End-to-End Differentiable Molecular Mechanics Force Field Construction

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A graph net is used to generate latent atom embeddings describing local chemical environments.

These atom embeddings are transformed into symmetry-encoded feature vectors for atom, bond, angle, and torsion.

Molecular mechanics parameters are predicted from these feature vectors using feed-forward layers.

3.4966\(^4\) 4.4098 kcal/mol test set RMSE, compared to 3.7365\(^4\) 4.4559 kcal/mol for Open Force Field 1.2.1 “Parsley”.

![Diagram showing the process of generating latent atom embeddings and predicting molecular mechanics parameters.](image-url)