

An Essay on the Rashomon Set

My father is an ardent admirer of Akira Kurosawa's movies. As a child, I remember watching *Rashomon*, a bizarre tale of a murder retold in many different ways. In today's world, each successful machine learning or deep learning model is orders of magnitude better than its own predecessors [1]. However, the cost of highly accurate models is their lack of interpretability, as is elucidated by Prof. Rudin [2].

The assertion by the 'Rashomon' argument is that if there are enough complex models that make diverse predictions and are highly accurate, there must be some models whose inner mathematical qualities may be distilled down to more interpretable functions. Prof. Rudin highlights three excellent examples in favour of her Rashomon argument, in areas where the model accuracy/interpretability trade off occurs. Accurate *and* interpretable models must a) provide a robust series of logical conditions b) have excellent scoring systems and c) be tailored for specific domains.

Biological and molecular data have relied on machine learning models created for other applications, for far too long. For instance, convolutional neural networks work very well on images. The public knowledge of CNNs is rapidly diminishing, as the mechanics of models are neatly hidden in wrapper functions and therefore make no sense to the scientist. DeepChem[3] and MoleculeNet[4] are two major advances in the creation of novel AI tools tailored specifically for molecular datasets. DeepChem includes a variety of graph convolutional network [5] models that were created primarily for molecular data, whose structures are conveyed neatly via SMILES[6] (another brilliant idea in representing the stereochemistry of a molecule via a string) and featurized efficiently by GCNS.

Another interesting example of an interpretable model in the biological community is the ability to predict the lab-of-origin of a DNA [7]. In an increasingly competitive world with an inbound 'biorevolution', engineered DNA may be considered as intellectual property with rigorous norms and regulations. A CNN is trained on Addgene data and can efficiently output the top n labs-of-origin.

Finally, it is my personal belief that the principles of synthetic biology could give rise to simple, logical models. Till the synthetic biology boom of the last decade, genetic sequences and components lacked standardization due to the lack of proper gene annotation, part boundaries, and overall modularity. Now, with modular biological components such as BioBricks [8] and databases such as the Registry of Standard Biological Parts [9], models have been used to predict the efficacy of genetic components, analyse gene expression, use AI to automate genetic circuit design and beyond [10]. It truly is possible to extend the Rashomon argument to the biological sciences as well!

References

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