

# Targeted Adversarial Learning Optimized Sampling

Jun Zhang, Yi Isaac Yang, Frank Noé

Submitted date: 22/05/2019 • Posted date: 22/05/2019

Licence: CC BY-NC-ND 4.0

Citation information: Zhang, Jun; Yang, Yi Isaac; Noé, Frank (2019): Targeted Adversarial Learning Optimized Sampling. ChemRxiv. Preprint.

Abstract Boosting transitions of rare events is critical to modern-day simulations of complex dynamic systems. We present a novel approach to modify the potential energy surface in order to drive the system to a user-defined target distribution where the free energy barrier is lowered. The new approach, called targeted adversarial learning optimized sampling (TALOS) combines the strengths of statistical mechanics and deep learning. By casting the enhanced sampling problem as a competing game between a real sampling engine and a virtual discriminator, TALOS enables unsupervised construction of bias potential on an arbitrary dimensional space and seeks for an optimal transport plan that transforms the system into target. Through multiple experiments we show that on-the-fly training of TALOS benefits from the state-of-art optimization techniques in deep learning, thus is efficient, robust and interpretable. Additionally, TALOS is closely connected to actor-critic reinforcement learning, giving rise to a new approach to manipulating the Hamiltonian systems via deep learning.

## File list (2)

MainText.pdf (659.92 KiB)

[view on ChemRxiv](#) • [download file](#)

SI.pdf (1.23 MiB)

[view on ChemRxiv](#) • [download file](#)

## Other files

---

MainText.pdf (659.92 KiB)

[view on ChemRxiv](#) • [download file](#)

---

Sl.pdf (1.23 MiB)

[view on ChemRxiv](#) • [download file](#)

---