COMPUTATIONAL RESEARCH IN BOSTON AND BEYOND SEMINAR

Friday, January 3, 2025

12:00 PM – 1:00 PM

https://mit.zoom.us/j/96155042770

Solid Solubility Prediction at the Limit of Experimental Accuracy

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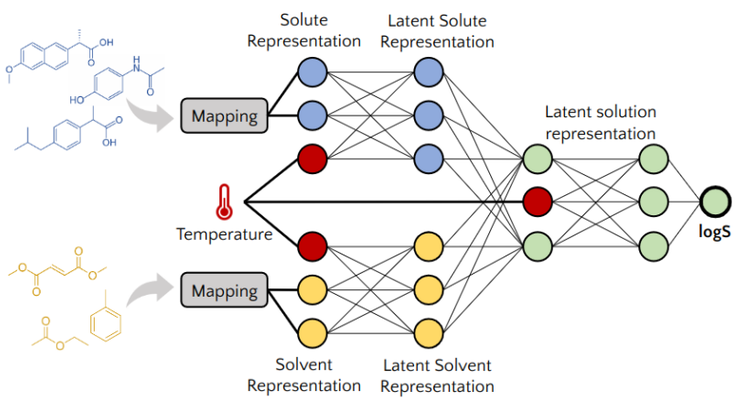
Abstract:

Small molecule solubility is a critically important property which affects the efficiency, environmental impact, and phase behavior of synthetic processes. Experimental determination of solubility is a time- and resource-intensive process and existing methods for in silico estimation of solubility are limited by their generality, speed, and accuracy. This work presents two models derived from the fastprop and chemprop architectures and trained on BigSolDB which are capable of predicting solubility at arbitrary temperatures for any small molecule in organic solvent. Both extrapolate to unseen solutes 2-3 times more accurately than the current state-of-the-art model and we demonstrate that they are approaching the aleatoric limit (0.5-1 logS), suggesting that further improvements in prediction accuracy require more accurate datasets. These models, collectively referred to as fastsolv, are open source, freely accessible via a Python package and web interface, highly reproducible, and up to 50 times faster than the next best alternative.



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