# Deep Learning for Rare Event Sampling


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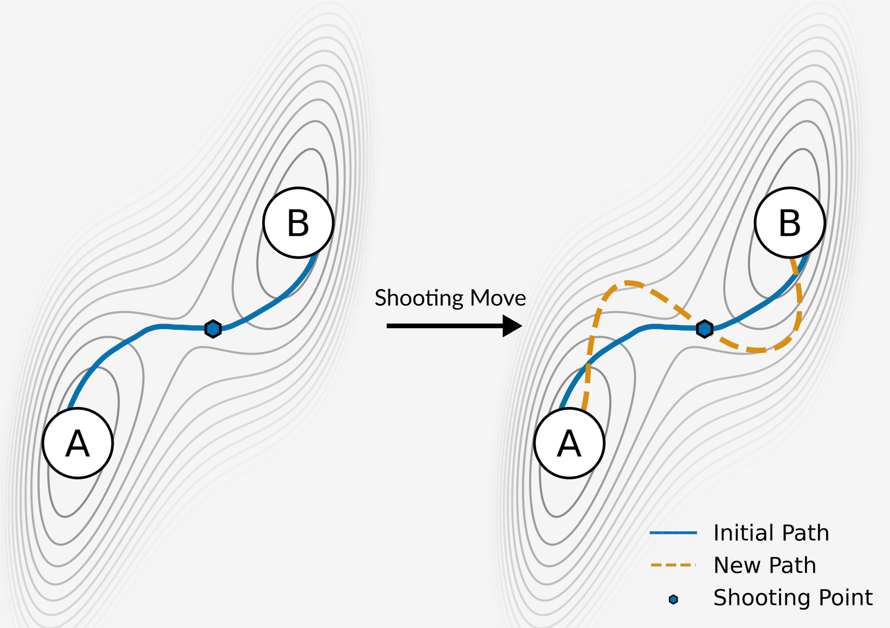
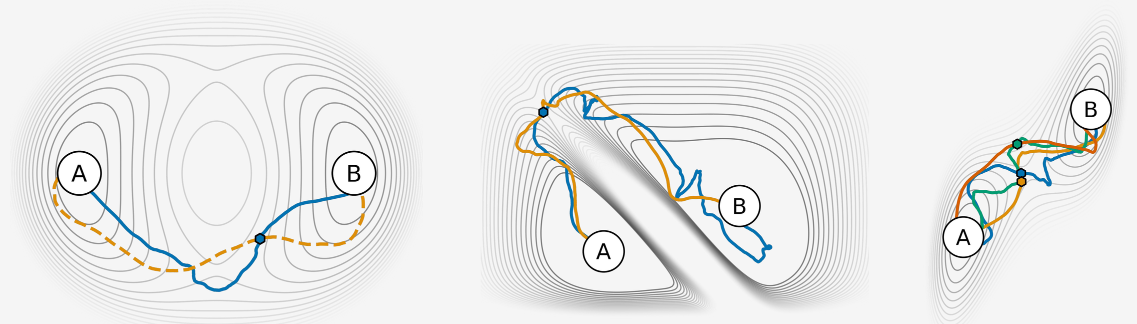
## Transition Path Sampling

### Sampling the Path Ensemble




- TPS aims at sampling the ensemble of reactive trajectories connecting stable states
- On an initial path, a configuration is randomly selected and optionally modified
- Integration is performed forward and backward in time to generate a new path
- If an acceptance criterion is fulfilled, the path is added to the ensemble and the procedure is repeated

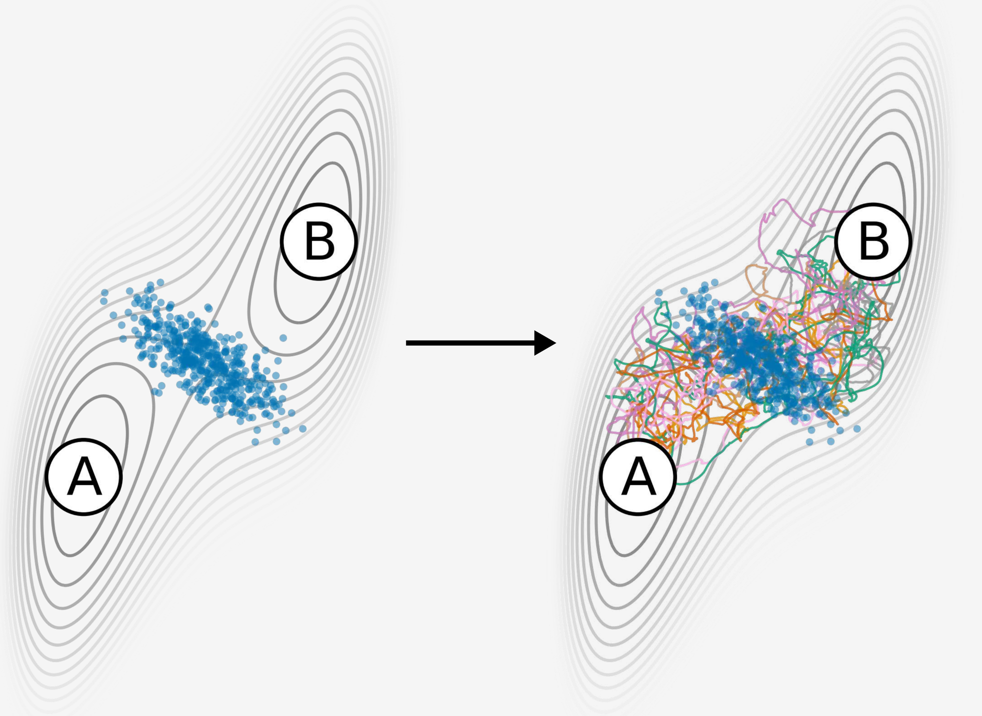
### Limitations of regular TPS




- Correlations between subsequently visited paths impact **exploration of path space**
- Low path generation probabilites in complex systems lead to waste of **computational resources**
- Inherently sequential sampling of the path ensemble limits **scalability**

## Reactive Path Sampling in Parallel

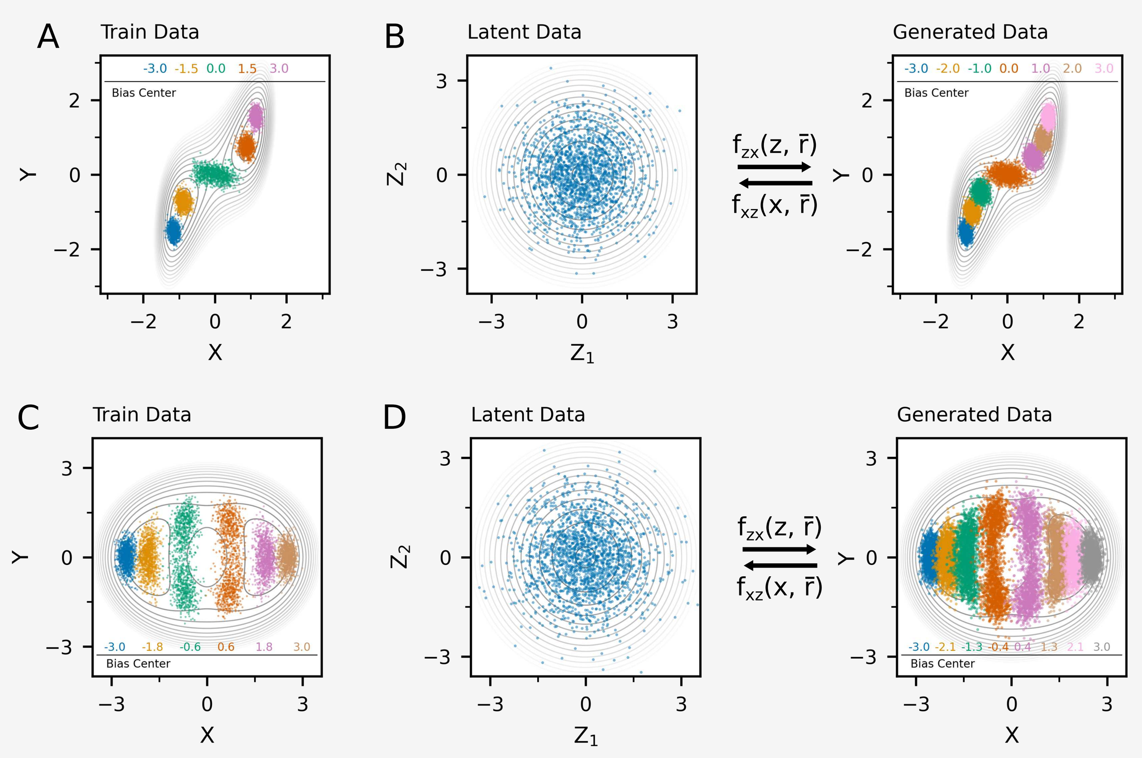
1. Sample Points
2. Integrate




3. Reweight Paths $w\left[X(\tau)\right] \propto \left[\sum_{k=0}^{\tau/\Delta t-1} \frac{p_{\mathrm{SP}}(x_{k\Delta t})}{p_{\mathrm{eq}}(x_{k\Delta t})}\right]^{-1}$

- Starting from a set of shooting points, paths can be generated in parallel
- Shooting points can be centered on regions with high probability to generate a reactive trajectory
- Less correlations between paths since they depend on correlations between shooting points
- Trajectories that dwell for a extended time in the biased region are sampled more often
- Paths can be reweighted to obtain an unbiased path ensemble

## Conditioning Boltzmann Generators

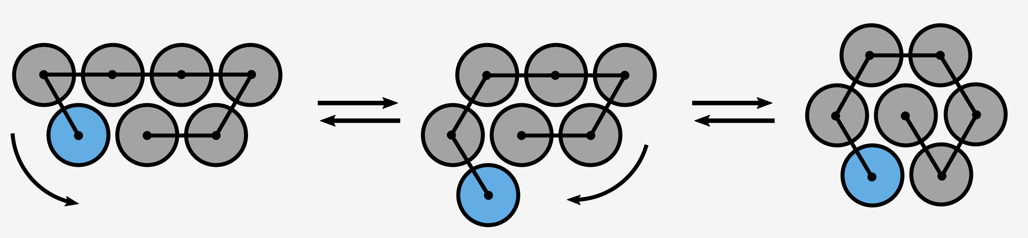


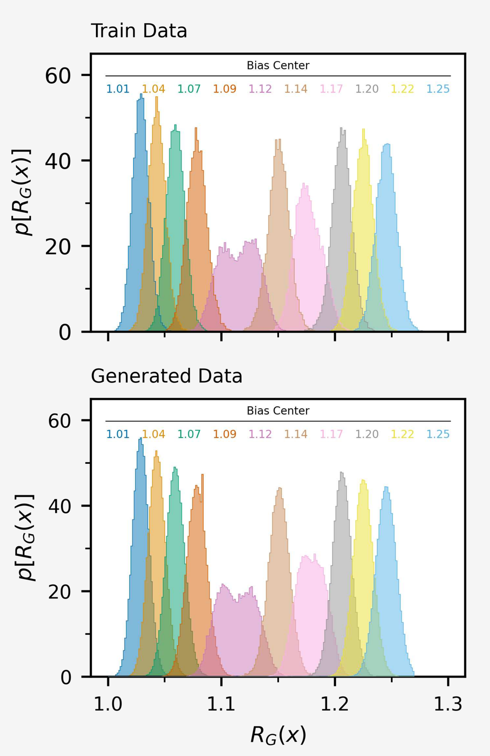

Biased Equilbrium Distribution:

$$p_{\mathrm{biased}}(x \mid \bar{r}) = \frac{1}{Z_x} e^{-\beta\left[U(x) + \frac{k}{2}(r(x)-\bar{r})^2\right]}$$

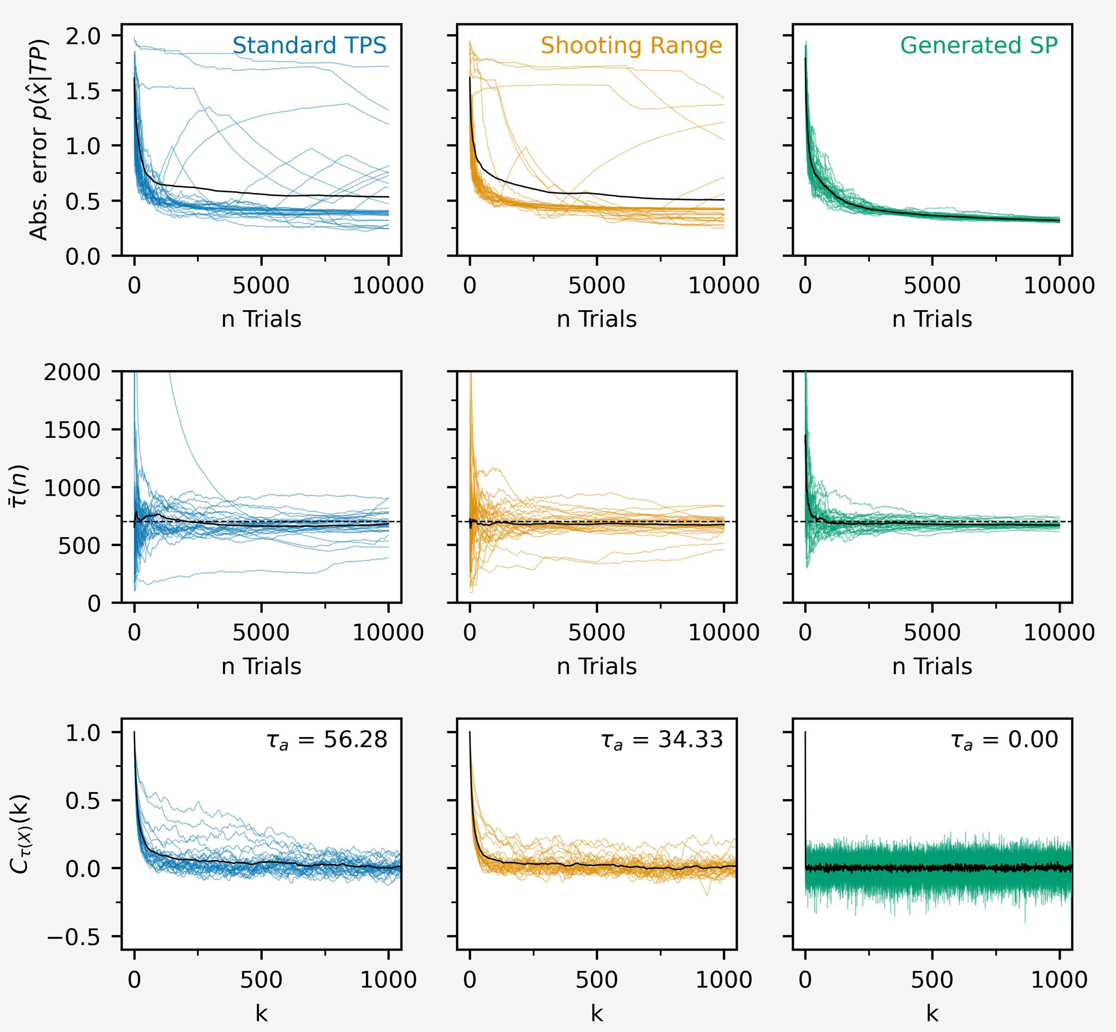
- Shooting points can be sampled using generative neural networks
- Boltzmann generators have been shown to be able to generate uncorrelated configurations
- Configurations are generated via a learnable, invertible transformation between the Boltzmann distribution and a latent space distribution
- Conditioning the transformation allows for biasing different regions in configuration space
- Harmonic potentials, as applied in umbrella sampling, are used for efficient biasing

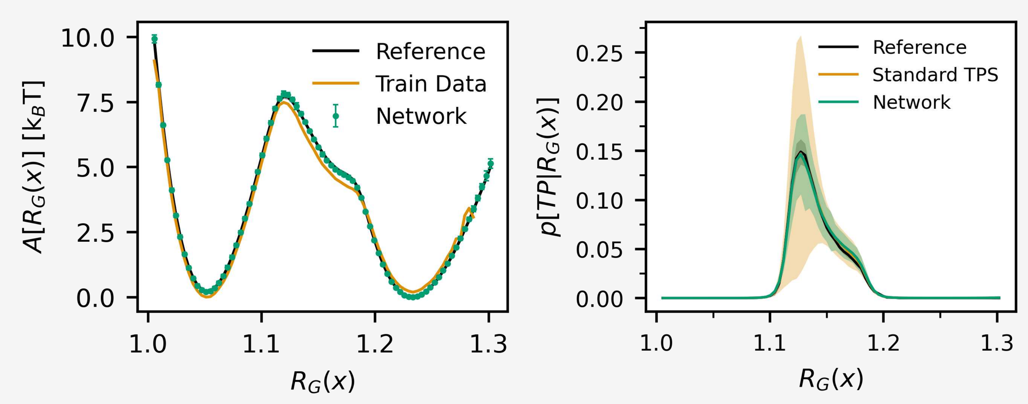
## Application






- Polymer model as a complex test system for path sampling algorithms
- Generation is biased along radius of gyration (left)
- Efficient path sampling due to reduced correlations (middle)
- Thermodynamics of the transition region can be resolved (right)




Free Energy

Transition Path Probability

References: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