Coping With Simulators That Don't Always Return

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TL;DR

- Deterministic simulators are often converted to stochastic simulators by adding random perturbations to state.
- Simulators can fail for invalidly perturbed inputs wasting computational resources and reduce effective sample size.

- We show these simulators are a rejection sampler.
- We train a flow-based proposal over perturbations targeting the distribution over permissible perturbations.
- Use of this proposal reduces the rejection rate, increasing the effective sample size yielding, lower variance evidence approximations in particle-based inference methods.

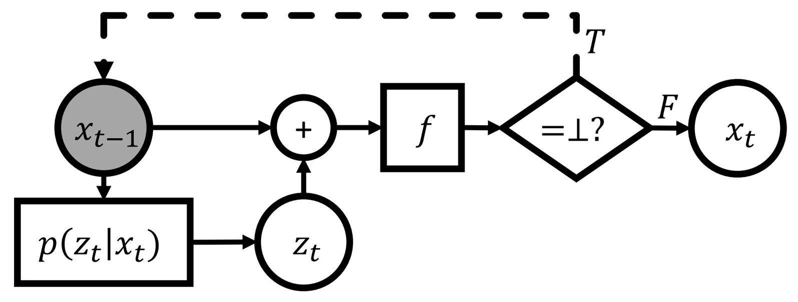

Figure 1a: sampling x_t in original model as a rejection sampler.

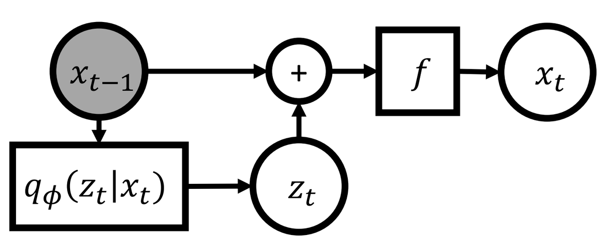

Figure 1b: replacing p with q_ϕ to eliminate rejection.

Method

- Simulator $F : X \to \{X, \perp\}$
- Perturbation proposal $p(z_t \mid x_t)$
- Simulator iteration $x_t \leftarrow f(x_{t-1} + z_t)$
- Define $\bar{p}(z_t|x_{t-1}) = \begin{cases} M\, p(z_t \mid x_{t-1}) & \text{if } f(x_{t-1}+z_t) \neq \perp \\ 0 & \text{otherwise} \end{cases}$

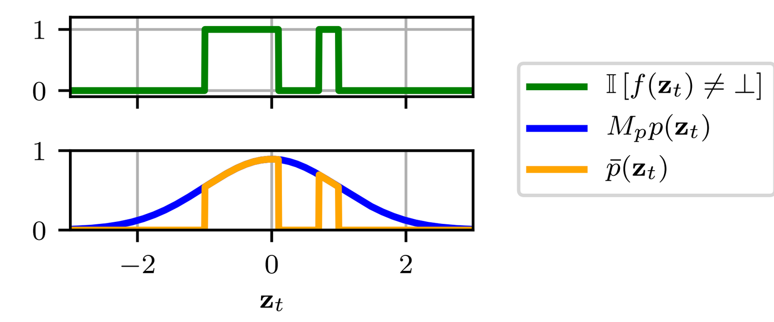

Figure 2: Graphical depiction of the scenario. Top: The simulator fails for some inputs. Bottom: The user-specified proposal distribution (blue) and resulting target distribution (gold).

- Target $q_{\phi^*}(z_t|x_t) = \bar{p}(z_t|x_t)$
- Where $\phi^* = \operatorname{argmax}_\phi \mathrm{E}_{z_t \sim \bar{p}(z_t|x_t),\, x_t \sim p(x_t)}[\log q_\phi(z_t|x_t)]$

- Directly replace p with q_ϕ to increase sample efficiency while targeting the same joint distribution.
- q_ϕ structured as a masked autoregressive flow (AF) [1] using one-layer MADE blocks [2].

Toy Example

- Observed data is Gaussian perturbed circular orbit.
- Model is linear velocity only.
- Failure if radius changes by more than a threshold.

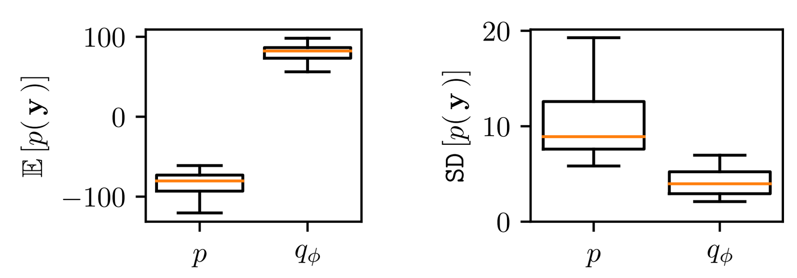

Figure 3a: Left: Much higher model evidence is achieved. Right: Dramatically lower variance SMC [2] evidence approximations are produced.

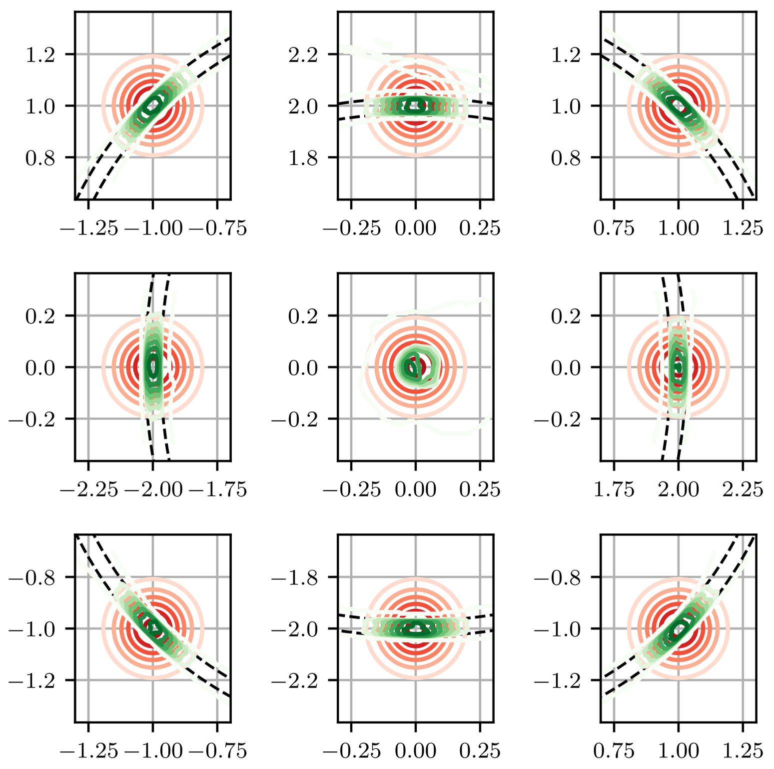

Figure 3b: A-priori specified perturbation proposal distribution (red) and learned permissible distribution (green).

Bouncing Balls

- Two elastically colliding balls.
- Failure if objects overlap.

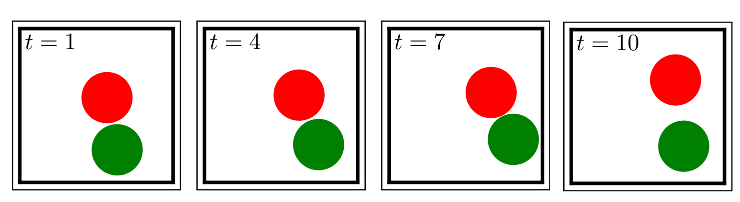

Figure 4a: Two balls bounce elastically in a square enclosure.

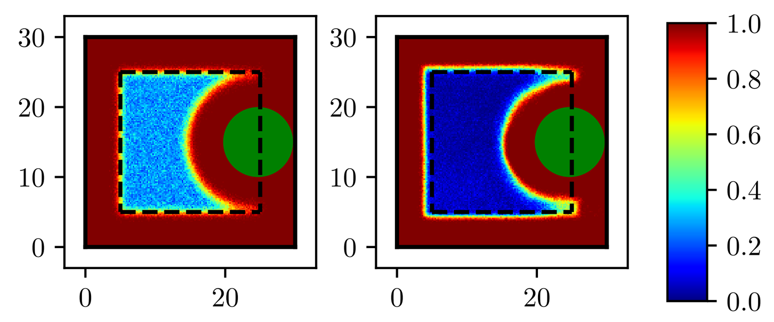

Figure 4b: rejection rate over position for red ball with green ball fixed in shown position using p (left) and trained AF (right).

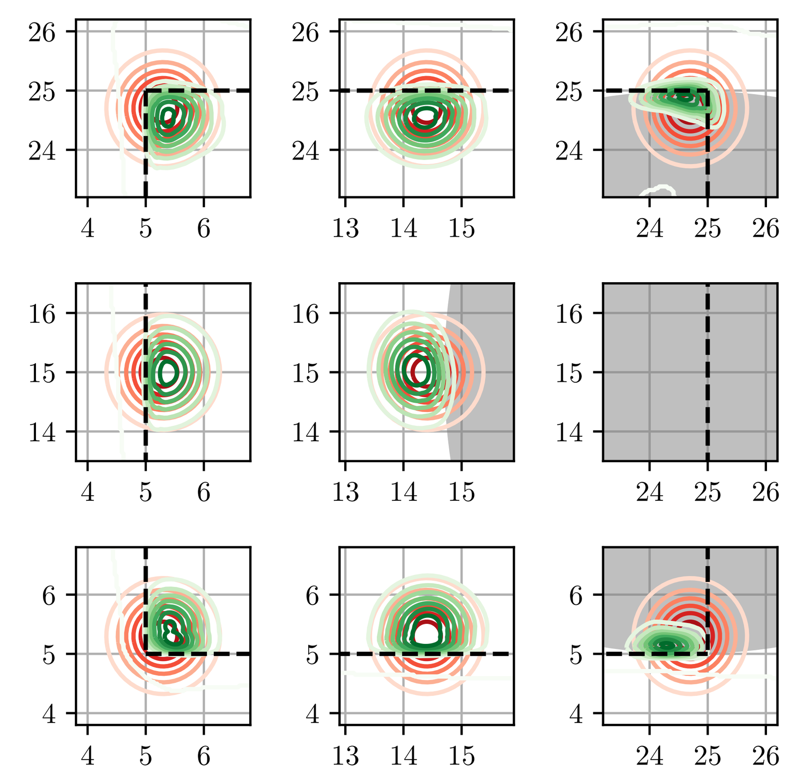

Figure 4c: learned proposal density over perturbations (green) and original density (red).

MuJoCo

- Perturb MuJoCo [3] simulator state with Gaussian noise.
- Failure if objects overlap above a threshold.

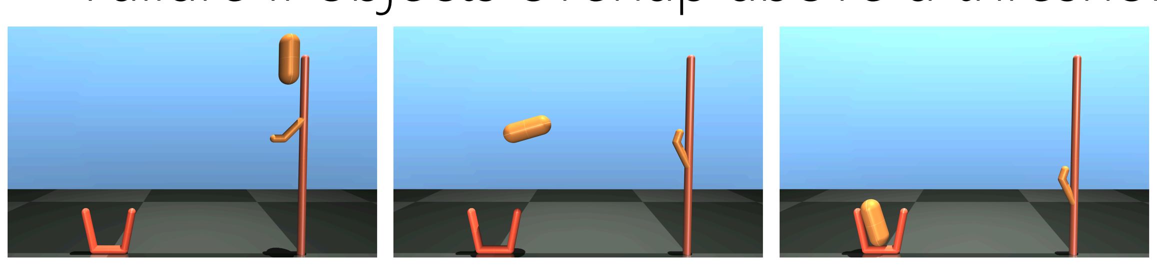

Figure 5a: "Tosser" MuJoCo environment.

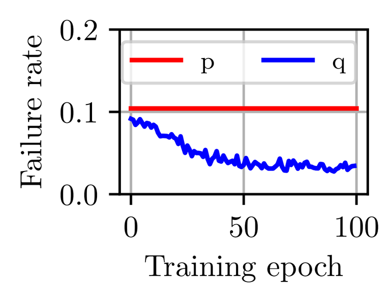

Figure 5b: AF learns to propose fewer rejections.

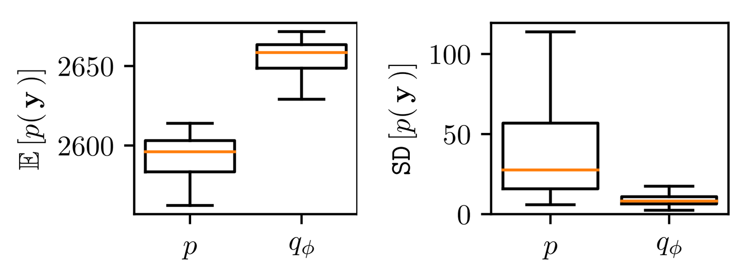

Figure 5c: Left: higher evidence using learned proposal. Right: dramatically lower variance evidence approximations.

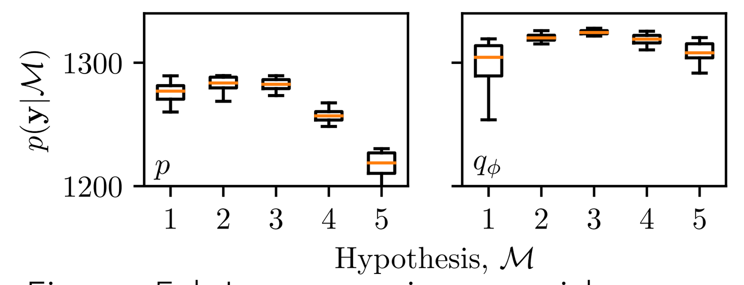

Figure 5d: Lower variance evidence approximations improve hypothesis testing.

Future Work

- Amortizing over simulator parameter values.
- Gradient-based optimization of simulator parameters.
- Ameliorate imperfect learned proposal distribution.

References

[1] G. Papamakarios, T. Pavlakou, and I. Murray. Masked autoregressive flow for density estimation. In Advances in Neural Information Processing Systems, pages 2338–2347, 2017.

[2] M. Germain, K. Gregor, I. Murray, and H. Larochelle. Made: Masked autoencoder for distribution estimation. In International Conference on Machine Learning, 2015.

[3] A. Doucet, N. De Freitas, and N. Gordon. An introduction to sequential Monte Carlo methods. In Sequential Monte Carlo methods in practice, pages 3–14. Springer, 2001.

[4] E. Todorov, T. Erez, and Y. Tassa. Mujoco: A physics engine for model-based control. IEEE/RSJ International Conference on Intelligent Robots and Systems, pages 5026–5033. IEEE, 2012.

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