Interpolation of Molecular Dynamics Trajectories with Bi-Directional Neural Networks

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- Solution is a trajectory in phase space

$$x(t) = \begin{bmatrix} r(t) \\ p(t) \end{bmatrix} = \int_{t_0}^{t} f\left(\begin{bmatrix} r(t) \\ p(t) \end{bmatrix}, t \right) dt$$

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Can we learn the phase space dynamics with a ML algorithm?

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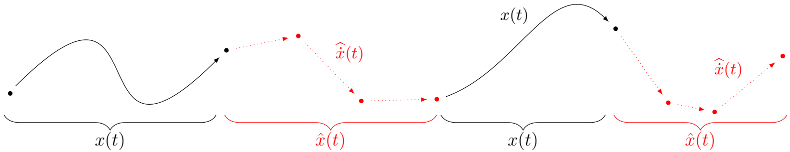

- ODENetwork

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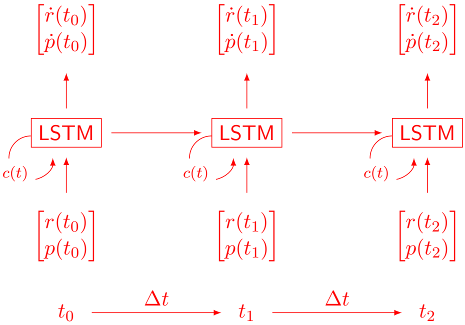
- RNN and LSTM

$$\dot{x}(t) = \begin{bmatrix} \dot{r}(t) \\ \dot{p}(t) \end{bmatrix} = f_\theta\left(\left[\begin{bmatrix} r(t_0) \\ p(t_0) \end{bmatrix}, \ldots, \begin{bmatrix} r(t) \\ p(t) \end{bmatrix}\right], t\right)$$

Learning Dynamical Systems with LSTM

- Best performing due to fewest assumptions and flexible parameterization
- Memory cell $c(t)$ to selectively read and write information
- Outputs $[\dot{r}(t), \dot{p}(t)]^T$ are integrated to obtain solution $\hat{x}(t)$



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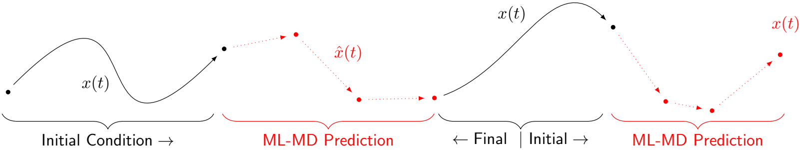

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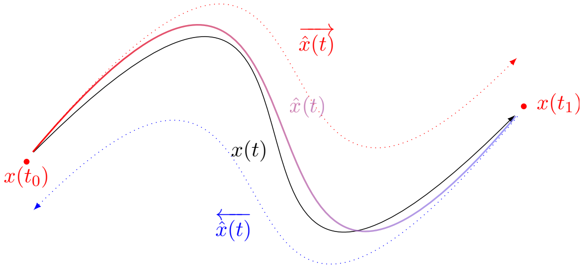
$$\hat{x}(t) = (1 - \lambda(t))\ \overrightarrow{\hat{x}(t)} + \lambda(t)\ \overleftarrow{\hat{x}(t)} \tag{1}$$

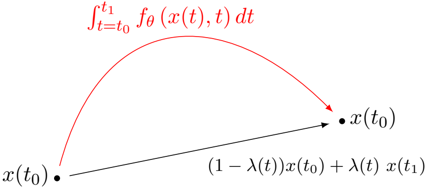


Bi-Directional Interpolation of Differential Equation

- For time-reversible solutions, we obtain

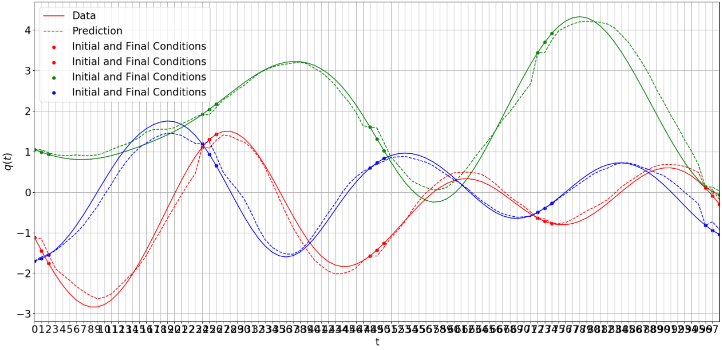
$$\begin{aligned}\hat{x}(t) &= (1-\lambda(t))\ \overrightarrow{\hat{x}(t)} + \lambda(t)\ \overleftarrow{\hat{x}(t)} \\ &= \underbrace{(1-\lambda(t))x(t_0) + \lambda(t)x(t_1)}_{\text{low frequency components}} + \underbrace{\int_{t=t_0}^{t_1} f_\theta\,(x(t),t)\,dt}_{\text{high frequency components}}\end{aligned}$$

- Adiabatic connection frees the ML model to model high frequency signals



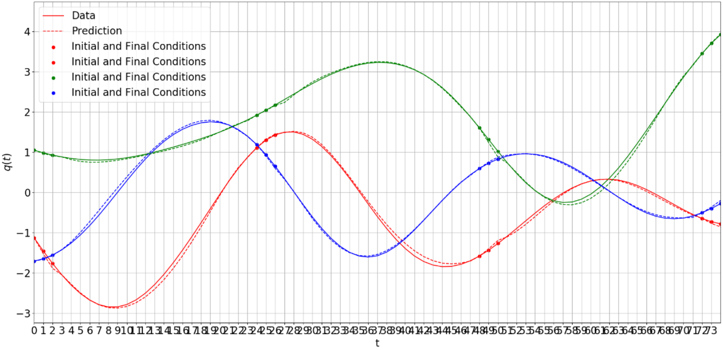
Bi-Directional Interpolation of Differential Equation

- Unidirectional LSTM architecture for Benzene MD trajectory interpolating over 20 time steps



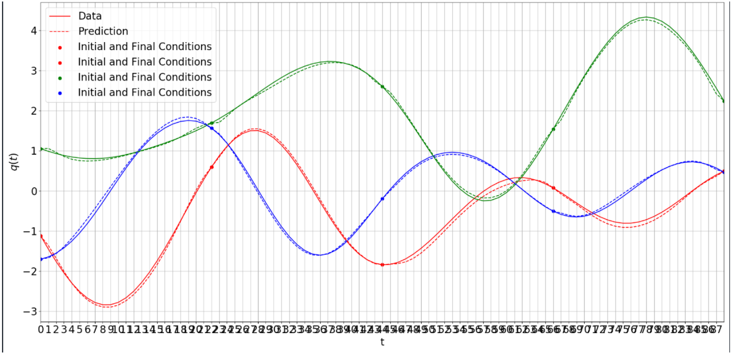
Bi-Directional Interpolation of Differential Equation

- Bidirectional LSTM architecture for Benzene MD trajectory interpolating over 20 time steps
- Final condition and additional bidirectional training smooth trajectories significantely



Bi-Directional Interpolation of Differential Equation

- Single initial and final condition already good for sufficient performance by bidirectional LSTM



Analysis of Interpolations

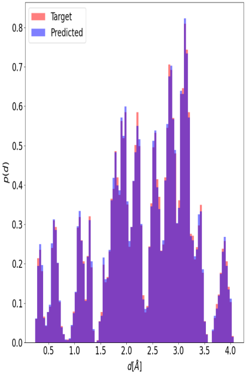


Figure: Keto-Malonaldehyde $(100K)$

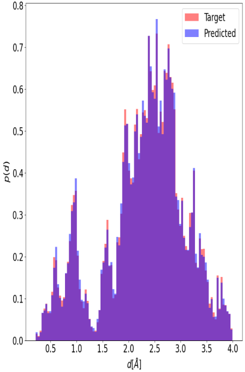


Figure: Keto-Malonaldehyde $(300K)$

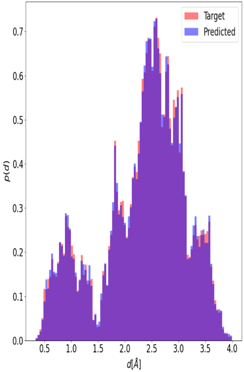


Figure: Keto-Malonaldehyde $(500K)$

Analysis of Interpolations

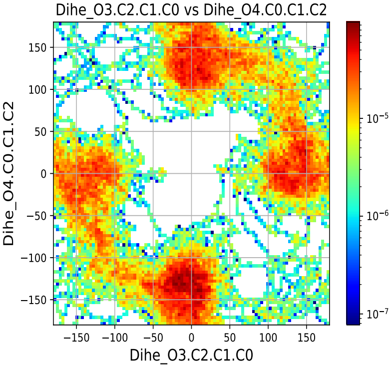


Figure: Ground Truth Free Energy Keto-Malonaldehyde $(300K)$

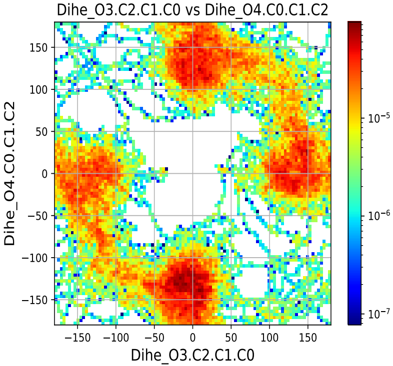


Figure: Predicted Free Energy Keto-Malonaldehyde $(300K)$