Two possible projects with autoencoders

Introduction

The discovery of collective variables of stochastic systems is a problem of great interest in a variety of contexts, including those of our REU. Specifically, we often choose to model such systems either with full Langevin dynamics

$$dq = \frac{p}{m} dt$$
$$dp = -(\nabla V(q) - \gamma p)\, dt + \sqrt{2\gamma m \beta^{-1}} dW_t$$

or the overdamped simplification:

$$dq = -\nabla V(q) d\tau + \sqrt{2\beta^{-1}} dW_\tau.$$

In many contexts, there is actually a map $\xi : \mathbb{R}^D \to \mathbb{R}^d$, i.e the *collective variable* that *coarse grains* these systems in the low dimensional space $\mathbb{R}^d$ such that the original dynamics in q can be described/understood/modeled in terms of the dynamics in $\xi(q)$. Our goal is to find ξ.

Autoencoders

An autoencoder is a neural network $f = f_d \circ f_e$ that approximates the identity function. However, the most important components of f are the encoder f_e which takes the input to a low-dimensional latent space ($\mathbb{R}^d$) and the decoder f_d which takes the latent representation back into ambient space ($\mathbb{R}^D$). In our case, we will think of f_e as the collective variable, and our goal will be to design this using two approaches taking inspiration from

Diffusion Nets by Mishne, Shaham, Cloninger, Cohen (2016) and from the PE for ED paper by Lelievre and Zhang.

Project 1: Target measure diffusion Nets

In diffusion nets, the training set is X with diffusion map Ψ. The encoder is trained to approximate the diffusion map:

$f_e = argmin_{W_e} \sum_{i=1}^{n} \|f_{W_e}(x_i) - \Psi(x_i)\|$

The decoder is trained to reconstruct the inputs from the outputs of this decoder. In this project, instead of the diffusion map, we will use the Target Measure Diffusion map (TMD map) Ψ_{TMD}. The benefits of TMD map are numerous, one of which is that it can approximate the generator of the overdamped Langevin dynamics through arbitrarily sampled data. Surprisingly this has not been done before for collective variable discovery!

Important papers:

1. Diffusion Nets by Mishne, Shaham, Cloninger, Cohen (2016)
2. Target Measure Diffusion maps by Banisch, Trstanova, Klus, Koltai, Bittracher (2018)

Project 2: CV through CE autoencoder

In the PE for ED paper by Lelievre and Zhang (2018), the authors suggest an interesting criterion for assessing the quality of a vector-valued collective variable ξ. In particular, with a as the diffusion tensor in the SDE (for O.L.D it could just be the identity matrix, for instance) if we define

$$\Phi_{ij} = \nabla \xi_i \cdot (a \nabla \xi_j)$$

Then set

$$\Pi = I - \sum_{1 \le i,j \le m} (\Phi^{-1})_{ij} \nabla \xi_i \otimes (a \nabla \xi_j)$$

And finally define:

$$\begin{aligned}
\mathcal{L}_0 &= \frac{e^{\beta V}}{\beta} \sum_{1 \le i,j \le n} \frac{\partial}{\partial x_i} \left(e^{-\beta V} (a\Pi)_{ij} \frac{\partial}{\partial x_j} \right), \\
\mathcal{L}_1 &= \frac{e^{\beta V}}{\beta} \sum_{1 \le i,j \le n} \frac{\partial}{\partial x_i} \left(e^{-\beta V} (a(I - \Pi))_{ij} \frac{\partial}{\partial x_j} \right).
\end{aligned}$$

Then the generator of OLD can be written as

$$\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_1$$

Lelievre and Zhang posit that a good choice of ξ corresponds to the case where

operator $\mathcal{L}_0$ contains large coefficients, while $\mathcal{L}_1$ does not.

Let us call this criterion (*). In effect, ξ is a good collective variable if (*) is met. In fact, for systems of the form

$$V(x) = V_0(x) + \frac{1}{\epsilon} V_1(x)$$

This condition is exactly true. This suggests an interesting loss function for an encoder. Essentially, let the encoder be f_e and plugging this into the above construction, let $\mathcal{L}_0^e, \mathcal{L}_1^e$ be the respective operators. Criterion (*) suggests minimizing a loss of the form

$$L(e) = \sum_{x_i} \frac{\|\mathcal{L}_1^e(x_i)\|_F^2}{\|\mathcal{L}_0^e(x_i)\|_F^2}$$

Minimizing this loss would potentially shrink the coefficients of L_1 w.r.t L_0, thus meeting criterion (*). We can also come up with different loss functions whose extrema meet criterion (*). So we should explore designing such an encoder! Or at least tell me why it definitely wouldn't work.

Important papers:

1. Pathwise estimates (PE) for effective dynamics (ED): the case of nonlinear vectorial reaction coordinates