



Project: Transition path theory

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Consider the depicted potential with two 'deep' minima at $\mathbf{x}_1 = (-1, 0)$ and $\mathbf{x}_2 = (1, 0)$ and a 'shallow' minimum at $\mathbf{x}_3 = (0, 5/3)$.

1. Using the provided python script, `trajectory.py`, generate a trajectory at inverse temperature, $\beta = 1.5$
2. Choose a 50×50 regular grid discretization of the depicted rectangle, $\Omega = [-1.8, 1.8] \times [-1.2, 2.2]$, to discretize the generated trajectory.
3. Using the discretized trajectory construct a *reversible* Markov model
4. Choose disks around \mathbf{x}_1 and \mathbf{x}_2 as reactant and product sets A, B and compute forward and backward committor functions.
5. Plot the committor function and the potential function on the domain Ω . You can find the function for the potential in the `trajectory.py` file.
6. Compute the dominant reaction pathways and plot them together with the potential function. You only need to compute 10% of all reaction pathways.

Repeat your experiment at inverse temperature $\beta = 3.0$. Compare your results and discuss your findings.