Project 2. Variational neural network-based solvers and PINNs.

Submit two IPYNB files, one for each problem. All figures and numbers must be displayed in them.

1. The committor problem with the rugged Mueller potential and high-dimensional noise is a popular test problem used e.g. in [1]: Lai and Lu (2017), [2]: Khoo, Lu, Ying (2018), [3]: Li, Lin, Ren (2019) (Section IV, page 6), and [4]: Yuan et al. (2023) (Section 6.2, page 15, Fig. 6). Please take problem parameters from Yuan et al. (2023) (Eqs. (82) and (71)) and training set generation details either from Li et al. (2019) or from Yuan et al. (2023). Set $\beta = 0.1$, which corresponds to temperature $T = 10$.

   (a) Solve the committor problem using a neural network solver based on the variational formulation as it is done in Face_NN_deltanet.ipynb.

   (b) Check your solution using the approach called *committor analysis*. This approach is used when the reference solution is unknown. This approach was used in Li et al. (2019). Do the following.

   - Extract the isocommittor curve $q = 0.5$ of the committor function projected onto the (x_1, x_2)-space.
   - Generate $N = 50$ or 100 points (if your computer is slow, set $N = 50$, if it is alright, set $N = 100$) on it sampled according to the probability measure $e^{-\beta V}$ restricted to this surface. For example, generate many points on this curve, prescribe weights to it equal to $e^{-\beta V}$. Sum all these weights dived these weights by their sum to obtain the probability distribution. Then sample N points according to this probability distribution.
   - For each of these N points, launch $M = 200$ stochastic trajectories and terminate them as soon as they reach A or B. For each point, find the probability to reach B rather than A. This is exactly the committor probability!
   - Plot a histogram of these probability data. If your isocommittor curve $q = 0.5$ is at the right location, the histogram must peak at $p = 0.5$. You can look at an example of such a histogram in [5]: Evans et al (2021) (Fig. 11, page 21).

2. (a) Use PINNs [6]: Raissi, Perdikaris, Karniadakis (2019) to solve the initial-boundary-value problem for the Allen-Cahn PDE (Eq. (12) on page 6 of the PDF). Use the continuous-time setting described in [6] (Section 3.1) and used for the nonlinear Schroedinger equation example in this paper and implemented in NLSE_PINNs.ipynb.

(b) Generate a reference solution to the same problem using the spectral method in NLSE_spectral.ipynb.

(c) Compare these two solutions by plotting their heatmaps, plotting the solutions at times $t = 0.1$ and $t = 0.9$, and computing the MAE (mean absolute error) and RMSE (root-mean-squared) errors.

References

[1] R. Lai and J. Lu, "Point cloud discretization of fokker–planck operators for committor functions," *Multiscale Modeling & Simulation*, vol. 16, no. 2, pp. 710–726, 2018.

[2] Y. Khoo, J. Lu, and L. Ying, "Solving for high-dimensional committor functions using artificial neural networks," *Research in the Mathematical Sciences*, vol. 6, p. 1, 2019.

[3] Q. Li, B. Lin, and W. Ren, "Computing committor functions for the study of rare events using deep learning," *The Journal of Chemical Physics*, vol. 151, p. 054112, 08 2019.

[4] J. Yuan, A. Shah, C. Bentz, and M. Cameron, "Optimal control for sampling the transition path process and estimating rates," *Communications in Nonlinear Science and Numerical Simulation*, vol. 129, p. 107701, 2024.

[5] L. Evans, M. K. Cameron, and P. Tiwary, "Computing committors in collective variables via mahalanobis diffusion maps," *Applied and Computational Harmonic Analysis*, vol. 64, pp. 62–101, 2023.

[6] M. Raissi, P. Perdikaris, and G. Karniadakis, "Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations," *Journal of Computational Physics*, vol. 378, pp. 686–707, 2019.