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

Martha A Zaidan[1,2], Filippo F Canova[1,2], Lasse Laurson[1] and Adam S Foster[1,3]

[1]Centre of Excellence in Computational Nanoscience, Aalto University, Finland

[2]Aalto Science Institute, Aalto University, Finland

[3]Division of Electrical Engineering and Computer Science, Kanazawa University, Japan

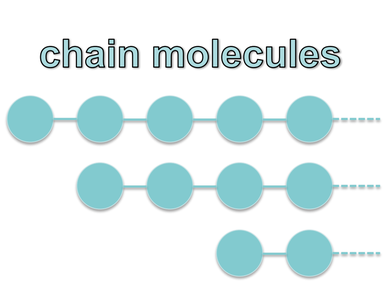
Aalto University
School of Science

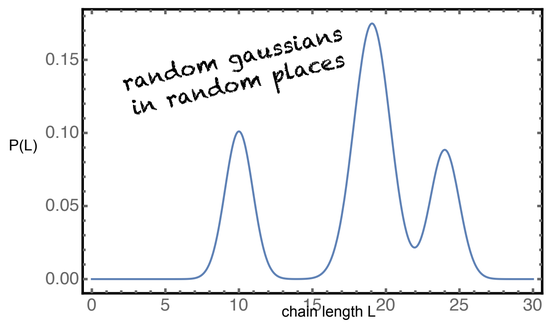
Introduction

- Friction is the principal cause of failure in mechanical system
- 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!

Lubricant Model

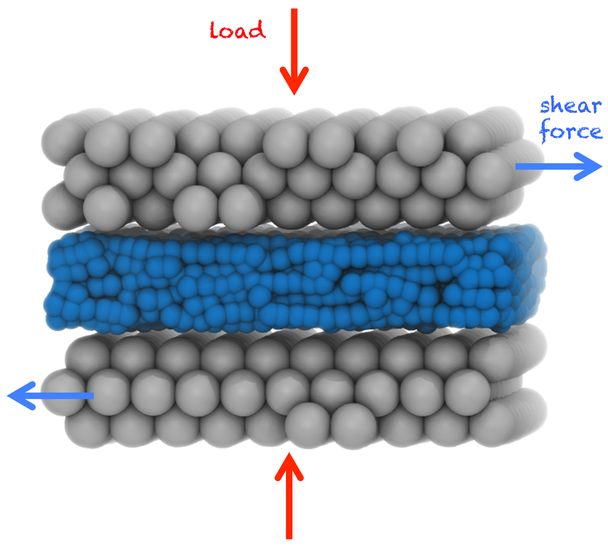
- Since there is no extensive database of real lubricants, we calculate one for model fluids!



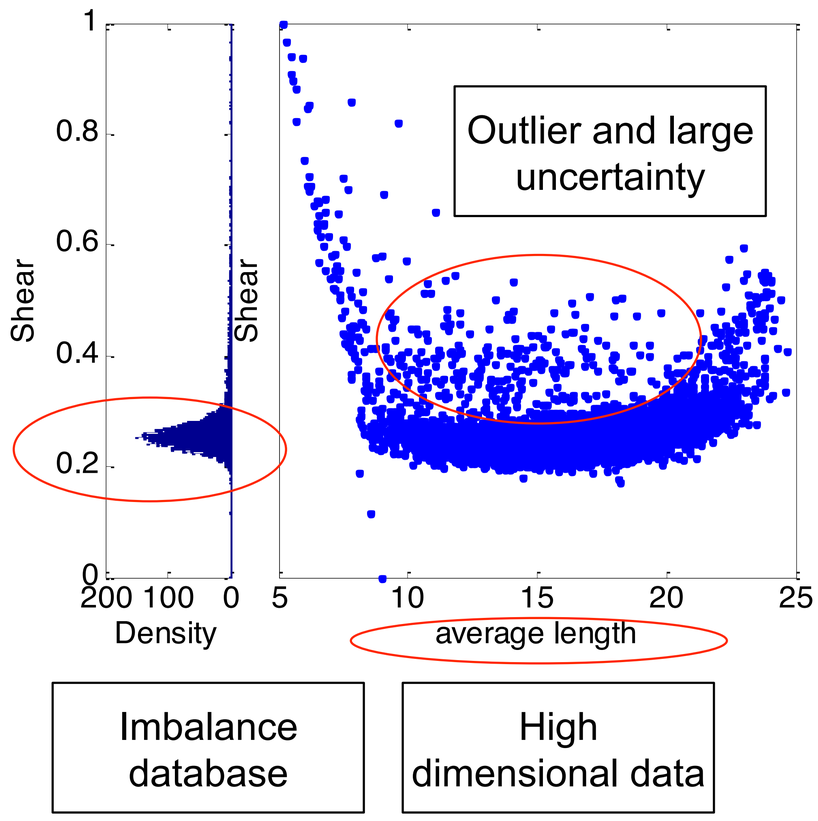


- The liquid is a mixture of chain-like molecules of random length.

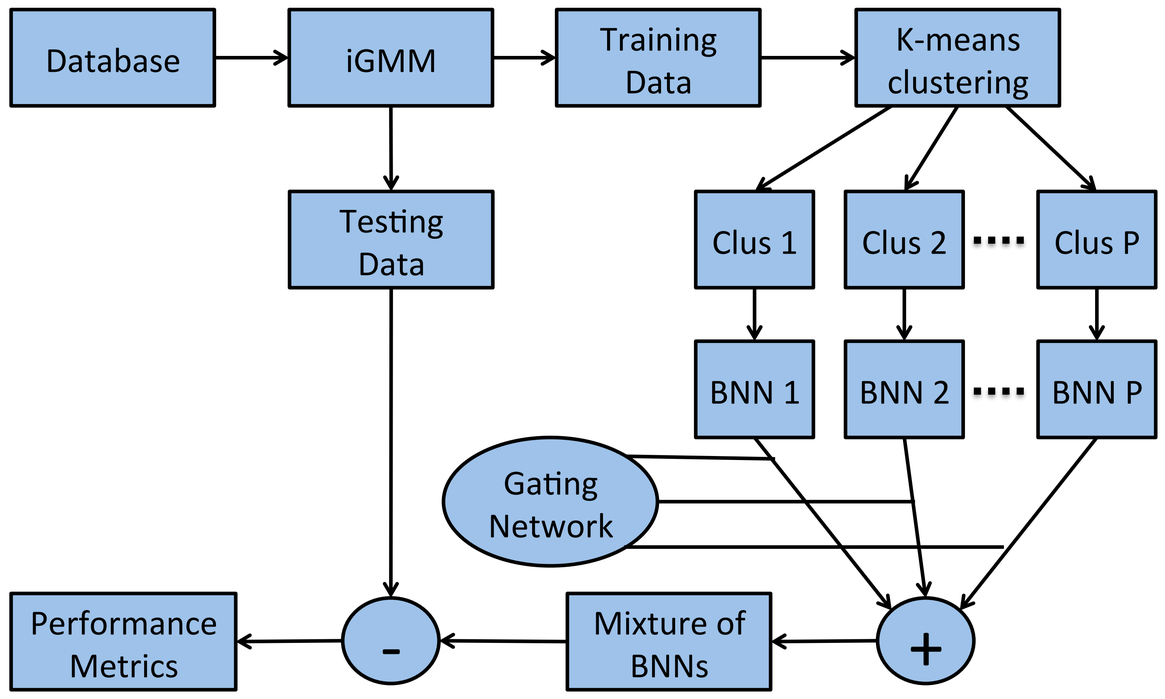
- The mixture is confined between model surfaces that squeeze it and shear.
- Interatomic forces are modelled with Lennar-Jones and Mose pair interactions for the liquid and solids respectively.
- Harmonic potentials keep the chains bonded and straight.



Challenges: Data Modelling

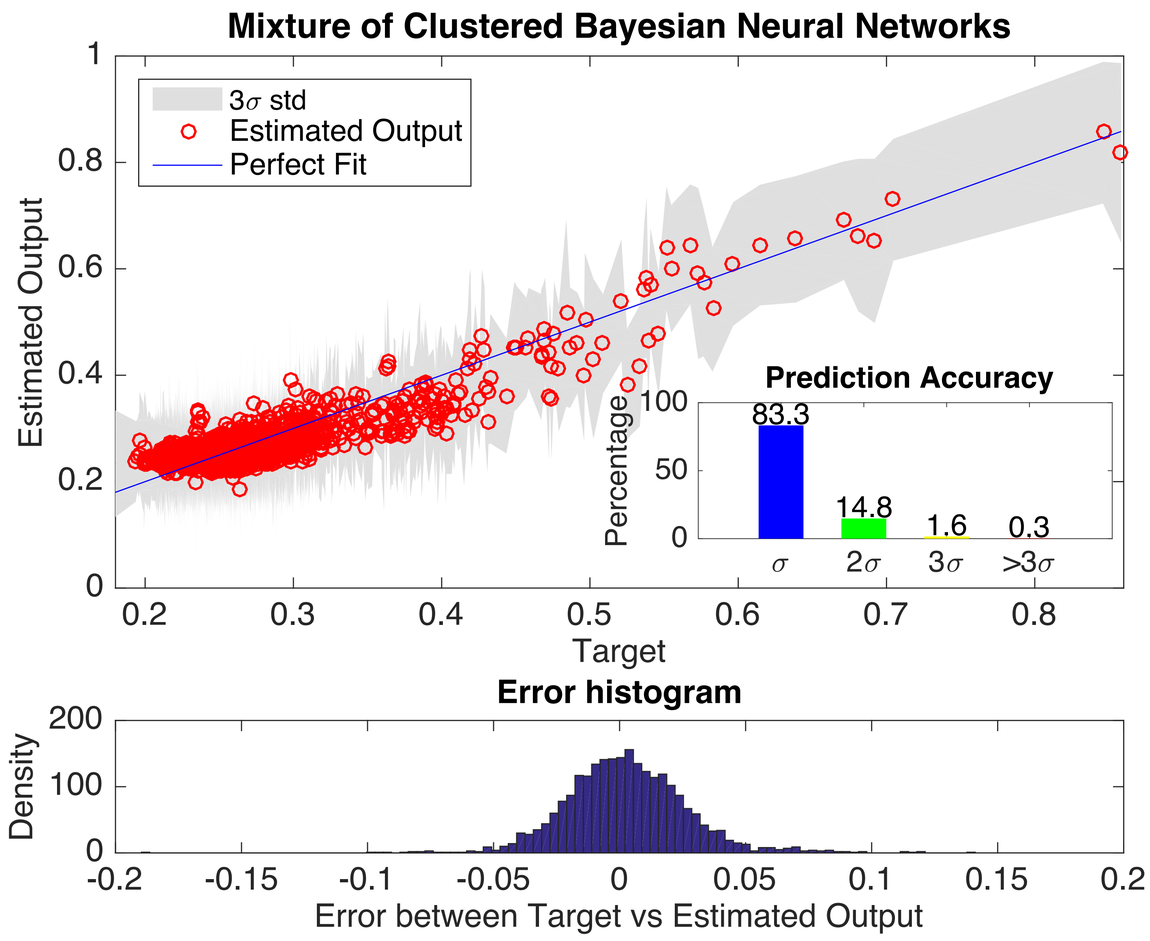


Machine Learning Strategy



Results and Conclusion

METHODS	RMSE	1-R^2
Average Individual. Neural Networks.	0.0262	0.1297
Ensemble Learning of Neural Networks	0.0260	0.1284
Average Individual. Bayesian Neural Networks	0.0251	0.1182
Ensemble Learning of Bayesian Neural Networks	0.0250	0.1173
Mixture of Bayesian Neural Networks	0.0250	0.1175
Mixture of Clustered Bayesian Neural Networks	0.0248	0.1144



Remarks:

- 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.