End-to-End Differentiable Molecular Mechanics Force Field Construction

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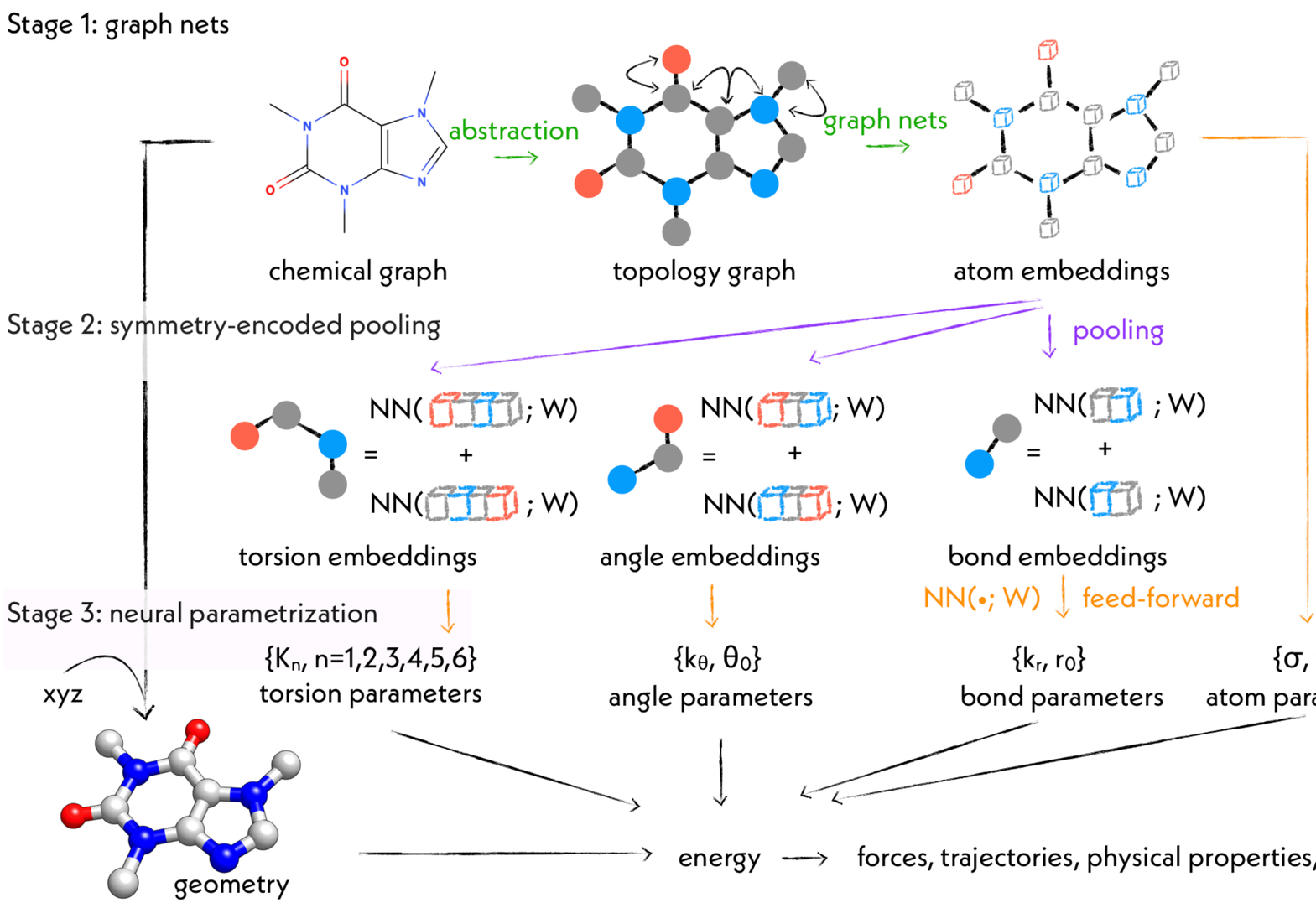
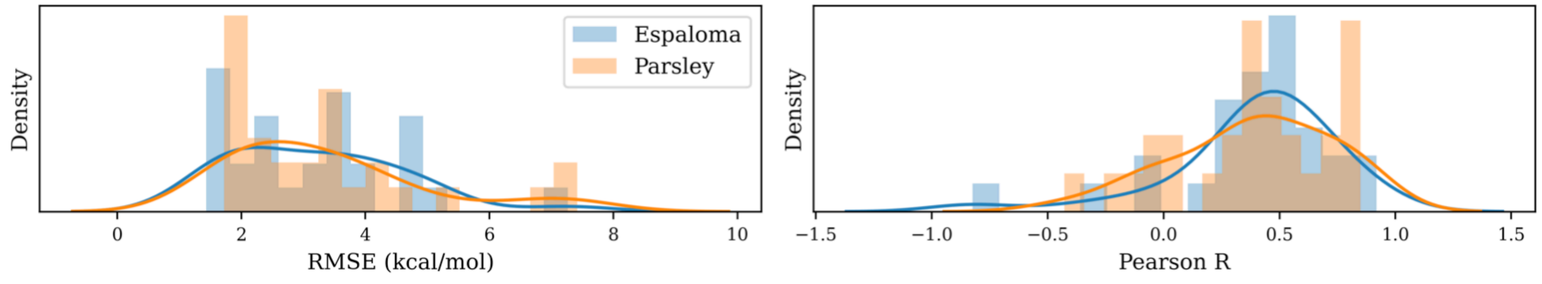


a graph net is used to generate latent atom embeddings describing local chemical environments

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

$3.4966^{4.4098}_{2.9526}$ kcal/mol test set RMSE, compared to $3.7365^{4.4559}_{3.0299}$ kcal/mol for Open Force Field 1.2.1 "Parsley".



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