Unravelling intermittent features in single particle trajectories by a local convex hull method

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Many biological transport processes are intermittent [1, 2], with two or several alternating phases of motion. These phases can be distinguished by a change in their dynamical properties e.g. change in diffusivity, in drift, in autocorrelations, in distribution of increments or in dimensionality. Identification of such distinct phases is of major importance for describing relevant properties such as biochemical reaction rates, or biophysical mechanisms as translocation, transcription or drug delivery. This identification is challenging by two factors: the amount of experimental data is limited and different phases are not known *a priori*. We address the problem of identification of change points between distinct phases in a single random trajectory without prior knowledge of the underlying stochastic model.

We introduce two model-free estimators based on a local convex hull (LCH) constructed over trajectory points. The basic idea consists in considering a weighted *local* functional of the trajectory, $S(n)$, which depends on 2τ points around a point x_n. When applied to successive points along the trajectory, this local functional transforms the trajectory into a new time series, which can then be used to discriminate between different phases. The points x_n with $S(n)$ below some threshold are assigned to one phase while the remaining points are assigned to the other phase. We consider two functionals based on the local convex hull, the volume and the diameter (the largest distance in the hull).

Being based on purely geometrical properties of a trajectory, this method is sensitive to various changes in the dynamics and can be applied to a trajectory in any dimension. Its integral-like form makes it robust even in very noisy situations. We validate the LCH method by applying it to several models of intermittent processes. The recognition score R (the fraction of correctly recognized points) was computed by averaging over 1000 independent trajectories. Figure 1 illustrates one example of heterogeneous diffusion, in which the particle diffuses in a composite medium with high and low diffusivities.

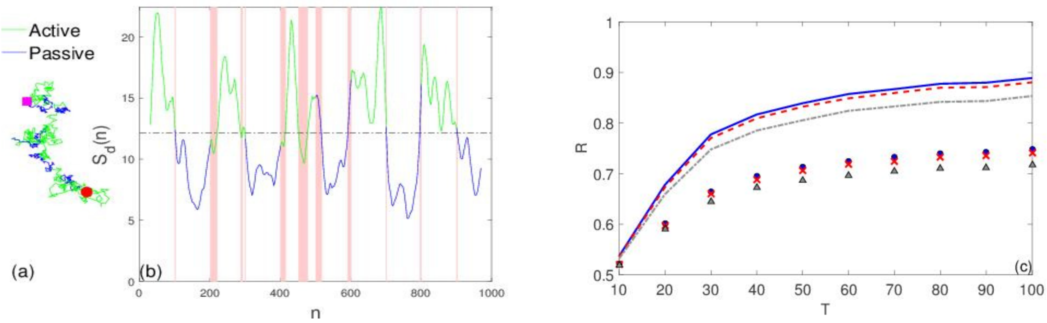

Figure 10: **(a)** A single trajectory with 1000 points of planar Brownian motion alternating a “slow” phase (D_1 = *1/4*, dark blue) and a “fast” phase (D_2 = *1*, light green), each phase duration *T=100*. **(b)** The weighted LCH diameter $S_d(n)$ with the window size τ = *10*, applied to this trajectory. Pink shadow highlights the false identification zones. Dashed horizontal line shows the empirical mean S_d over that trajectory. **(c)** Recognition score *R* of the diameter-based discriminator $S_d(n)$ as a function of the mean phase duration *T*. Lines show the results for the case D_2 =*1/4* with three noise levels σ_n: *0* (blue solid), 0.5 σ (red dashed), and σ (gray dash-dotted) (σ being the empirical standard deviation of increments calculated for each trajectory). Symbols correspond to the case D_2 = *1/2* with the same levels of noise.

References

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