Singular Nature of the Continuous Time Limit of the Onsager-Machlup Functional

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CCP 2014, Boston MA

August 12, 2014

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Main point

We have made progress since the abstract was submitted and I have modified the talk to reflect this progress.

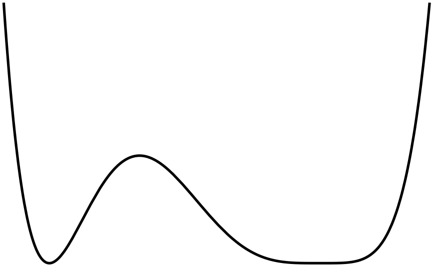
Purpose

Explain the singular nature of the continuous-time Onsager-Machlup functional. We use a novel approach to show the unphysical nature of this limit.

Outline

1. Brownian Dynamics and the OM Function
2. The Continuous-Time formulation: Ito and Girsanov
3. New perspective based on a MC method
4. Results and Discussion

Starting point



- Particles moving in a potential, U, with Force $F = -\nabla U$
- In contact with a thermal bath at temperature ε.
- Spatial distribution given by Boltzmann distribution:

$$\exp(-U(x)/\varepsilon)$$

Brownian dynamics

- ε is temperature
- $F(x)$ is the force $\qquad F(x) = -\nabla U(x)$
- W represents the Wiener process (White noise)

Stochastic Differential Equation (SDE)

$$dx = F(x)dt + \sqrt{2\varepsilon}\, dW$$

With a finite time step Δt, $dW \to \sqrt{\Delta t}\, \xi_i$, and the SDE becomes

$$x_{i+1} - x_i = F(x_i)dt + \sqrt{2\varepsilon\Delta t}\, \xi_i$$

Quadratic Variation

$$\sum |\Delta x|^2 \to 2N\ \Delta t\ \varepsilon = 2\ T\ \varepsilon$$

Onsager-Machlup (OM) functional

$$x_{i+1} - x_i = F(x_i)dt + \sqrt{2\varepsilon\Delta t}\,\xi_i$$

Eliminate the random variables and express the path probability in terms of the path variables themselves.

Path probability for the SDE

$$\begin{aligned} -\ln P_{OM} &= \sum \frac{1}{2}\xi_i^2 \\ &= \frac{\Delta t}{2\varepsilon}\sum_i \frac{1}{2}\left|\frac{\Delta x}{\Delta t} - F(x_i)\right|^2 \end{aligned}$$

Continuous-time OM functional

$$-\ln P_{OM} = \frac{\Delta t}{2\varepsilon} \sum_i \frac{1}{2} \left| \frac{\Delta x}{\Delta t} - F(x_i) \right|^2$$

Use Ito's formula and Girsinov's theorem to find the probablity of the path.

Continuous-time limit path probability

$$-\ln P_{Ito} = \frac{U(T) - U(0)}{2\varepsilon} + \frac{1}{2\varepsilon} \int_0^T dt \left[\frac{1}{2} \left(\frac{dx}{dt} \right)^2 + G(x_t) \right]$$

where G is the *path potential*:

$$G = \frac{1}{2}|F|^2 - \varepsilon \nabla^2 U$$

A New Perspective (HMC)

It is difficult to understand the continuous-time limiting process within Brownian dynamics. Require a method where the finite-time-step errors are known (single step Hybrid Monte Carlo).

Starting parameters: x_0 $v_0 = \sqrt{\varepsilon}\ \xi_0$ h (time step)

Leap-Frog integrator (symplectic)

$$x_1 = x_0 + h\ v_0 + \frac{h^2}{2} F(x_0)$$

$$v_1 = v_0 + \frac{h}{2} F(x_1) + \frac{h}{2} F(x_0)$$

The error in energy $\delta e = \frac{1}{2} v_1^2 - \frac{1}{2} v_0^2 + U(x_1) - U(x_0)$

Note: If $\Delta t = h^2/2$, we recover Brownian dynamics.

Single step probability

$$-\ln P_{MB} = \frac{v_0^2}{2\varepsilon} = \frac{1}{2\varepsilon}\left[\frac{1}{2}v_0^2 + \frac{1}{2}v_1^2 + \Delta U - \delta e\right]$$

$$-\ln P_{MC} = -\ln\{\min[1, \exp(-\delta e/2\varepsilon)]\} = \frac{|\delta e| + \delta e}{2\varepsilon}$$

Probability for the entire path

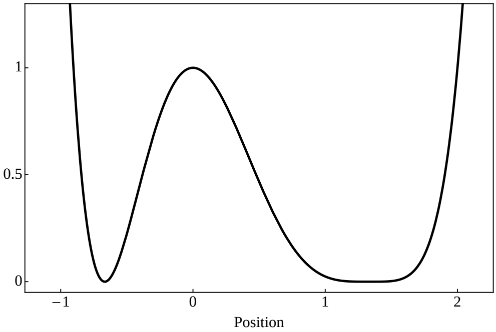
$$-\ln P_{New} = \frac{\Delta U}{2\varepsilon} + \frac{\Delta t}{2\varepsilon}\sum_i \left(\frac{1}{4}\left|\frac{\Delta x}{\Delta t} + F_{i+1}\right|^2 + \frac{1}{4}\left|\frac{\Delta x}{\Delta t} - F_i\right|^2 + \frac{|\delta e|}{\Delta t}\right)$$

- cross terms: $\frac{1}{2}\frac{\Delta x}{\Delta t}(F_{i+1} - F_i) \rightarrow \frac{1}{2}\frac{\Delta x^2}{\Delta t}\frac{\Delta F}{\Delta x} \rightarrow \varepsilon \nabla F$

Except for the first term, this process is symmetric in time: no spurious entropy production.
When $\Delta t \rightarrow 0$, the quadratic variation is satisfied and δe is small.

A small detour: 1D potential

I will use a simple one dimensional potential to illustrate my results.



$$U(x) = \frac{(3x-4)^4(3x+2)^2}{1024}$$

- Minima: $-\frac{2}{3}$ and $\frac{4}{3}$
- Barrier Height: $U_B = 1$
- $\varepsilon = 0.15$

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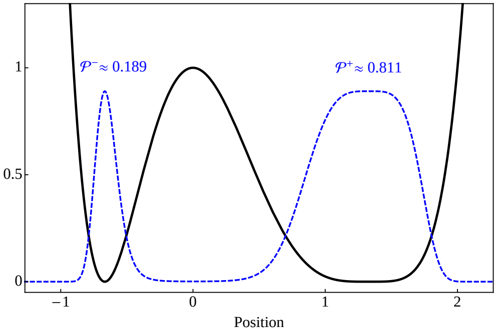

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Boltzmann probability: entropy drives the particle to spend more time in the broad well.

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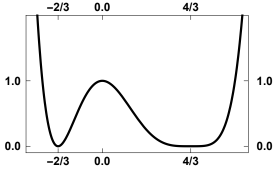
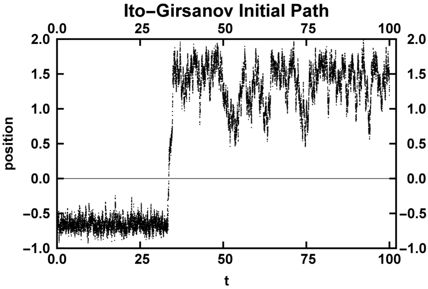
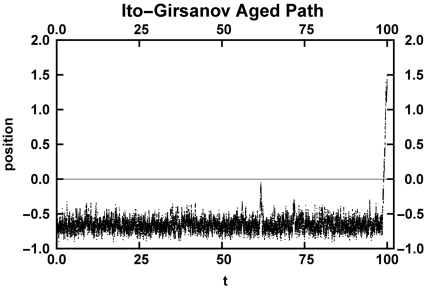
Ito-Girsanov formalism

$$\sum \left(\frac{1}{2} \left| \frac{\Delta x}{\Delta t} \right|^2 + \frac{1}{2} |F|^2 - \varepsilon \nabla^2 U \right)$$





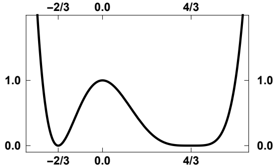


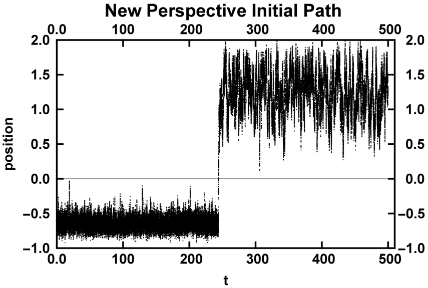
The initial path is constructed to be consistent with Boltzmann. Clearly the final path cannot represent physical transitions.

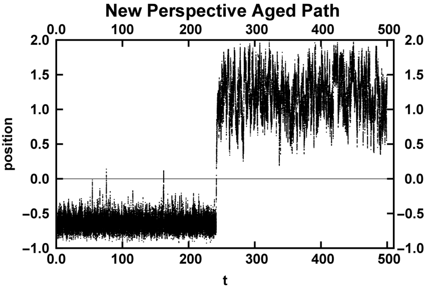
The curvature term is driving the collapse!

New perspective

$$\sum \left(\frac{1}{4}\left|\frac{\Delta x}{\Delta t} + F_{i+1}\right|^2 + \frac{1}{4}\left|\frac{\Delta x}{\Delta t} - F_i\right|^2 \right)$$







The **quadratic structure is essential** for recovering the Boltzmann distribution along the path.

Lessons to take home

- The Onsager-Machlup functional is singular in the continuous time limit.
- Using the Ito-Girsanov leads to unphysical results.
- Using a small (but nonzero) time step in the new formulas leads to sensible and physical results.

Thank You

Acknowledgments

This work would not have happened without many conversations with *Andrew Stuart*, *Robin Ball*, *Gideon Simpson* and *Hendrik Weber*.

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