Mixture of Clustered Bayesian Neural Networks for Modeling Friction Process at the Nanoscale

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Introduction

Friction

- Friction is the principal cause of failure in mechanical systems.
- Lubricants can help!
- We need to engineer lubricants for nano electromechanical systems, or they won’t work!
- Since we do not understand how they work, we cannot design a lubricant from scratch.
- Maybe we can machine-learn the complex physics!

Lubricants

- Since there is no extensive database of real lubricants, we calculate one for model fluids!


Chain molecules

- The liquid is a mixture of chain-like molecules of random length.

- The mixture is confined between model surfaces that squeeze it and shear.
- Interatomic forces are modelled with Lennar-Jones and Morse pair interactions for the liquid and solids respectively.
- Harmonic potentials keep the chains bonded and straight.

Challenges: Data Modelling

- Outlier and large uncertainty
- Imbalance database
- High dimensional data

Machine Learning Strategy

- Database → iGMM → Testing Data → K-means clustering
- Clus 1 → Clus 2 → Clus P
- BNN 1 → BNN 2 → BNN P
- Performance Metrics → Mixture of BNNs

Results and Conclusion

<table>
<thead>
<tr>
<th>METHODS</th>
<th>RMSE</th>
<th>1-R²</th>
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<tbody>
<tr>
<td>Average Individual. Neural Networks.</td>
<td>0.0262</td>
<td>0.1297</td>
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<tr>
<td>Ensemble Learning of Neural Networks</td>
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<td>Average Individual. Bayesian Neural Networks</td>
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<td>Mixture of Clustered Bayesian Neural Networks</td>
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</table>

- ML strategy is promising to approximate experiments/simulations in much faster computational speed and cheaper cost.
- Physical data is complex and ill behaved.
- The estimated shears lie within 3σ, reaching 99.7% accuracy.
- The presence of uncertainty around the ML prediction is useful for decision making by a lubricant designer.