Interpolation of Molecular Dynamics with Bi-Directional Neural Networks

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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_θ with NN
- Train f_θ to predict the true solutions $x(t)$

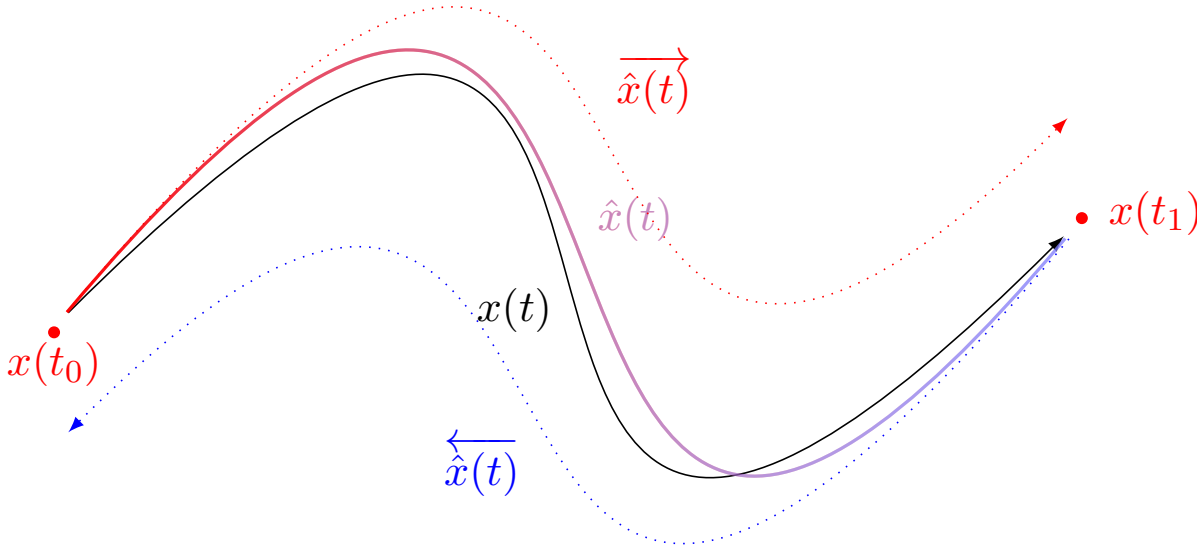
- Integrate approximate dynamics f_θ to obtain approximate solution $\hat{x}(t)$

- 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

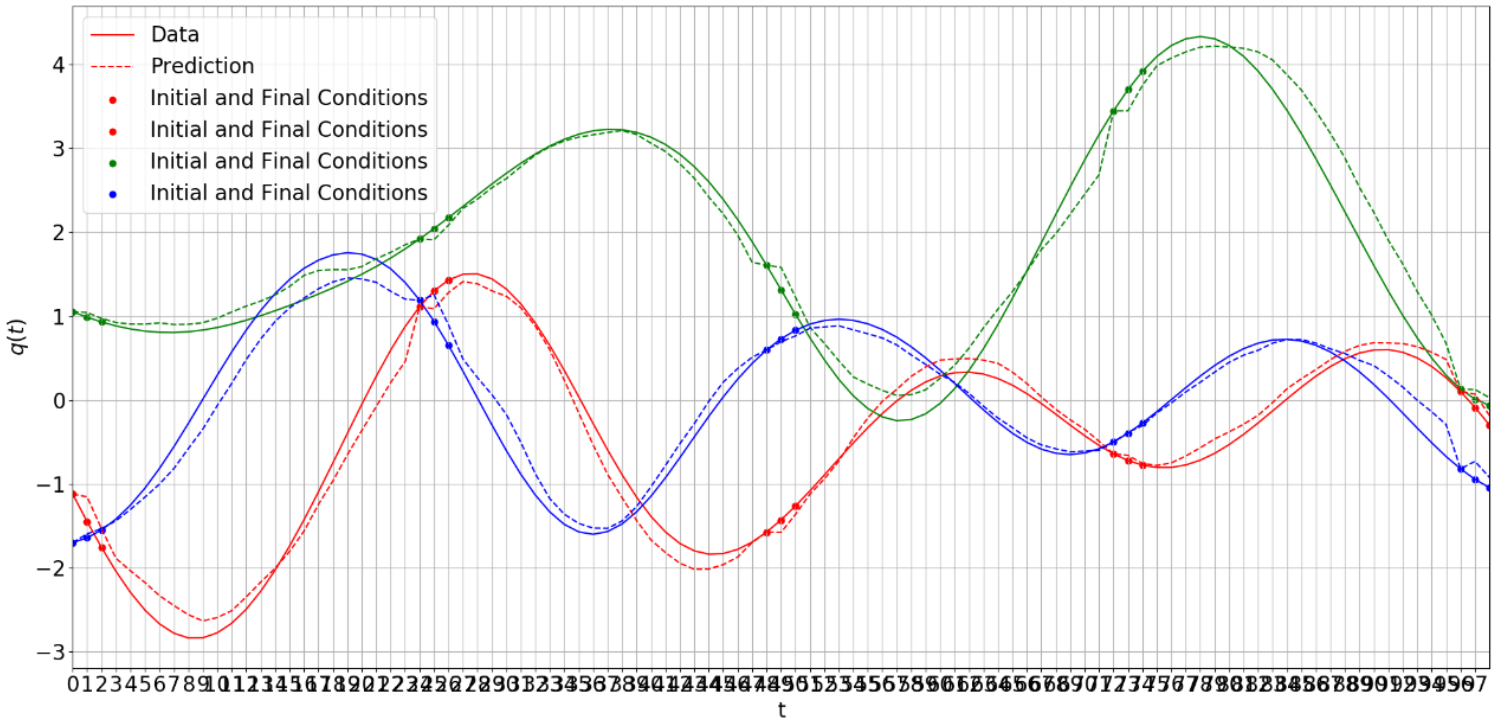
- Predict forward solution $\overrightarrow{\hat{x}(t)}$ and backward solution $\overleftarrow{\hat{x}(t)}$ with the **same** dynamics f_θ
- Use adiabatic connection to interpolate $\overrightarrow{\hat{x}(t)}$ and $\overleftarrow{\hat{x}(t)}$ to $\hat{x}(t)$

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



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 significantely