Toy NETS Simulation in a 1D Double-Well Potential

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Goal

Compare the effect of NETS-inspired drift with standard Langevin dynamics when applied to barrier crossing in a 1D double-well potential. The goal is to understand how this drift can accelerate transitions while slightly biasing the stationary distribution.

Model

- **Potential:** $V(x) = (x^2 - 1)^2$ (minima at $x = \pm 1$, barrier at $x = 0$)
- **Baseline Langevin:** $dx = -V'(x)dt + \sqrt{2/\beta}\, dW_t$
- **Toy NETS drift:** $u_\alpha(x) = -\alpha \tanh(x)$ Full dynamics: $dx = [-V'(x) + u_\alpha(x)]dt + \sqrt{2/\beta}\, dW_t$
- **Parameters used:** $\beta = 5$, $\alpha = 0.5$, $dt = 0.01$, $T = 200$, $N = 100$ trajectories

Key Metrics Computed

- Sample trajectories $x(t)$
- Transition counts per trajectory
- Mean first-passage times (MFPT)
- Stationary histograms vs theoretical Boltzmann: $p_{\text{Boltz}}(x) \propto e^{-\beta V(x)}$
- α-sweep: transition rate vs histogram distortion (L1, KL)

Results

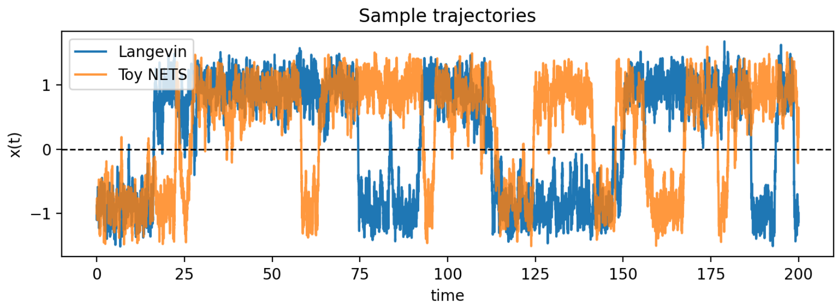

Figure 1: Sample trajectories starting in the left well ($x_0 = -1$). Langevin dynamics occasionally crosses the barrier at $x = 0$ but remains mostly trapped in the left well. The toy NETS-inspired drift (with $\alpha = 0.4$) produces multiple barrier crossings, demonstrating accelerated transitions. Time step $\Delta t = 0.01$, $\beta = 3.0$.

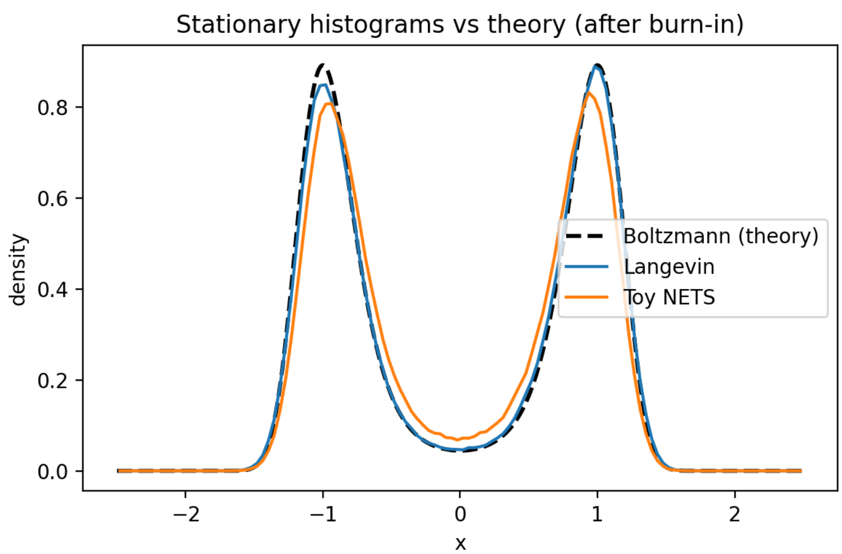

Figure 2: Stationary position distributions (after burn-in) from $N = 100$ trajectories. NETS drift slightly biases the histogram toward the barrier, while Langevin reproduces the Boltzmann distribution.

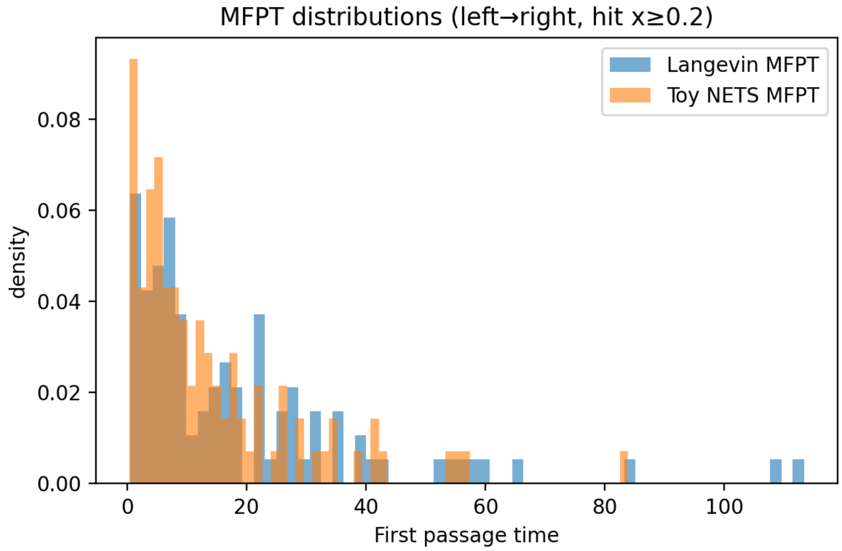

Figure 3: Mean first-passage times (left well to $x \geq 0.2$). NETS reduces MFPTs and increases the number of successful crossings compared to Langevin.

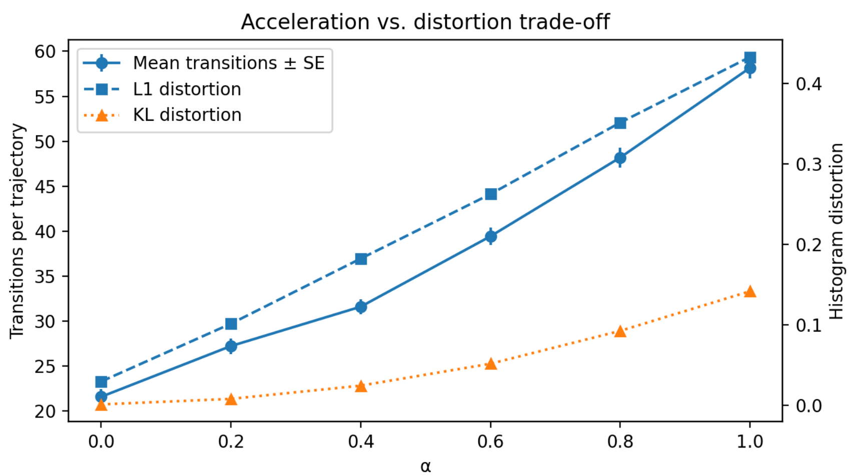

Figure 4: Tradeoff between acceleration (mean transitions) and histogram distortion (L1, KL) as α is varied. Larger α increases transitions but biases stationary distribution.

Summary Table

Method	Mean transitions	Mean MFPT	# trajectories reached
Langevin	21.54 ± 0.84	19.08 ± 2.11	100/100
Toy NETS α=0.4	31.57 ± 0.85	13.78 ± 1.47	100/100

Table 1: Comparison of Langevin and Toy NETS trajectories in the 1D double-well potential. MFPT measured from left well ($x < 0$) to $x \geq 0.2$.

Takeaways

- NETS-inspired drift accelerates transitions and reduces MFPT compared to standard Langevin dynamics.
- Stationary distribution is slightly biased, demonstrating the tradeoff between kinetic acceleration and equilibrium accuracy.
- Provides a computationally tractable toy model to explore concepts underlying NETS and rare-event acceleration.