- **Goal**: To develop a machine-learning methodology for discovering reaction paths in multi-dimensional potential landscapes of chemical reactions.
- **Methodology**: Given a potential, identified for instance by the techniques of computational chemistry, the problem is to find the most probable path from the reactants to the products. As the underlying Langevin equation can be lifted to the corresponding Fokker-Planck description, the most probable path is found by an Onsager-Machlup path integral [4, 2, 1]

$$P[q(t)] = \int_{q_0,t_0}^{q_1,t_1} \exp(-S[x(t)])\mathcal{D}[x(t)] \tag{1}$$

where $S[x(t)]$ is the Onsager-Machlup action for path $q(t)$. Figure 1 shows how the optimal path between the reactants and products can be found by minimization of the action.

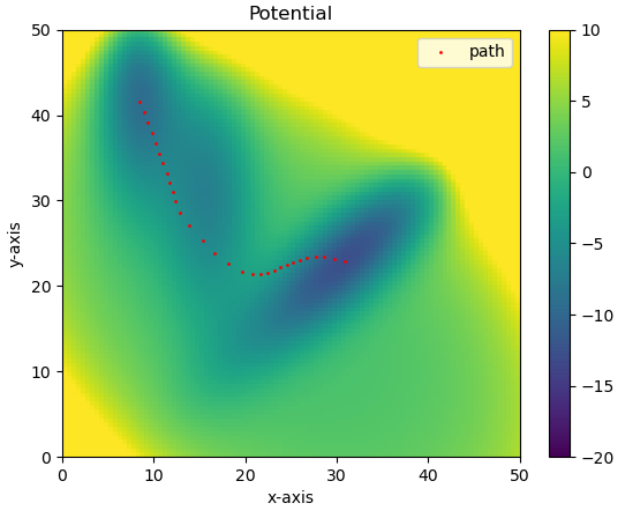

Figure 1: A prototype potential between two basins of attraction (the Müller-Brown potential [3]). The x-and-y axes denote the tentative collective variables significant for a chemical reaction (for instance a dihedral angle and a distance [5]). By minimizing the Onsager-Machlup action (using the PyTorch framework), we are able to find the optimal transition path from the reactants to the products. The method is suitable for potentials defined by trained neural networks.

- **Specific tasks**:
  1. Implementation of the Onsager-Machlup optimization within the Julia programming language (alternatively, passing form the PyTorch implementation to JAX).
  2. Extension of the method from the Müller-Brown potential to a simple but realistic chemical potential encoded by neural networks.
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