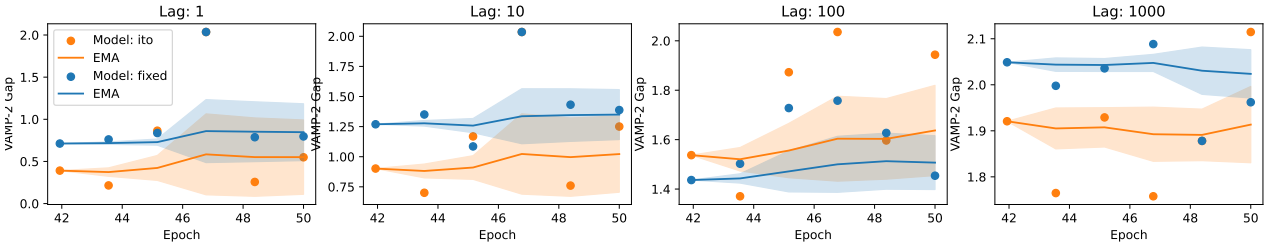

Figure 1: Alanine dipeptide, VAMP2 gaps. We show the gaps at multiple model checkpoints (epochs). Exponential moving average (EMA), exponentially moving standard deviation (EMSD), are shown with lines and shaded areas, respectively.

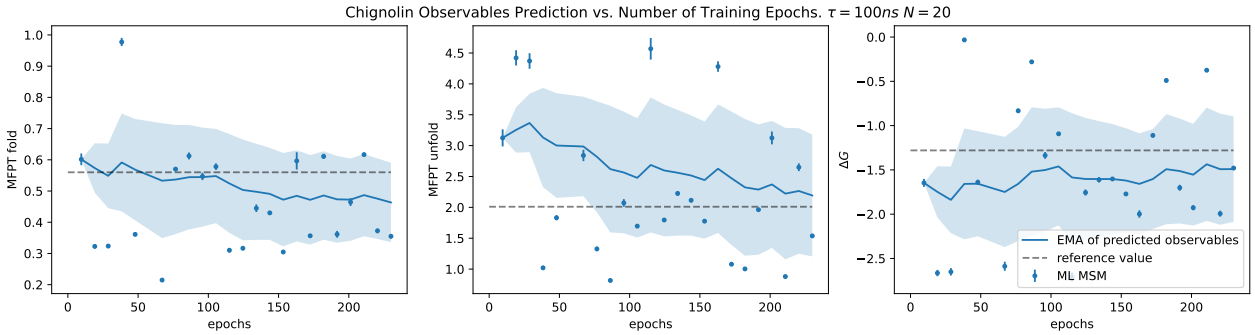

Figure 2: Observables of Chignolin. We show the values at multiple model checkpoints (epochs). EMA, EMSD and five fold cross validated errors, are shown with lines, shaded areas, and errorbars, respectively. While fluctuations persist during training, the amplitudes are small.

Lag	Stochastic lag	Fixed lag
1	0.55(44)	0.85(34)
10	1.02(32)	1.35(21)
100	1.64(18)	1.51(11)
1000	1.91(8)	2.02(5)

Table 1: VAMP2 gaps for alanine dipeptide. Values reported are the values of EMA and EMSD as shown in fig 1 at the last epoch of training.

Observable	ITO	MD
MFPT Fold	0.46 (12)	0.565(4)
MFPT Unfold	2.2 (9)	2.01(2)
Free Energy of Folding ΔG	-1.5 (6)	-1.28(1)

Table 2: Observables of Chignolin. Values reported are the values of EMA and EMSD as shown in fig 2 at the last epoch of training.

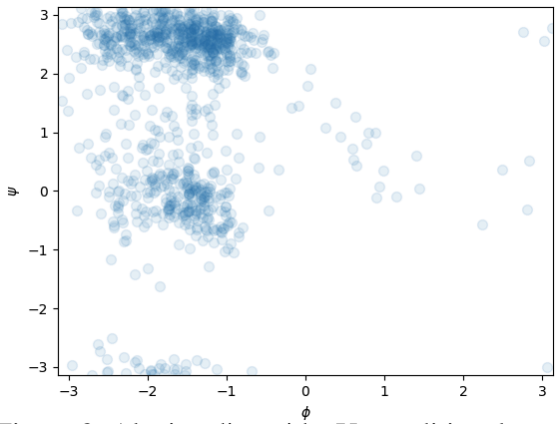

Figure 3: Alanine dipeptide. Unconditional samples from SE3 equivariant model

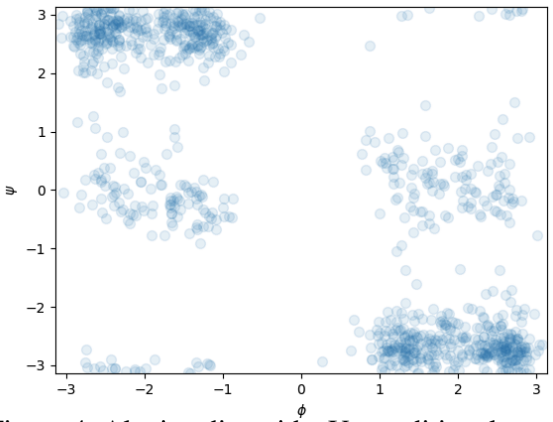

Figure 4: Alanine dipeptide. Unconditional samples from E3 equivariant model. It is essentially Fig. 3 and its mirror image through $\phi = \psi$.