Analyzing Phase Transitions through Deep Learning

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Problem description

This project seeks to classify atoms in crystalline or interface states based on geometric parameters calculated during molecular dynamics simulations. Classification is of critical importance when determining the mechanism(s) by which atoms transition between the two states (**Fig. 1a**). [1-5]
A model trained on silicon data is applied to water data to determine feasibility of transfer learning. The two have similar underlying geometric bonding structures. (**Fig. 1b**)

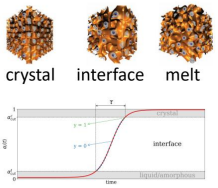


Fig. 1a Melt and interface [1]

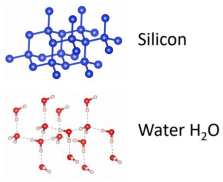


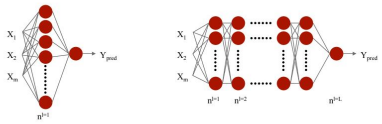
Fig. 1b Ambient structures

Data acquisition and preprocessing

This project utilizes 500,000-atom datasets from molecular dynamics simulations on silicon and water. Each atom has defined local structure based on spherical harmonics, which relates its position and classification (crystal y=1 or interface y=0) to surrounding atoms. This yields 21 features and 1 label per atom based on radial structure functions.

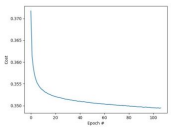
Implemented network architectures

Iterating through several network architecture parameters showed that f1 and precision scores are maximized with a 10-layer (L = 10) deep neural network with 100 neurons per layer ($n^l = 100$) and dropout regulation (**Fig. 2**).



Model	Precision	Recall	f1	Accuracy
Linear SVM, sample weight = 1:1	0.0	0.0	--	80%
Linear SVM, sample weight = 3:1	0.42	0.80	0.55	74%
NN, 1 layer (100 neurons), sample weight = 1:1	0.46	0.74	0.57	78%
NN, 10 layers (100 neurons), sample weight = 1:1	0.47	0.70	0.56	78%
NN, 10 layers (100 neurons) + dropout, sample weight = 1:1	0.50	0.68	0.57	80%

Fig. 2 Iterating architectures and several hyperparameters



For the selected 10-layer neural network with 100 neurons per layer, the cost during training monotonically decreases and stabilizes by 100 epochs (**Fig. 3**).

Fig. 3 Cost vs. training epoch

Results and discussion

Hyperparameter tuning on the 10-layer neural network with 100 neurons per layer using the silicon dataset revealed optimal thresholds and the relationship between the precision and recall for both train and test sets (**Fig. 4**).

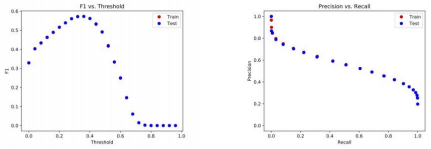


Fig. 4 Hyperparameter tuning and results on silicon data

Transfer Learning

Freezing up to 5 Si-trained layers of the network does not achieve comparable performance as fully re-training the model on water data. (**Fig. 5**)
Initializing with Si-trained weights does accelerate training (**Fig. 6**).

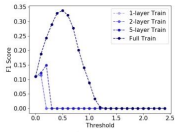


Fig. 5 Transfer learning to H_2O

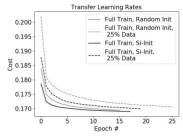


Fig. 6 Weight initialization for H_2O

Future work

Apply NN classifier to new materials (i.e germanium, tin)
Incorporate time dependence into model parameters

References

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[3] Valderrama, José O., Claudio A. Faúndez, and Vilma J. Vicencio. "Artificial neural networks and the melting temperature of ionic liquids." Chemistry Research 53.25 (2014): 10504-10511.
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Acknowledgements

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