Interpolation of Molecular Dynamics Trajectories with Bi-Directional Neural Networks

Ludwig Winkler & Huziel Sauceda

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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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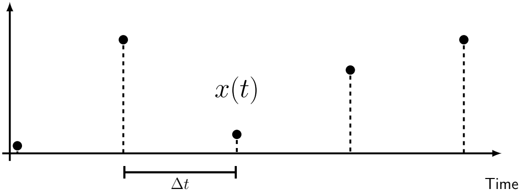

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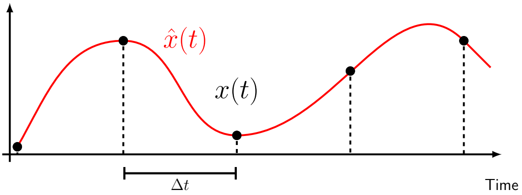

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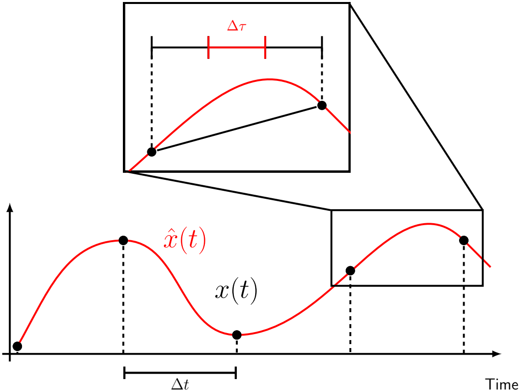

- ODENetwork

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- HamiltonianNetwork

$$\dot{x}(t) = \begin{bmatrix} \dot{r}(t) \\ \dot{p}(t)) \end{bmatrix} = \begin{bmatrix} \frac{\partial \mathcal{H}(r(t), p(t), t)}{\partial p(t)} \\ -\frac{\partial \mathcal{H}(r(t), p(t), t)}{\partial r(t)} \end{bmatrix}$$

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- RNN and LSTM

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

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$$\begin{bmatrix} \dot{r}(t_0) \\ \dot{p}(t_0) \end{bmatrix}$$

$$\uparrow$$

$$\boxed{\text{LSTM}}$$

$$\uparrow$$

$$\begin{bmatrix} r(t_0) \\ p(t_0) \end{bmatrix}$$

$$t_0$$

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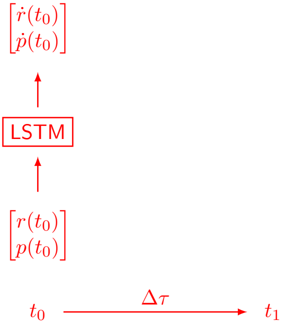

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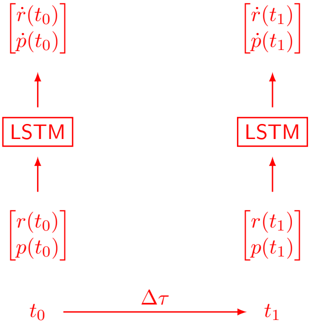

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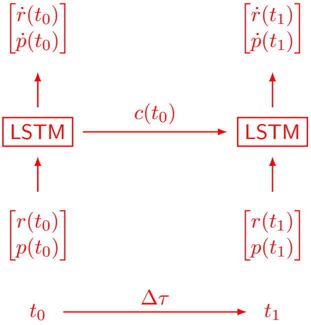

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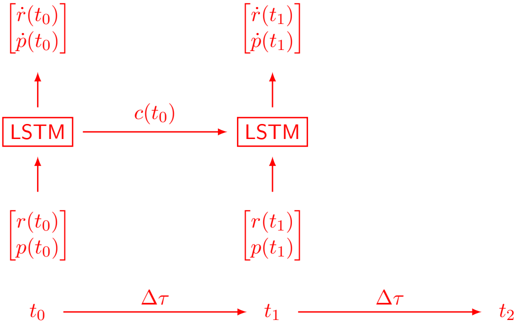

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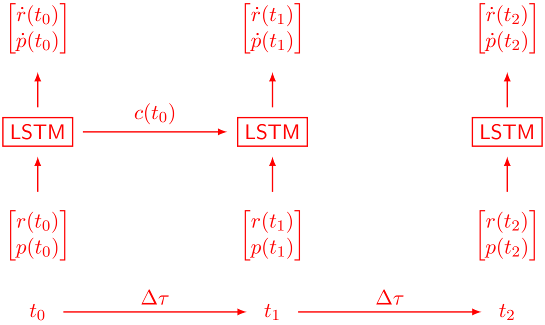

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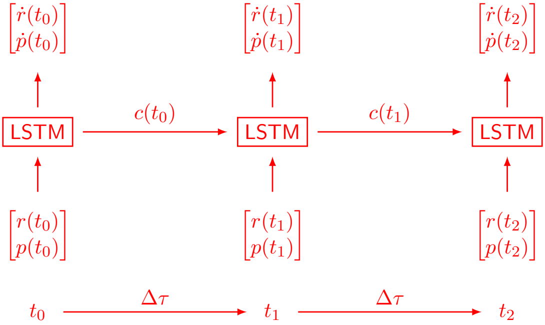

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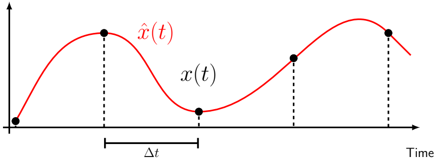

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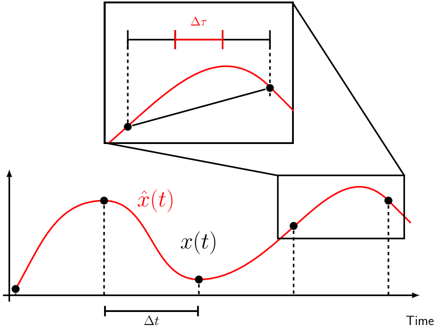

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- Use coarse, analytical MD to provide initial and final conditions
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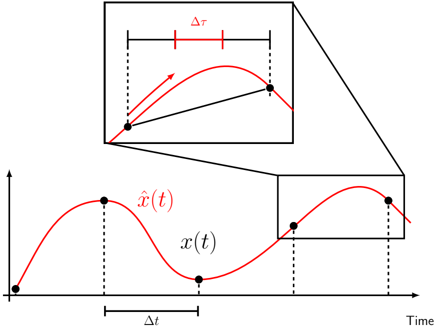
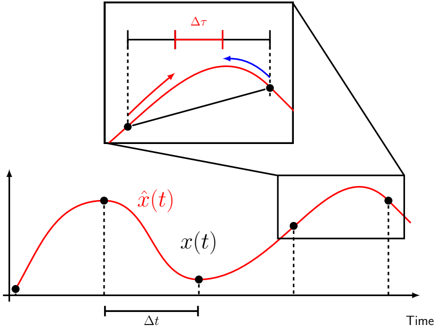


Bi-Directional Interpolation of Differential Equation

- Use coarse, analytical MD to provide initial and final conditions
- Integrate dynamics forward and backward through time



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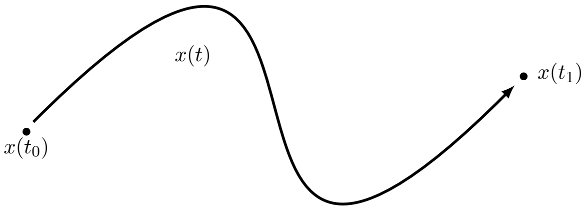

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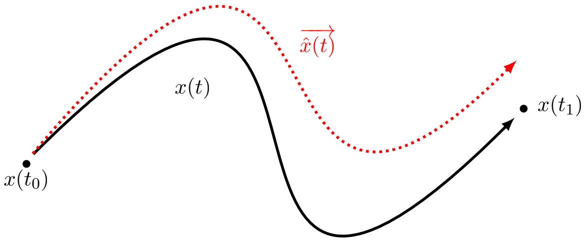

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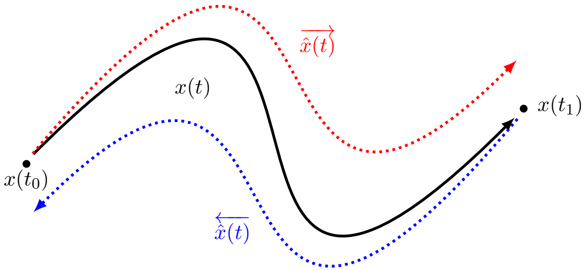

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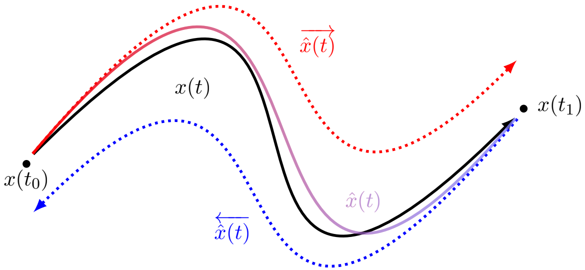
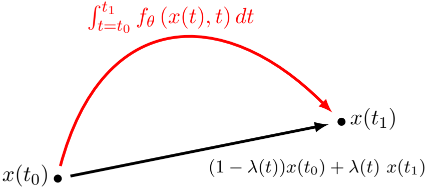


Bi-Directional Interpolation of Differential Equation

- For time-reversible solutions, we obtain

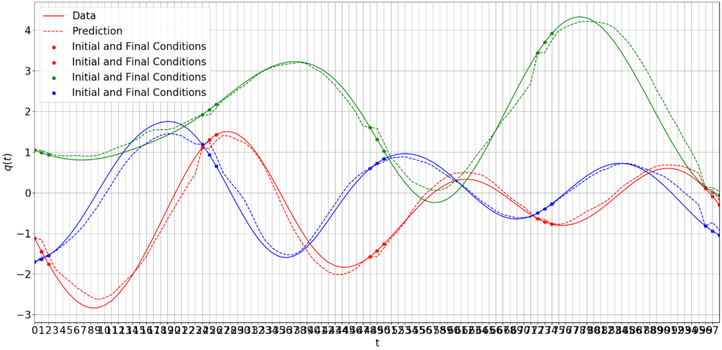
$$
\begin{aligned}
\hat{x}(t) &= (1-\lambda(t))\ \overrightarrow{\hat{x}(t)} + \lambda(t)\ \overleftarrow{\hat{x}(t)} \\
&= \underbrace{(1-\lambda(t))x(t_0) + \lambda(t)x(t_1)}_{\text{low frequency components}} + \underbrace{\int_{t=t_0}^{t_1} f_\theta\left(x(t), t\right) dt}_{\text{high frequency components}}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

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



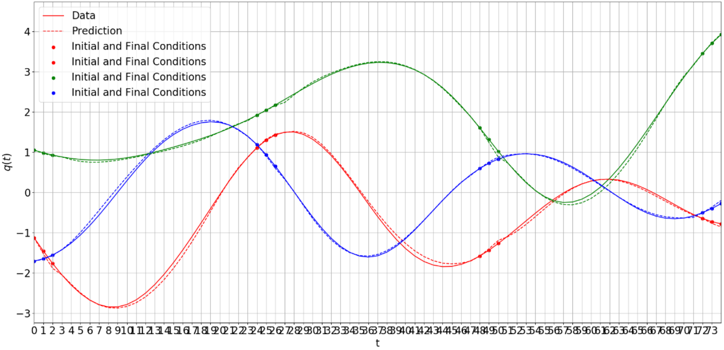
Uni-Directional Interpolation of Differential Equation

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



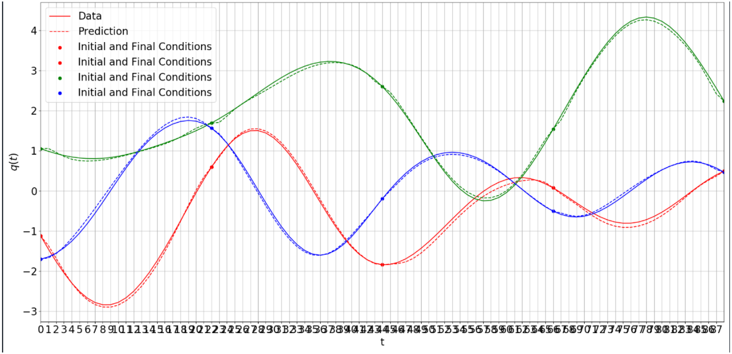
Bi-Directional Interpolation of Differential Equation

- 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

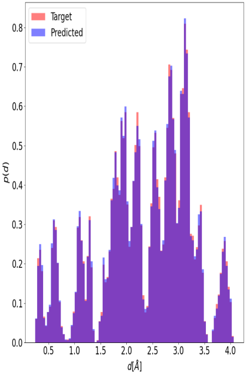


Figure: Keto-Malondialdehyde $(100K)$

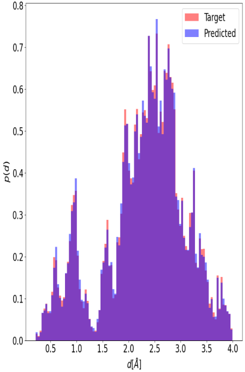


Figure: Keto-Malondialdehyde $(300K)$

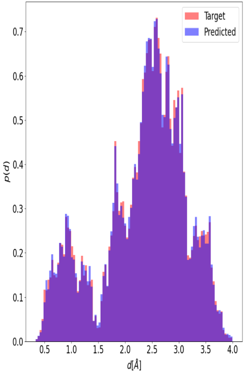


Figure: Keto-Malondialdehyde $(500K)$

Analysis of Interpolations

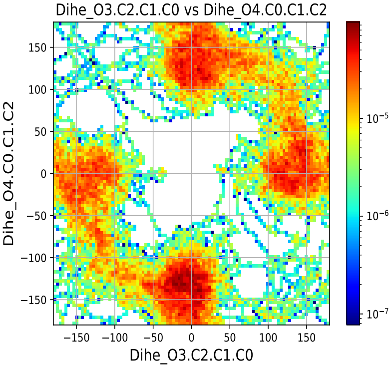


Figure: Ground Truth Free Energy Keto-Malondialdehyde $(300K)$

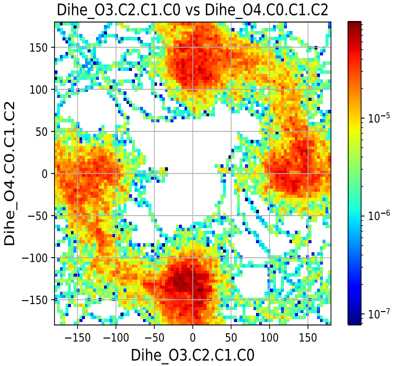


Figure: Predicted Free Energy Keto-Malondialdehyde $(300K)$

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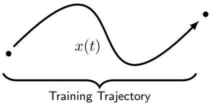

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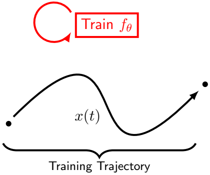

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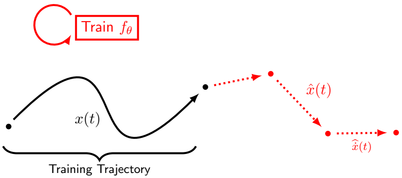

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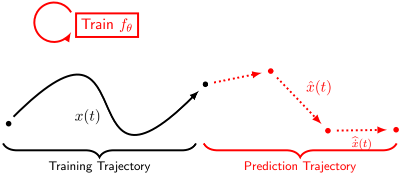

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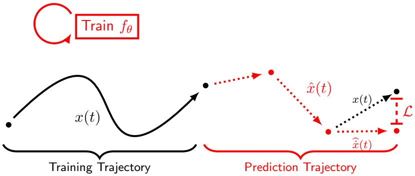

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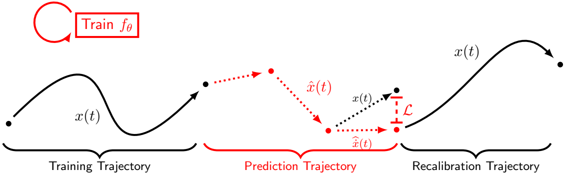

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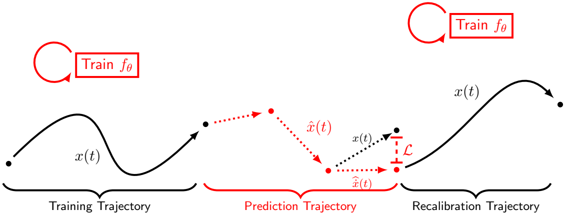

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