Correction to: Hybrid Monte Carlo methods for sampling probability measures on submanifolds

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Shiva Darshan and Miranda Holmes–Cerfon (Courant Institute, NYU) pointed out a mistake in the projection functions to enforce the momentum constraint when rewriting the algorithm in Numerical Algorithm A of Section 3.1. Two different projection functions are actually needed, see indeed the formula for the Lagrange multiplier $\lambda^{n+1}$ after Equation (7) for the RATTLE step, and Remark 5 for the Ornstein–Uhlenbeck step.

We provide below a corrected version of the pseudo-code for the complete algorithm; see Numerical algorithms 1, 2 and 3. Changes are highlighted in blue. The sampling algorithm consists in iterating procedure ConstrainedGHMC of the algorithm (Numerical algorithm 1), which uses the procedures LAGRANGE_MOMENTUM_OU (Numerical algorithm 2) and LAGRANGE_MOMENTUM_RATTLE (Numerical algorithm 3) to compute the Lagrange multiplier for momentum constraints in the fluctuation/dissipation and RATTLE steps, respectively. The procedure NEWTON to compute the Lagrange multiplier for position constraints is unchanged.

Numerical algorithms 2 and 3 differ by a multiplication by $\left(\text{Id} + \Delta t \gamma M^{-1}/4\right)^{-1}$, which arises from the specific choice of the discretization of the fluctuation/dissipation part in Algorithm 3.

The original article can be found online at https://doi.org/10.1007/s00211-019-01056-4.

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Numerical algorithm 1 One step of the practical constrained HMC algorithm with reverse projection

\textbf{Parameters:} $\gamma$ (friction), $\Delta t$ (timestep), $\eta_{\text{rev}}$ (tolerance for reverse check)

\begin{verbatim}
procedure CONSTRANDEDGHMC(q, p)
\end{verbatim}
\begin{verbatim}
G \sim \mathcal{N}(0, \text{Id})
\end{verbatim}
\begin{verbatim}
p \leftarrow (\text{Id} + \Delta t \gamma M^{-1}/4)^{-1} \left[(\text{Id} - \Delta t \gamma M^{-1}/4)p + \sqrt{\gamma \Delta t} G\right]
\end{verbatim}
\begin{verbatim}
\lambda = \text{LAGRANGE\_MOMENTUM\_OU}(q, p)
\end{verbatim}
\begin{verbatim}
p \leftarrow p + (\text{Id} + \Delta t \gamma M^{-1}/4)^{-1} \nabla \xi(q) \lambda
\end{verbatim}  \hspace{1em} \triangleright Integration of the fluctuation/dissipation for $\Delta t/2$

\begin{verbatim}
\text{Reject} = \text{TRUE}
\end{verbatim}
\begin{verbatim}
\tilde{p} = p - \Delta t \nabla V(q)/2 \text{ and } \tilde{q} = q + \Delta t M^{-1} \tilde{p}
\end{verbatim}
Compute $(\text{Success\_forward\_RATTLE, } \theta) = \text{NEWTON}(\tilde{q}, \tilde{p})$

\begin{verbatim}
if Success\_forward\_RATTLE then
\end{verbatim}
\begin{verbatim}
\tilde{p} \leftarrow \tilde{p} + \nabla \xi(\tilde{q})\theta/\Delta t \text{ and } \tilde{q} \leftarrow \tilde{q} + M^{-1} \nabla \xi(\tilde{q})\theta
\end{verbatim}
\begin{verbatim}
\tilde{p} \leftarrow \tilde{p} - \Delta t \nabla V(\tilde{q})/2
\end{verbatim}
\begin{verbatim}
\lambda = \text{LAGRANGE\_MOMENTUM\_RATTLE}(\tilde{q}, \tilde{p})
\end{verbatim}
\begin{verbatim}
\tilde{p} \leftarrow \tilde{p} + \nabla \xi(\tilde{q})\lambda
\end{verbatim}  \hspace{1em} \triangleright Constrained RATTLE – proposition

\begin{verbatim}
\text{Compute } (\text{Success\_backward\_RATTLE, } \theta) = \text{NEWTON}(\hat{q}, \hat{p})
\end{verbatim}

\begin{verbatim}
if Success\_backward\_RATTLE then
\end{verbatim}
\begin{verbatim}
\hat{p} \leftarrow \hat{p} + \nabla \xi(\hat{q})\theta/\Delta t \text{ and } \hat{q} \leftarrow \hat{q} + M^{-1} \nabla \xi(\hat{q})\theta
\end{verbatim}
\begin{verbatim}
\hat{p} \leftarrow \hat{p} - \Delta t \nabla V(\hat{q})/2
\end{verbatim}
\begin{verbatim}
\lambda = \text{LAGRANGE\_MOMENTUM\_RATTLE}(\hat{q}, \hat{p})
\end{verbatim}
\begin{verbatim}
\hat{p} \leftarrow \hat{p} + \nabla \xi(\hat{q})\lambda
\end{verbatim}  \hspace{1em} \triangleright Constrained RATTLE – reverse move

\begin{verbatim}
if \|\hat{q} - \tilde{q}\| < \eta_{\text{rev}} then
\end{verbatim}  \hspace{1em} \triangleright Constrained RATTLE – checking reversibility
\begin{verbatim}
U \sim \mathcal{U}([0, 1])
\Delta H = H(\hat{q}, \hat{p}) - H(q, p)
\end{verbatim}
\begin{verbatim}
if \log(U) \leq -\Delta H then
\end{verbatim}  \hspace{1em} \triangleright Constrained RATTLE – Metropolis acceptance/rejection
\begin{verbatim}
\text{Reject} = \text{FALSE}
\end{verbatim}

end if
\begin{verbatim}
end if
\end if
\end if
\begin{verbatim}
if \text{Reject then}
\end{verbatim}
\begin{verbatim}
\tilde{p} = -p \text{ and } \tilde{q} = q
\end{verbatim}
end if
\begin{verbatim}
\hat{G} \sim \mathcal{N}(0, \text{Id})
\end{verbatim}
\begin{verbatim}
\tilde{p} \leftarrow (\text{Id} + \Delta t \gamma M^{-1}/4)^{-1} \left[(\text{Id} - \Delta t \gamma M^{-1}/4)\tilde{p} + \sqrt{\gamma \Delta t} \tilde{G}\right]
\end{verbatim}
\begin{verbatim}
\lambda = \text{LAGRANGE\_MOMENTUM\_OU}(\tilde{q}, \tilde{p})
\end{verbatim}
\begin{verbatim}
\tilde{p} \leftarrow \tilde{p} + (\text{Id} + \Delta t \gamma M^{-1}/4)^{-1} \nabla \xi(\tilde{q}) \lambda
\end{verbatim}  \hspace{1em} \triangleright Integration of the fluctuation/dissipation for $\Delta t/2$

return $\hat{q}, \hat{p}$
\end{verbatim}
\begin{verbatim}
end procedure
\end{verbatim}

Numerical algorithm 2 Computation of the Lagrange multiplier for momentum constraints in OU part

\begin{verbatim}
procedure LAGRANGE\_MOMENTUM\_OU(q, p)
\end{verbatim}
\begin{verbatim}
S = [\nabla \xi(q)]^{T} M^{-1} \left[(\text{Id} + \Delta t \gamma M^{-1}/4)^{-1} \nabla \xi(q)\right]
\end{verbatim}
\begin{verbatim}
b = [\nabla \xi(q)]^{T} M^{-1} p
\end{verbatim}
\begin{verbatim}
return $\lambda = -S^{-1}b$
\end{verbatim}
\end{verbatim}
\begin{verbatim}
end procedure
\end{verbatim}
**Numerical algorithm 3** Computation of the Lagrange multiplier for momentum constraints in RATTLE part

```
procedure LAGRANGE_MOMENTUM_RATTLE(q, p)
    S = (∇ξ(q))^T M^{-1} ∇ξ(q)
    b = (∇ξ(q))^T M^{-1} p
    return λ = -S^{-1} b
end procedure
```

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