

# Improving Explorability in Chemical Space with Annealed Variational Objectives.

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## Abstract

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Despite the advances in the representational capacity of approximate distributions for variational inference, the optimization process can still limit the density that is ultimately learned. We demonstrate the drawbacks of biasing the true posterior to be unimodal, and introduce Annealed Variational Objectives (AVO) into the training of hierarchical variational methods. Inspired by Annealed Importance Sampling, the proposed method facilitates learning by incorporating energy tempering into the optimization objective. In our experiments, we demonstrate our method's robustness to deterministic warm up, and the benefits of encouraging exploration in the latent space.

# References

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