean trajectory \( \overline{\lambda} \) gives
\[
S^a = S \bigg|_{\lambda=\overline{\lambda}} + \sum_{n=1}^{N} \frac{\partial S}{\partial \lambda_k(n)} \bigg|_{\lambda=\overline{\lambda}} \chi_k'(n) + \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \frac{\partial^2 S}{\partial \lambda_k(n) \partial \lambda_l(m)} \bigg|_{\lambda=\overline{\lambda}} \chi_k'(n) \chi_l'(m)
\]

where \( \chi' = \lambda - \overline{\lambda} \)

To facilitate computation we introduce the following symbols
\[
T_i(n) \equiv \frac{\lambda_i(n) - \lambda_i(n-1)}{\Delta t} - \frac{1}{2} \left( \Theta_i(n) + \Theta_i(n-1) \right)
\]
\[ G_{ij}^+(n) \equiv \frac{2\delta_{ij} - \partial\Theta_i(n)}{\Delta t} = 2 \frac{\partial T_i(n)}{\partial \lambda_j(n)} \]

\[ G_{ij}^-(n) \equiv \frac{-2\delta_{ij} - \partial\Theta_i(n)}{\Delta t} = \frac{2\partial T_i(n+1)}{\partial \lambda_j(n)} \]

\[ R_{kl}^i(n) \equiv \frac{\partial^2 n_{kl}^i}{\partial \lambda_i(n)\partial \lambda_j(n)} = 2 \frac{\partial h_{kl}^i(n)}{\partial \lambda_i(n)} = \frac{2h_{kl}^i(n+1)}{\partial \lambda_i(n)} \]

\[ V_{kij}(n) \equiv \frac{\partial^2 \Theta_k}{\partial \lambda_i(n)\partial \lambda_j(n)} = \frac{\partial G_{kl}^+(n)}{\partial \lambda_i(n)} = -\frac{\partial G_{kl}^-(n)}{\partial \lambda_i(n)} \]

\[ U_{ij}^k(n) \equiv \frac{\partial^2 g_{ij}^k}{\partial \lambda_i(n)\partial \lambda_j(n)} = \frac{\partial R_{ij}^k(n)}{\partial \lambda_i(n)} \] (18)

in which notation we have

\[ S = \Delta t dt \sum_{n=1}^N \{ T_i(n)h^{ij}T_j(n) + \Psi(n) \} \]

Differentiating \( S \) once using (18) and also using the fact that the metric tensor \( g \) is symmetric we obtain

\[
\frac{1}{\alpha} \frac{\partial S}{\partial \lambda_i(n)} = G_{ki}^+(n)h^{kl}(n)T_l(n) + \frac{1}{2} R_{kl}^i(n)T_k(n)T_l(n) + G_{ki}^-(n)h^{kl}(n+1)T_l(n+1) + \frac{1}{2} R_{kl}^i(n)T_k(n+1)T_l(n+1) + \frac{\partial \Psi(n)}{\partial \lambda_i(n)} \]

\[ \alpha \equiv \Delta t dt \]

Differentiating again using (18) and again using the metric tensor symmetry we obtain the Hessian matrix

\[
\frac{1}{\alpha} \frac{\partial^2 S}{\partial \lambda_i(n)\partial \lambda_j(n)} = \delta_{r,n} \left[ -V_{kij}(n)h^{kl}(n)T_l(n) + \frac{1}{2} G_{kij}^+(n)R_{kl}^i(n)T_l(n) + \frac{1}{2} G_{kij}^+(n)h^{kl}(n)G_{kl}^+(n)T_l(n) + \frac{1}{2} G_{kij}^+(n)h^{kl}(n)G_{kl}^+(i)T_l(n) + \frac{1}{2} U_{ij}^k(n)T_k(n)T_l(n) + \frac{1}{2} R_{ij}^k(n)G_{kl}^+(n)T_l(n+1) + \frac{1}{2} R_{ij}^k(n)G_{kl}^+(n)T_l(n+1) + \frac{\partial^2 \Psi(n)}{\partial \lambda_i(n)\partial \lambda_j(n)} \right] + \delta_{r(n-1),n} \left[ \frac{1}{2} G_{kij}^+(n)R_{kl}^i(n-1)T_l(n) + \frac{1}{2} G_{kij}^+(n)h^{kl}(n)G_{kl}^+(n-1) + \frac{1}{2} R_{ij}^k(n)G_{kl}^-(n-1)T_l(n) \right]
\]
Furthermore in the second partial derivative deriving from this drop in the expressions above for the partial derivatives. Not occur in the discrete action due to the truncation adopted. Thus all terms defined. One can now identify we have

\[ \delta_{r(n+1)} \left[ \frac{1}{2} G_{ki}^-(n) R_{kj}^R(n+1) \right. \]

Since \( \Theta, \Psi \) and \( g \) are known functions of \( \lambda \), the second order Taylor series is defined. One can now identify \( G \) above because when constructing \( (10) \) for \( k = m \) one needs to take into account equal contributions from \( \frac{1}{\alpha \lambda_i(n)} \partial \lambda_i \delta \lambda_i(n) \) and from \( \frac{1}{\alpha \lambda_i(n+1)} \partial \lambda_i(n) \). Explicitly we have

\[
G_{ij}^r(m) = -V_{kij}(r) h^{kl}(r) T_l(r) + \frac{1}{2} G_{ki}^+(r) R_{kj}^R(r) T_l(r) \\
+ \frac{1}{2} G_{ki}^+(r) h^{kl}(r) G_{lj}^+(r) \quad + \frac{1}{2} U_{ij}^R(r) T_k(r) T_l(r) + \frac{1}{2} R_{ki}^R(r) G_{kj}^+(r) T_l(r) \\
- V_{kij}(r) h^{kl}(r+1) T_l(r+1) + \frac{1}{2} G_{ki}^+(r) R_{kj}^R(n) T_l(r+1) \\
+ \frac{1}{2} G_{ki}^+(r) h^{kl}(r+1) G_{lj}^+(n) + \frac{1}{2} U_{ij}^R(r) T_k(r+1) T_l(r+1) \\
+ \frac{1}{2} R_{ki}^R(r) G_{kj}^+(r) T_l(r+1) + \frac{\partial \Psi(r)}{\partial \lambda_i(r)} \partial \lambda_i(r) \\
H_{ij}^r(m) = G_{ki}^+(r) R_{kj}^R(r - 1) T_l(r) + G_{ki}^+(r) h^{kl}(r) G_{lj}^+(r - 1) + R_{ki}^R(r) G_{kj}^+(r - 1) T_l(r) \\
H_{ij}^R(m) = G_{ki}^+(r) R_{kj}^R(r + 1) T_l(r + 1) + G_{ki}^+(r) h^{kl}(r + 1) G_{lj}^+(r + 1) + R_{ki}^R(r) G_{kj}^+(r + 1) T_l(r + 1) \\
K_i^r(m) = \frac{\partial \Psi(r)}{\partial \lambda_i(r)} + G_{ki}^+(r) h^{kl}(r) T_l(r) + \frac{1}{2} R_{ki}^R(r) T_k(r) T_l(r) \\
+ G_{ki}^+(r) h^{kl}(r + 1) T_l(r + 1) + \frac{1}{2} R_{ki}^R(r) T_k(r + 1) T_l(r + 1)
\]

### 8.1 Endpoint conditions

At \( n = 1 \) we need to define \( T_i(1) \). This we do by assuming that \( \lambda_i(0) \) is fixed by some prescribed initial condition. At \( n = N \) we note that \( T_i(N + 1) \) does not occur in the discrete action due to the truncation adopted. Thus all terms deriving from this drop in the expressions above for the partial derivatives. Furthermore in the second partial derivative \( m = N + 1 \) is not present due to the truncation so we obtain the following simpler expressions:

\[
\frac{1}{\alpha} \frac{\partial S}{\partial \lambda_i(N)} = G_{ki}^+(N) h^{kl}(N) T_l(N) + \frac{1}{2} R_{ki}^R(N) T_k(N) T_l(N) + \frac{\partial \Psi(N)}{\partial \lambda_i(N)} \\
\frac{1}{\alpha} \frac{\partial^2 S}{\partial \lambda_i(N) \partial \lambda_j(m)} = \delta_{mn} \left[ -V_{kij}(N) h^{kl}(N) T_l(N) + \frac{1}{2} G_{ki}^+(N) R_{kj}^R(N) T_l(N) + \frac{1}{2} G_{ki}^+(N) h^{kl}(N) G_{kj}^+(N) T_l(N) + \frac{1}{2} U_{ij}^R(N) T_k(N) T_l(N) + \frac{1}{2} R_{ki}^R(N) G_{kj}^+(N) T_l(N) + \frac{\partial^2 \Psi(N)}{\partial \lambda_i(N) \partial \lambda_j(N)} \right]
\]
\[ + \delta_{m(N-1)} \left[ \frac{1}{2} G_{ki}^+(N) R_{jl}^{kl}(N-1) T_{i}(N) + \frac{1}{2} G_{kj}^+(N) h^{kl}(N) G_{lj}^-(N-1) T_{l}(N) \right] \]

**9 Endpoint considerations**

Path integrals calculated as above have fixed endpoints since the action calculation detailed above demands this. For our application however only the initial condition is fixed by the prescribed initial trial density. Once a delta function for the initial consistency distribution is prescribed then consistency distributions are determined for all times since they satisfy a Euclidean Schrödinger equation. Thus the final endpoint at \( t = T \) must be sampled from a determined consistency distribution. For a fixed final endpoint the consistency distribution is proportional to the following sum of path weights

\[ \rho(x_0, x(T)) = \sum_{\lambda(0) = x_0, \lambda(T) = x(T)} \exp \left[ - \Delta t S(\lambda) \right] \]  \hfill (19)

This equation is just a restatement of the generalized Boltzmann principle for paths assumed in the present approach. By choosing a variety of endpoints \( x \) we can clearly calculate the relative magnitude of the consistency distribution at time \( T \) for various choices of \( x \). For many applications however \( x \) is a vector and so only a sample of possible such final time vectors will be available. The question then becomes how to ensure that these follow the appropriate consistency distribution. We proceed as follows: Construct a moderate sample \( N \) of the \( x(T) \) using a trial density \( \phi(x) \). For each sample member perform the fixed endpoints MCMC calculation as detailed previously and then calculate \( \rho \) using (19). This calculation will be straightforward since \( S \) is central to the MCMC method. Consider now a small volume \( dV \) surrounding \( x \). The number of paths sampled will be

\[ n_t(x) = N \phi(x) dV \]

as opposed to the desired

\[ n(x) = N \rho(x_0, x(T)) dV \]

Thus the contribution of each path ending in \( x \) in calculating such things as moments at any time along the path, will need to be reweighted by the factor

\[ \Phi(x_0, x) = \rho(x_0, x(T))/\phi(x) \]

which may well vary significantly with each different sampled value \( x \) if the trial density differs from the actual density there.

\[ ^1 \text{Such as an appropriate multivariate Gaussian calculated from a linearization of the problem} \]
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