# Transfer Learning
## for Ionic Liquid Property Prediction


**Nathan Culmer**
**University of Akron**
**Dept. of Computer Science**
**nrc61@uakron.edu**

**Mark Earl**
**University of Akron**
**Dept. of Computer Science**
**mpe12@uakron.edu**

**Dr. Zhong-Hui Duan**
**University of Akron**
**Dept. of Computer Science**
**duan@uakron.edu**


## Purpose

**Modelling can be used to predict the properties of materials without the need for expensive experiments. We use neural networks to model properties of ionic liquids and show that transfer learning, a "technique in which knowledge gained through one task or dataset is used to improve model performance on another related task," can be used to improve the training process. Knowledge can be shared between models that predict density, viscosity, and surface tension.**

## Modelling Ionic Liquid Properties

Kamil Paduszyński uses several machine learning models, including neural networks, to predict properties of ionic liquids in a series of papers.[1][2][3] The properties investigated are detailed below. He makes the following contributions:

- A **large database** of ionic liquid data is compiled.
- Predictions are **based on functional groups** present in the ionic liquid.
- Modelling is **divided into two tasks**:
  1. The *reference term* predicts the property at a temperature of 298.15K.[1]
  2. The *correction term* adjusts this value for temperature/pressure.[1]

## Reference Term Neural Networks

We focus on the neural network models that predict the reference term. These are feed-forward neural networks, which consist of three layers:

1. **Input layer**: Each input is the count of a functional group in the liquid.
2. **Hidden layer**: uses hyperbolic tangent as the activation function.[1]
3. **Output layer**: Single node whose value is the predicted value.

## Modelled Properties

Paduszyński uses his method to investigate three properties:

**Density**: model uses 162 groups for input, contains 2 hidden nodes, and outputs the molar volume of the liquid, which is used to find the density with the following equation:

$$\hat{\rho}_0(\mathbf{n}) = \frac{M(\mathbf{n})}{\hat{v}_0(\mathbf{n})}$$

where $\hat{\varrho}_0$ is the density, $M$ is the molecular weight and $\hat{v}_0$ is the molar volume.[1]

**Viscosity**: model uses 72 groups for input, contains 4 hidden nodes, and outputs the natural log of the viscosity.[2]

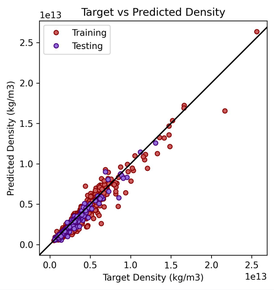
**Surface tension**: model uses 51 groups for input, contains 2 hidden nodes, and outputs the parachor, which can be used to find the surface tension with the following equation:

$$\hat{P}_0 \equiv \hat{V}_0 \hat{\sigma}_0^{\frac{1}{4}}$$

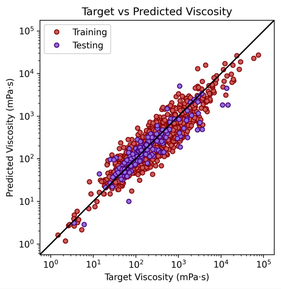
where $\hat{P}_0$ is the parachor, $\hat{\sigma}_0$ is the surface tension, and $\hat{V}$ is the molar volume.[3]

The predicted values of properties by the models are plotted against the true values below:

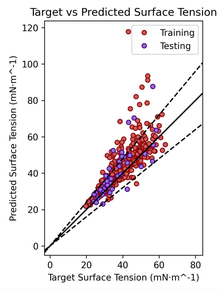
**Density**




**Viscosity**




**Surface Tension**




## Methods

To evaluate the utility of transfer learning, several transfer techniques are compared:

1. **Untrained model**: a model is trained to predict a property, based on a model architecture used by Paduszyński to predict a different property.
2. **Pre-trained model**: a model is trained to predict one property, based on Paduszyński's work, then re-trained to predict a different property.
3. **Pruned pre-trained model**: a model is trained to predict one property, based on Paduszyński's work, then pruned, then re-trained to predict a different property.

## Pruning

Pruning is "the task of reducing the size of a network by removing parameters". One method of this is *global magnitude pruning*, where the weights with the lowest values are removed from the network. We prune 20%-30% of the weights and fine-tune for 10-20 epochs, depending on the model. Only the weights into the hidden layer are pruned.

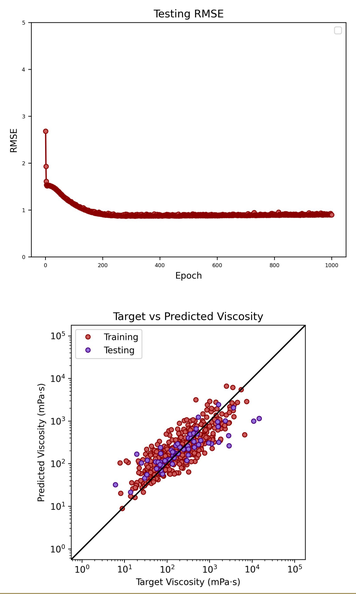
## References


[1] Paduszyński, K. (2019). *Extensive Databases and Group Contribution QSPRs of Ionic Liquids Properties. 1. Density*. Industrial & Engineering Chemistry Research 58 (13), 5322-5338. 10.1021/acs.iecr.9b00130
[2] Paduszyński, K. (2019). *Extensive Databases and Group Contribution QSPRs of Ionic Liquids Properties. 2. Viscosity*. Industrial & Engineering Chemistry Research 58 (36), 17049-17066. 10.1021/acs.iecr.9b03150
[3] Paduszyński, K. (2021). *Extensive Databases and Group Contribution QSPRs of Ionic Liquids Properties. 3. Surface Tension*. Industrial & Engineering Chemistry Research 60 (15), 15705-5720. 10.1021/acs.iecr.1c00783

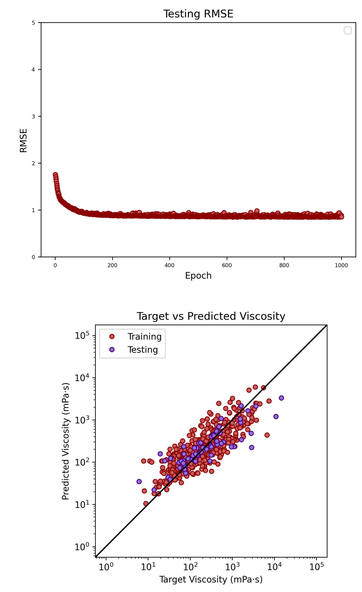

## Results

### Viscosity (Using Surface Tension Model)

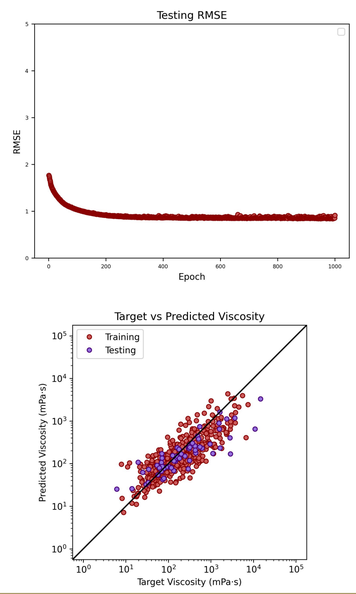
**Untrained**




**Pre-trained**

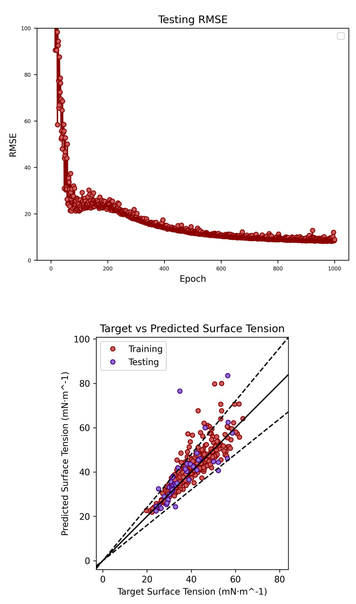



**Pruned**

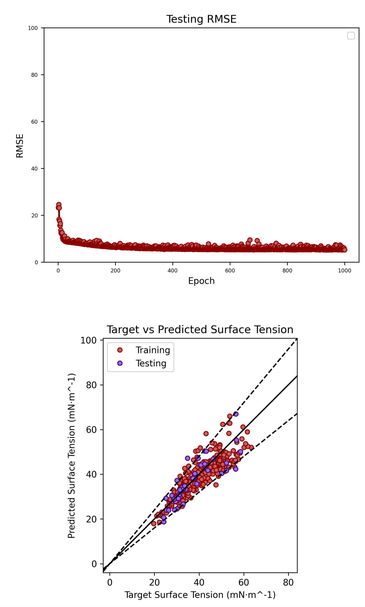



### Surface Tension (Using Density Model)

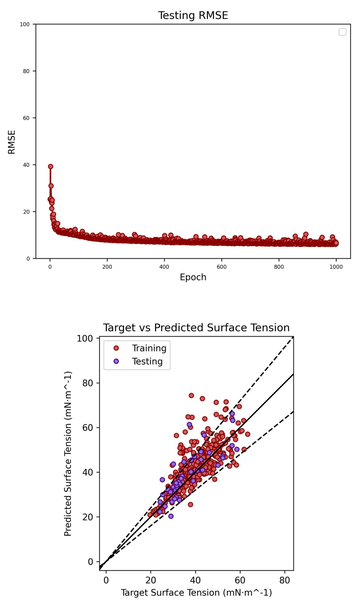
**Untrained**




**Pre-trained**

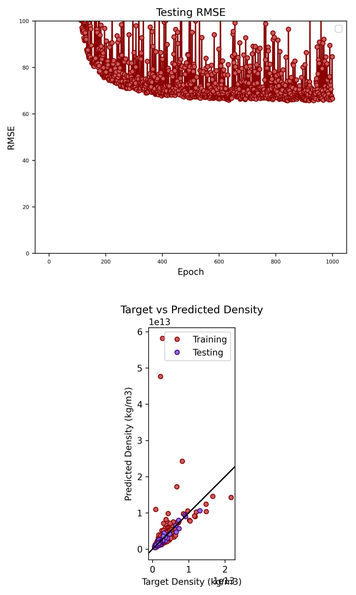



**Pruned**

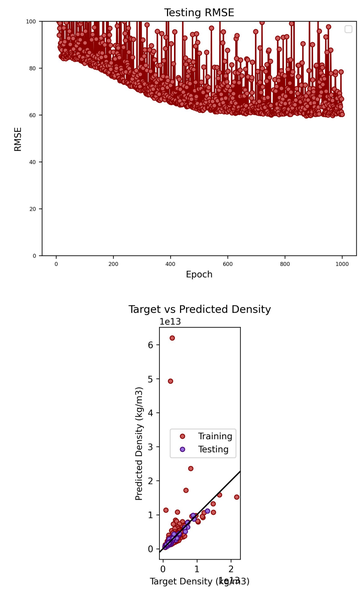



### Density (Using Surface Tension Model)

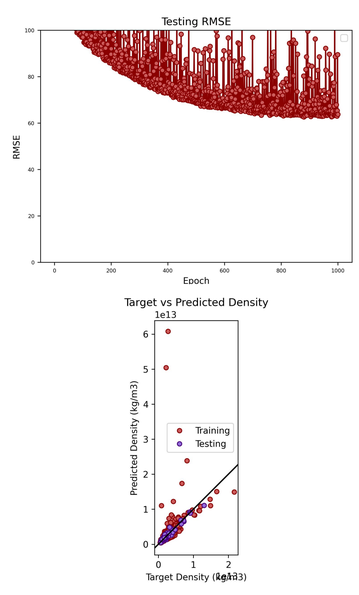
**Untrained**




**Pre-trained**




**Pruned**




## Discussion

- Overall, transfer learning produces comparable results to models trained from scratch.
- While final results do not improve, there are several indications that knowledge is imparted on the new model:
  - The training process is faster in several cases.
  - In the case of surface tension, training from a pre-trained network avoids the plateau encountered early in the training process.
  - Pruned models transfer knowledge with a minimal loss in effectiveness, compared to their unpruned counterparts.

## Acknowledgement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