Deducing molecular structure of plastics from flow data using Deep Learning

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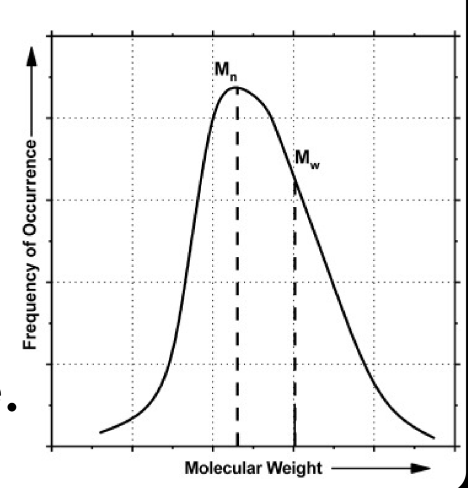
A. Motivation

- In 2022, global plastic production reached approximately **390.7 million** metric tons, with **50%** consisting of single-use plastics.
- It is hence crucial to recycle plastics quickly and efficiently.
- The efficiency of plastic recycling lies in the quick estimation of it's **molecular weight distribution.**

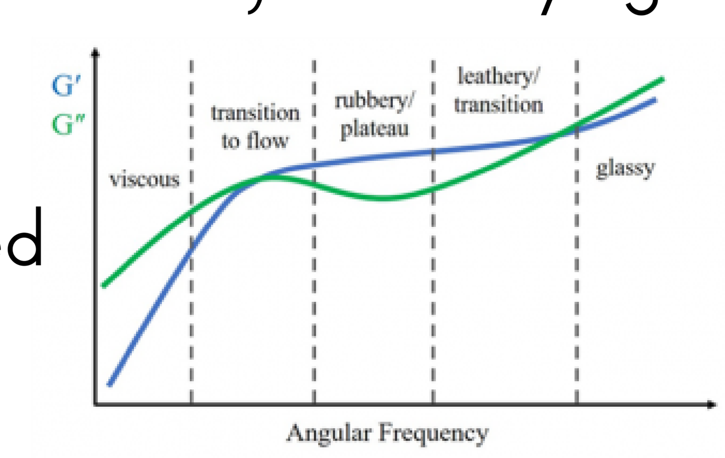
B. Molecular Weight Distribution

- The plastic mass is categorized into a polymer type.
- **Z** denotes the mean and **PDI**, the variance.



C. Linear Rheology

- An experiment on plastics observing changes in **G'** (storage modulus) and **G''** (loss modulus) with varying **angular frequency**.
- Data acquired is known as flow data.

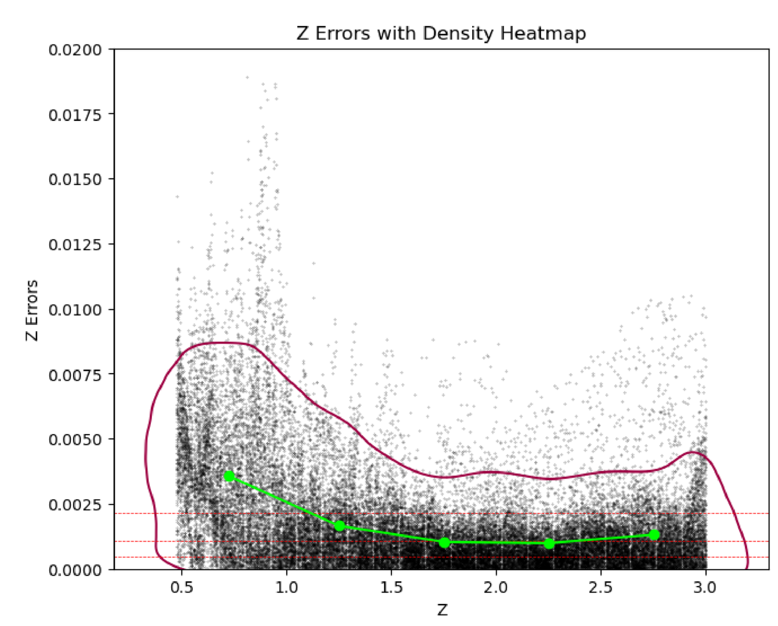


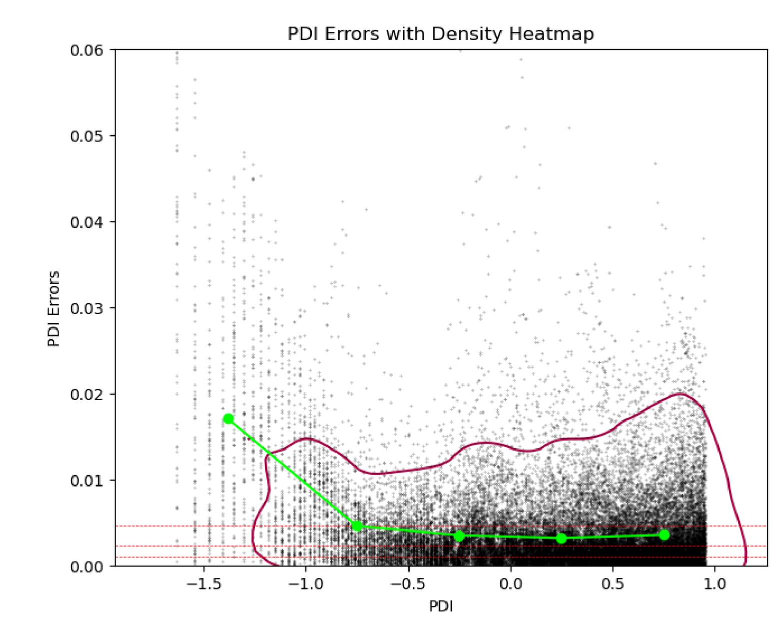
D. Aim

- A recently developed tube model by Chinmay Das and Daniel J. Read [1] generates flow data given the parameters of the Molecular Weight Distribution (Z and PDI).
- Can **Deep Learning** methodologies be used to predict **Z and PDI**, given the **flow data**?

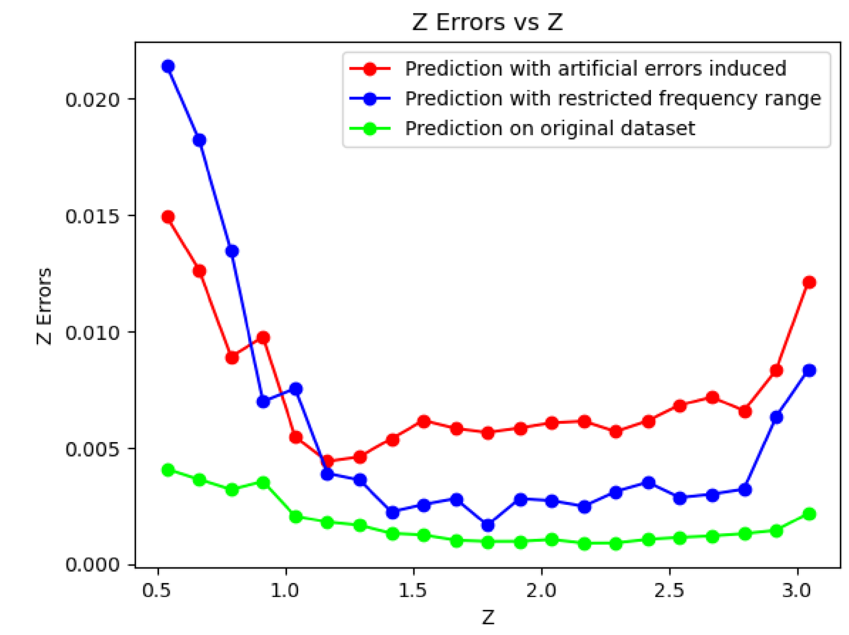
E. Analysis

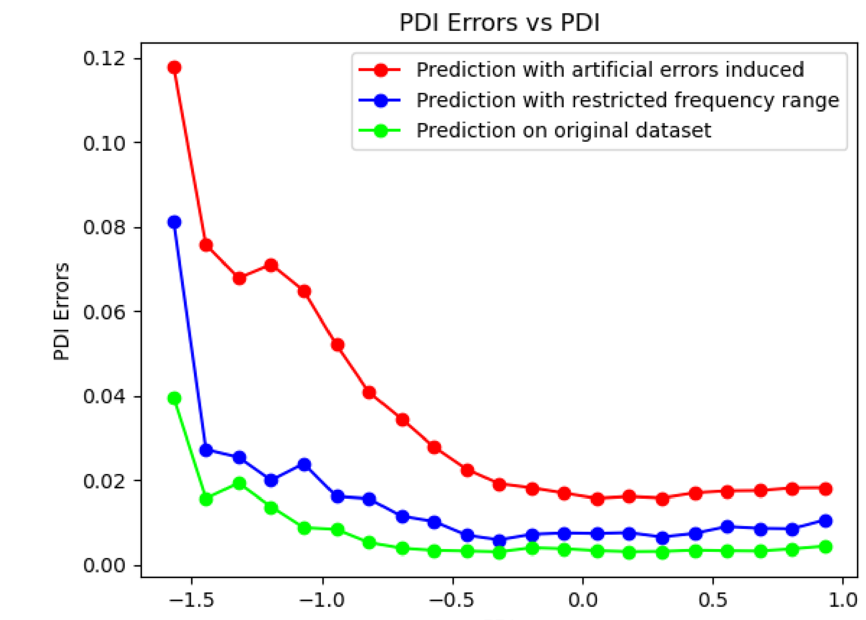
- Considering **linear polymers**, a dataset of 202500 rheology curves are generated with 450 distinct Z and PDI values in the log parameter space.
- An **RNN** architecture is utilized due to the temporal nature of the data. [2]
- The density plots showcased below are that of the errors produced in predicting Z and PDI respectively :





- In real life, however, the high range of frequency values present in our generated dataset will not be available to us.
- There is also expected to be a 5 to 7% error in measurement while conducting the Linear Rheology experiment.
- The graphs below showcase the average error trend of the model prediction when a certain constraint is introduced for Z and PDI respectively :





F. Conclusions and Future Work

- In conclusion, a deep learning approach is **definitely viable** for the analysis of plastic flow data.
- The accuracies attained even with data restrictions, are fruitful in nature and can be deployed in the industry.
- Low Z values seem to be more reliant on the entire frequency range for highly accurate predictions.
- Future work includes extending this approach to polymodal data and testing of model robustness on real-life data.

References :

[1] Das, Chinmay and Read, Daniel J. (2023). "A tube model for predicting the stress and dielectric relaxations of polydisperse linear polymers" (Access Date: 10th July 2024)

[2] Rmus, Milena AND Pan, Ti-Fen AND Xia, Liyu AND Collins, Anne G. E (2024). "Artificial neural networks for model identification and parameter estimation in computational cognitive models" (Access Date: 7th July 2024)

Further information :

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if you have a question or comment.