

# Interpolation of Molecular Dynamics with Bi-Directional Neural Networks

Ludwig Winkler & Huziel Saucedo

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# Bi-Directional Interpolation of Differential Equation

- Can we predict MD trajectories directly with a neural network (NN)?
- Use NN to predict solver for MD equations
- NN are trained on predicting change in position and momentum
- But we still want the accuracy of real MD simulations?
- Use coarse grained MD simulation to predict initial and final conditions of differential equation governing MD trajectories
- Reconstruct high dimensional components to interpolate smartly with NN between coarse grained solution

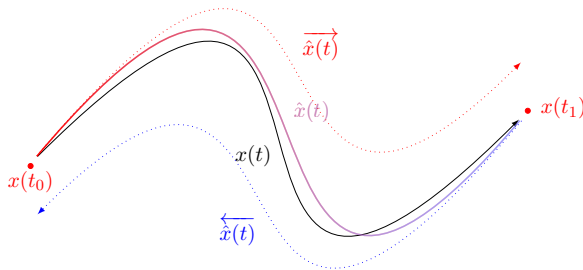
# Bi-Directional Interpolation of Differential Equation

- Given true dynamics  $f$  learn approximate dynamics  $f_\theta$  with NN
- Train  $f_\theta$  to predict the true solutions  $x(t)$
- Integrate approximate dynamics  $f_\theta$  to obtain approximate solution  $\hat{x}(t)$
- Use coarse grained MD simulation to predict initial and final conditions of differential equation governing MD trajectories
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# Bi-Directional Interpolation of Differential Equation

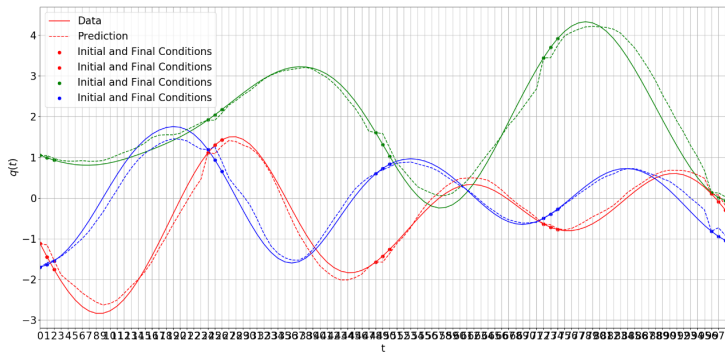
- Predict forward solution  $\overrightarrow{\hat{x}(t)}$  and backward solution  $\overleftarrow{\hat{x}(t)}$  with the **same** dynamics  $f_\theta$
- Use adiabatic connection to interpolate  $\overrightarrow{\hat{x}(t)}$  and  $\overleftarrow{\hat{x}(t)}$  to  $\hat{x}(t)$

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



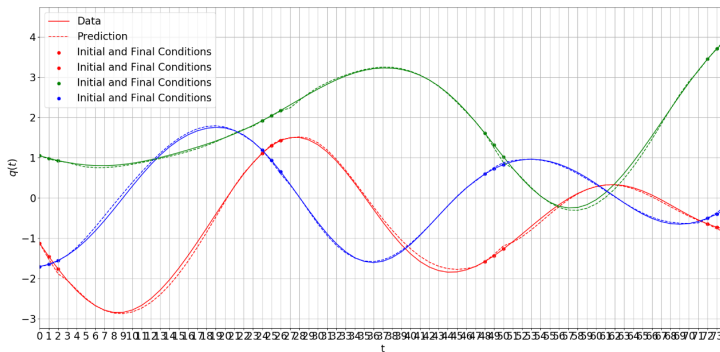
# Bi-Directional Interpolation of Differential Equation

- 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 significantly



# Bi-Directional Interpolation of Differential Equation

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

