Predicting Ionic Liquid Materials Properties From Chemical Structure

https://youtu.be/rrpmpZZOaao

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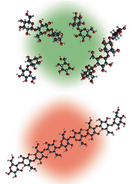
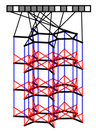
Motivation and Methods



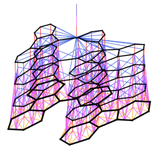
Ionic liquids (ILs) are of interest in fields ranging from batteries to carbon capture[1]. **Accurate prediction of their physiochemical properties enables high throughput screening and thus accelerates their practical application in tangible technologies.**

We aim to **predict the melting point and viscosity of ionic liquids**, **using the chemical structure of the anion and cation**.

1-D encodings are limited in complexity



Neural-Fingerprints allow for end to end learning of molecule



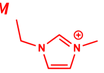
Rather than using a 1-D encoding of the molecule, **we adapted a neural fingerprinting technique[2] to encode the molecules.**

Dataset

The selected IL dataset contained experimentally determined physiochemical properties from over 400 peer-reviewed articles[2].

- **7,666 viscosity values at various temperatures**
- **2,212 melting points for unique ILs**

Chemical structure was fed into the network via a SMILES string

Chemical Structure	*SMILES String*
Cation: EMIM 	*CCN1C=C[N+](=C1)C*
Anion: TFSI 	*C(F)(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F*

A representative **entry in our dataset**:

Cation	Anion	Temperature [K]	$\log_{10}(\eta)$ [cP]	Melting Point [K]
CCN1C=C[N+](=C1)C	C(F)(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	298	1.51	257

Viscosity ranged over 8 orders of magnitude, so a **logarithmic transformation** was applied to allow large and small values to contribute more evenly during training. Melting point values were scaled between –1 and 1.

Neural Fingerprinting

Our model uses a **neural fingerprinting process**, adapted from St. John et al.[4] to capture features from **both the atoms in a molecule and each atom's local bonding environment**. For each time step, these message-passing steps are as follows:

$$m_v^{t+1} = \sum_{w \in N(v)} A_{e_{vw}} h_w^t$$

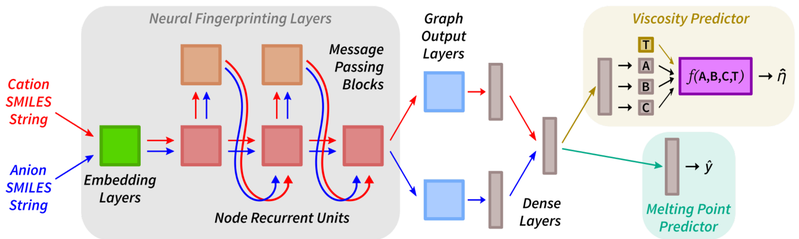
For each bond, the bonding atom's feature vector is multiplied with the corresponding bond matrix to generate the message

$$h_v^{t+1} = GRU(h_v^t, m_v^{t+1})$$

Atom feature vectors are updated based on the learned bond-dependence and the previous time step's feature vectors

After message-passing was performed, the graph output layers were summed to give a neural fingerprint of adjustable length which was then fed into the head of the network.

Model



Our model used an **existing relation for temperature dependence of viscosity** prior to the network output

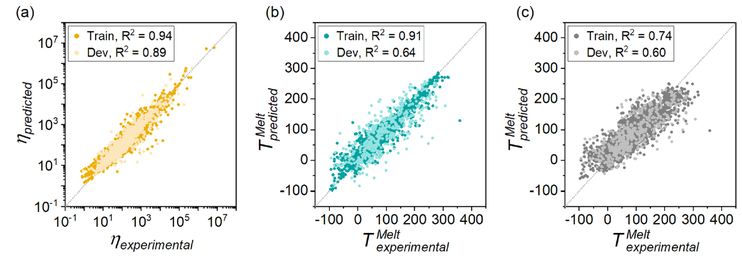
$$\log_{10}\eta = A + \frac{B}{T - C}$$

Hyperparameter Tuning

The architecture was first tuned to optimize for variance with learning rate later adjusted via step decay for highest accuracy.

Index	R^2_{train}	R^2_{dev}	Atom Features Size	Fingerprint Size	Mixing Size	Message Passing Steps
1	0.913162	0.708920	32	8	12	4
2	0.910837	0.691588	32	8	8	4
3	0.910206	0.683271	32	8	32	4
⋮	⋮	⋮	⋮	⋮	⋮	⋮
12	0.896435	0.674678	32	8	32	3
13	0.895648	0.713652	32	32	20	4
14	0.894692	0.664827	32	16	32	3
⋮	⋮	⋮	⋮	⋮	⋮	⋮

Results



Mean Absolute Error

Train	0.124 log(cP)	14.78 K	30.43 K
Dev	0.155 log(cP)	35.48 K	37.20 K

Discussion

Atom features size and **number of message passing steps** are critical hyperparameters. The viscosity model performance does not surpass the best models in literature, but does provide **reasonable accuracy considering its significantly larger, more diverse dataset**. **Melting point prediction struggled with large variance**, likely due to the small data set size. Transfer learning decreased apparent variance but increased melting point bias, possibly because the embedding was not trained on ILs unique to the melting point data set.

Future Work

Emphasis would be placed on **expanding both datasets** with additional unique ionic liquids. This is in hopes to reduce melting point variance and viscosity predictive performance of "unseen" ionic liquids. **Both models could also be combined to one** to train embedding matrices on the combined set of ILs.

Acknowledgements

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References

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[3] Venkatraman, V., Evjen, S. & Chellappan Lethesh, K. The Ionic Liquid Property Explorer: An Extensive Library of Task-Specific Solvents. *Data* **4**, 88 (2019).

[4] St John, P. C. *et al.* Message-passing neural networks for high-throughput polymer screening. *J. Chem. Phys.* **150**, 234111 (2019).