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Citation: Chin. Phys. B, 2025, 34 (**5**): 050205. DOI: 10.1088/1674-1056/adcb99
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SPECIAL TOPIC — Computational programs in complex systems

Trajectory tracking on the optimal path of two-dimensional quadratic barrier escaping

Zengxuan Zhao(赵曾轩)[1], Xiuying Zhang(张秀颖)[1], Pengchen Zhao(赵鹏琛)[1], Chunyang Wang(王春阳)[1,2,†], Chunlei Xia(夏春雷)[2], Mushtaq Rana Imran[1], and Joelous Malamula Nyasulu[1]

[1] *Institute of Theoretical Physics, School of Physics and Optoelectronic Engineering, Ludong University, Yantai* 264025, *China*
[2] *Yantai Institute of Coastal Zone Research, Chinese Academy of Sciences, Yantai* 264003, *China*

(Received 24 December 2024; revised manuscript received 9 April 2025; accepted manuscript online 11 April 2025)

The diffusion trajectory of a Brownian particle passing over the saddle point of a two-dimensional quadratic potential energy surface is tracked in detail according to the deep learning strategies. Generative adversarial networks (GANs) emanating in the category of machine learning (ML) frameworks are used to generate and assess the rationality of the data. While their optimization is based on the long short-term memory (LSTM) strategies. In addition to drawing a heat map, the optimal path of two-dimensional (2D) diffusion is simultaneously demonstrated in a stereoscopic space. The results of our simulation are completely consistent with the previous theoretical predictions.

Keywords: trajectory tracking, optimal path, two-dimensional barrier escaping, deep learning

PACS: 02.70.–c, 05.40.Jc, 07.05.Bx

DOI: 10.1088/1674-1056/adcb99 **CSTR:** 32038.14.CPB.adcb99

1. Introduction

The model of multi-dimensional (MD) barrier escaping is of great use in many fields of scientific studies. For example, in the fusion reaction of massive nuclei, where the asymmetrical or the neck degree of freedom of the compound nuclei needs to be considered,[1,2] MD barrier escaping is proved to be the most convenient model to reveal the complicated mechanism of the reactions. Based on these considerations, Abe and Boilley *et al.* presented an analytical matrix operation to calculate the MD fusion probability.[3] Zagrebaev and Greiner proposed a set of differential equations to describe the morphological change of the reactive nuclei.[4,5] Although there are still some other innovative methods to deal with this problem, the milestone progress in recent years is thought to be the prediction of a MD diffusion optimal path[6,7] which is in accordance with the maximum probability of successful fusion of the massive nuclei.

However, in the previous studies, there is actually not a clear image of the optimal path. What the authors provided in reality is only an optimal incidence angle and an analytical prediction on the existence of an optimal path. The diffusion of the particles along the optimal path has not yet been revealed genuinely. Recently, we noticed that this can be satisfactorily achieved by a numerical process of trace tracking based on deep learning.[8–10] Therefore in this paper, in order to obtain a clear illustration of the optimal path, we take the two-dimensional (2D) case as an example to track in detail the diffuse trajectory of the particles. The generative adversarial networks (GANs)[11,12] are used to generate and assess the rationality of the data in each step. The long short-term memory (LSTM)[13,14] is applied to optimize the path of trace tracking.

The paper is organized as follows. In Section 2, the research background of the 2D optimal path is reviewed briefly for cherry-picking of the deep learning strategies. The numerical procedure of how to generate and assess the rationality of the trajectory data by GANs and how to optimize them with LSTM is elucidated concisely. In Section 3, The results of trace tracking on the diffusion trajectory of the Brownian particles are presented as figures. The optimal path of the 2D quadratic barrier escaping is demonstrated clearly both in the heat map and the stereoscopic space. Section 4 serves as the concluding part of this article where some discussions and prospects are also presented.

2. Learning strategy selection

Mathematically, the dynamic process of a Brownian particle escaping from a multi-dimensional potential energy barrier can be described by the following generalized Langevin equation (GLE):

$$m_{ij}\ddot{x}_j(t)+\beta_{ij}\dot{x}_j(t)+\omega_{ij}x_j(t)=\xi_i(t), \tag{1}$$

where m_{ij}, β_{ij} and ω_{ij} are the tensors of inertia, friction and potential curvature, respectively. $\xi_i(t)$ is the tensor of random force, which is always supposed to be Gaussian with its second-order moment satisfying the fluctuation-dissipation theorem

$$\langle\xi_i(t)\xi_j(t')\rangle=k_{\rm B}Tm_{ik}^{-1}\beta_{kj}\delta(t-t'), \tag{2}$$

†Corresponding author. E-mail: wchy@foxmail.com

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where k_B is the Boltzmann constant and T the temperature. The Einstein summation convention is used here for the simplicity of mathematical expressions, i.e., the repeated subscripts represent the corresponding matrix elements of each tensor.

In the neighborhood of the saddle point, the barrier of the potential energy surface (PES) is generally approximated to be quadric, therefore, the potential can be described as

$$U(x_i,x_j)=\frac{1}{2}\omega_{ij}x_ix_j, \quad \text{with} \quad i,j=1,2,\ldots. \tag{3}$$

As an example illustrated in Fig. 1, the shape of the PES tends to be a hyperbolic paraboloid in the 2D case.

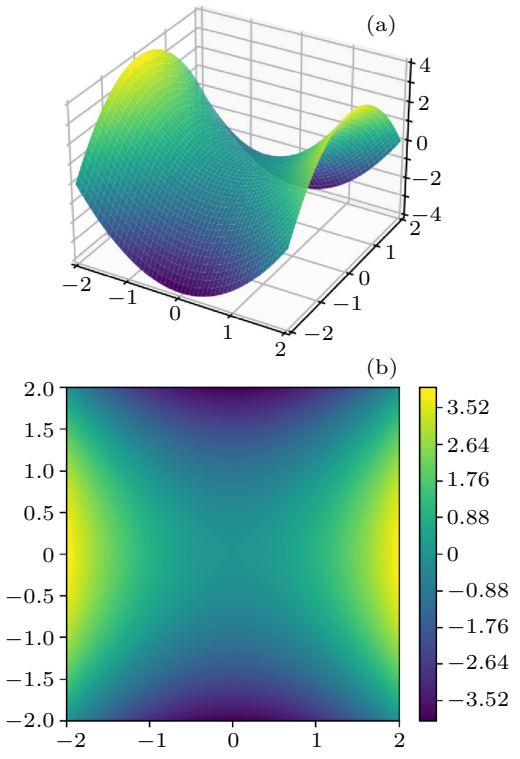


Fig. 1. (a) A 2D quadratic potential energy surface and (b) its heat map.

In the dynamic process of a 2D quadratic barrier escaping, the particles are generally supposed to start their motion from the initial position x_{10} with an initial velocity v_{10}. As time goes on, with the help of thermal diffusion in the system, they travel along the route which has the lowest obstacle of potential energy. Theoretically, this route is always suspected to be the valley of the 2D hyperbolic paraboloid. However, another route was predicted analytically as the optimal path in Ref. [6].

This is a starkly unexpected result from the viewpoint of energy criterion. Experimental proofs and numerical simulation results are needed urgently for its certification. But as far as we known, no further research has been conducted till now except for a theoretical prediction of the 3D optimal path.[7] In order to have a clear understanding on the existence of the optimal path, we take the 2D case as an example to show some microscopic insights into its inner mechanism.

Our basic idea is to rely on the numerical strategy of deep learning to track the motion trajectory of the Brownian particles in a hyperbolic saddle surface and determine the optimal path with the diffusing particle in a numerical way of less difficulty. The generative adversarial networks (GANs),[11,12] consist of two neural networks: one plays the role of a generator to produce samples from the target space, the other acts as a discriminator to evaluate the quality of these samples, are selected firstly at the beginning for a high efficiency of initial data training.

The long short-term memory (LSTM),[13,14] which is a variant of the recurrent neural network (RNN),[15,16] is applied succeedingly to optimize the results of trace tracking. LSTM is a gradient-based method that is specifically designed for processing and predicting sequential data. It can learn to bridge long-time lags by enforcing constant error flow through special units and capture more efficiently the long-term dependencies with the help of gating mechanisms and memory cells.

The benefit of choosing GANs and LSTM is that they can be used for learning deep representations without any extensive annotated data training. Although there are some limitations of GANs, such as lacking diversity as well as needing long training times, they still have many advantages in generating and assessing the rationality of the data. From the perspective of algorithm efficiency, LSTM can outperform other recurrent network algorithms in various kinds of artificial tasks.[17]

At the beginning of trace tracking, we use the generator of GANs firstly to generate a vector $\boldsymbol{r}$ from the random noise and then use it subsequently as a new input of the generator to generate a series of false trajectory data $G(\boldsymbol{r})\rightarrow(x(t),y(t),z(t))$. Then we input the generated false data $G(\boldsymbol{r})$ into the discriminator to obtain a probability of judgment $D(G(\boldsymbol{r}))$. The optimization of the generator in the learning process is then to maximize the probability of $D(G(\boldsymbol{r}))$.

At the same time, we solve the GLE analytically and then select a series of real data of the diffusion trajectory from the analytical results, marking it as r. Using r as the new input of the discriminator, we will obtain another probability of judgment $D(r)$. The optimization of the discriminator is then to maximize the probability of $D(r)$ while minimizing the probability of $D(G(\boldsymbol{r}))$. Then, by initializing the weights and performing multiple rounds of generative adversarial training, a series of trustworthy results can be finally obtained.

Another advantage of LSTM is its time sensitivity, which enables it to learn some specific patterns and features from the time series. Corresponding to the process of barrier escaping, after enough rounds of learning and training, the sports mode of the 2D diffusing Brownian particles will be grasped. The possible direction of moving can then be predicted based on the historical memory of trace tracking, resulting in at last a continuous path of diffusion under numerical optimization.

3. Results of trace tracking

In order to verify the rationality of the learning strategy and ensure the correctness of the results, we inspect first the incident angle which was defined in Ref. [6] as the angle $\theta_{\rm m}$ clockwise from the positive half to the negative half of the x_1 axis under the same set of system parameters. The difference between this prospection and the previous prediction is that the incident angle $\theta_{\rm in}$ is now defined to be the angle counterclockwise from the positive half to the negative half of the x_2 axis, i.e., they are complementary angles. Since the optimal value of $\theta_{\rm m}$ was predicted to be 0.258 rad ($\theta_{\rm m} \cong 15^\circ$) in Ref. [6], the optimal value of $\theta_{\rm in}$ is now expected to be 75° approximately.

For the convenience of future discussions, we need to go on to define another quantity of $P(t)$ in accordance with the probability of a Brownian particle successfully surmounting the barrier of the 2D PES. Its stationary value is described as $P_{\rm s}$, which can be detected conveniently during the process of trajectory tracking by counting the number of particles that have already arrived at the saddle point and calculating the proportion of it based on the total number of all the Brownian particles.

In Fig. 2, $P_{\rm s}$ is plotted as a function of $\theta_{\rm in}$ at different tracking accuracy, which is determined by the gap of each tracking step $g_{\rm t}$, i.e., the smaller the gap, the higher the accuracy. We can see that there are several peaks of each curve but their maximum emerges at the same value of $\theta_{\rm in} \cong 75^\circ$, implying that there is an optimal incident angle in this direction. This is obviously consistent with the previously predicted results.

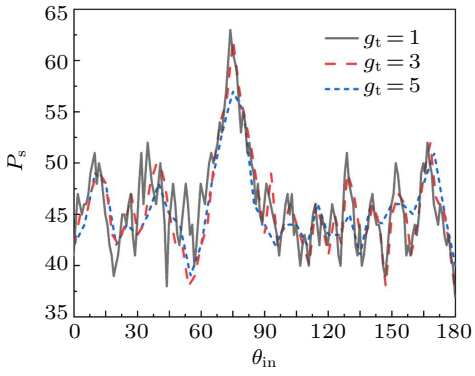


Fig. 2. The $\theta_{\rm in}$ dependence of $P_{\rm s}$ at various precisions of $g_{\rm t}$.

Based on these tests and inspections, we can find that the strategy of tracing with GANs and LSTM is reliable. The trajectory of the diffusing particles can be revealed correctly by these means. Therefore, to present some information on the tracing details, we track on the optimal path directly in the following with this learning strategy of combining GANs with LSTM.

The parameters in the GLE are rescaled to diagonally dimensionless numbers $m_{11} = m_{22} = 1.0$, $\beta_{11} = 0.5$, $\beta_{22} = 0.3$, $\omega_{11} = 2.0$, $\omega_{22} = 1.0$ for simplicity. The input dimension of the generator is set to be 100 and the number of nodes in each layer of dense is 256 and 512. The data generated from GANs are trained more than 1000 times before they are input into the LSTM.

Figure 3 shows the detailed diffusion trajectory of the Brownian particles obtained from trace tracking, where the starting point is set to be $x_{10} = -2.0$, $x_{20} = 0.0$ and the particles are supposed to diffuse freely on the PES under the combined influence of inertia, viscosity and perturbations emerging from the thermodynamic fluctuation and dissipation of the system.

In addition to displaying the results of trace tracking in a 2D heat map, we present simultaneously in Fig. 3 in the 3D space a stereoscopic illustration of the trajectories. We can see that the trajectory of the particles is relatively chaotic. There is no discernible pattern that can be excepted for it except for random walk.

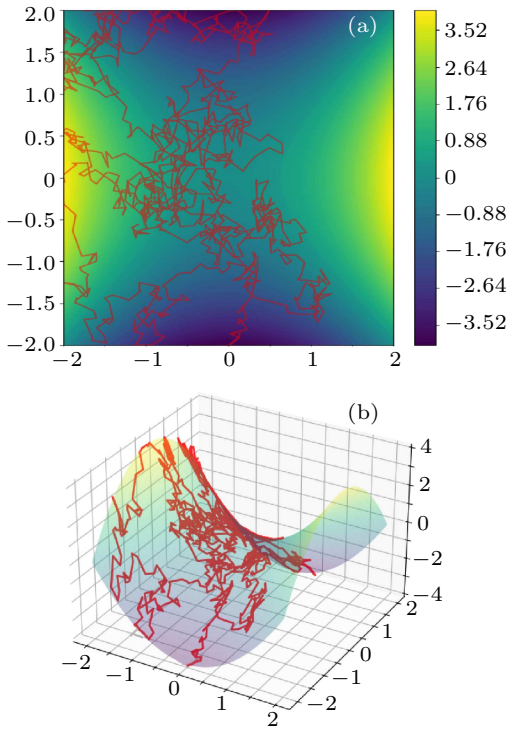


Fig. 3. Trace tracking results of the trajectories before noise reduction.

In order to obtain a clearer image of the diffusion optimal path, we tried some means to improve the degree of accuracy in the tracking of each step and reduced the noise of the above learning process as much as possible. The final appearance of the optimal path is then clearly shown in Fig. 4 in the heat map and stereoscopic space together with the image of a 2D quadratic PES. We can see that the trajectory of the particle still retains the obvious characteristic of random walking. But overall, it deviates from the route we speculated from the perspective of the lowest energy, i.e., the valley of the PES. Under

the combined effect of the thermodynamic factors of the system, the particles select to move along a route with relatively high potential energy.

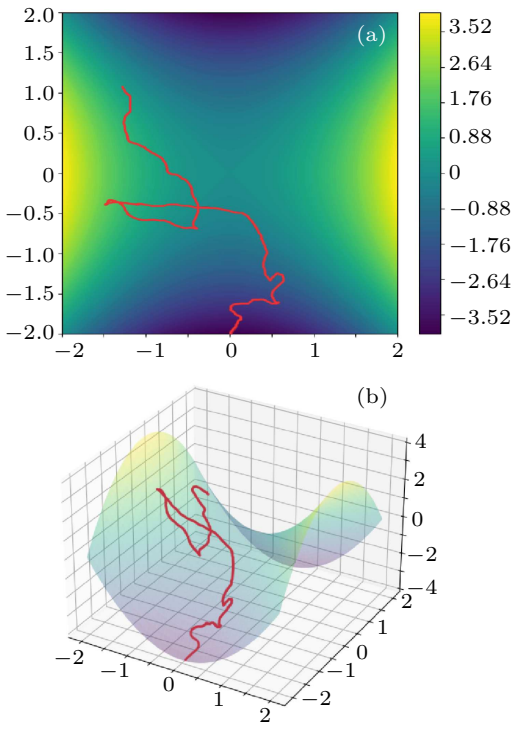


Fig. 4. (a) 2D and (b) 3D description of the optimal path after noise reduction.

4. Discussion and conclusion

In conclusion, we have tracked in this paper the trajectory of a Brownian particle diffusion on a 2D quadratic PES under the theoretical guidance of deep learning strategies. The originally determined optimal incident angle in Ref. [6] is re-enacted at different learning precisions as a detection and certification of the correctness of our research plan. The optimal path analytically predicted in the previous studies is depicted authentically in the heat map and 3D stereoscopic space. The theoretical and practical significance of this result is easy to be comprehended. Because as far as we know, this is the first time for us to obtain a clear description of the optimal path.

As has been mentioned in the introduction, the model of MD barrier escaping is of great use in many fields of scientific studies due to its convenience in describing various phenomena with mathematical equations such as the GLE. But it is always a hard work to solve these equations analytically. Because of this, numerical simulations, especially the rapidly developing machine learning strategies in recent years, become the indispensable approaches. But as far as we know, machine learning strategies are still rarely used in the study of barrier escaping problems. Our work may act as a starting point of these attempts in the near future.

As a prospect, we would like to say that the deep learning strategy of combining GANs with LSTM used in this paper has many advantages in tracking the trajectory of diffusion particles. It can be used more extensively in the future in the study of many analogous processes in chemistry, biology and nuclear physics to get more meaningful results of authenticity, for example, the diffusion in a bistable system,[18] the biochemical processes in solution and living cells,[19] the reaction mechanism and anomalous diffusion of some random dynamical systems concerning the amazing barrier crossing dynamics.[20–24]

Program availability

The source code is openly available in the Science Data Bank at https://doi.org/10.57760/sciencedb.j00113.00231 and https://doi.org/10.57760/sciencedb.j00113.00232.

Acknowledgements

This work was supported by the Natural Science Foundation of Shandong Province (Grant No. ZR2020MA092) and the Innovation Project for Graduate Students of Ludong University (Grant No. IPGS2024-048). The authors would like to express their sincere thanks to the open accesses of the original codes of GANs and LSTM.

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