Deep Probabilistic Surrogate Networks for Universal Simulator Approximation

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Introduction

A probabilistic programming framework that:
1. Allows for surrogate modeling in higher-order probabilistic programming languages.
2. Speeds up simulations/program execution.

Model the distribution, \( p \), over random variables \( x \) and their addresses \( a \) using a surrogate \( s \) based on neural networks \( f \) parameterized by \( \theta \):

\[
p(x, a) = \prod_i p(x_i|c_{x_i}, a_i) p(c_{x_i}|c_{x_{<i}}, a_{<i}, \theta),
\]

\[
e(x, a; \theta) = \prod_i e(c_{x_i}|c_{x_{<i}}, a_{<i}, \theta)|e(c_{x_{<i}}, a_{<i}, \theta)),
\]

In particular we note that the address transitions, \( p(c_{x_i}|c_{x_{<i}}, a_{<i}, \theta) \), are deterministic.

Surrogate modeling for higher-order programs requires modeling these address transitions.

\[
e(x, a; \theta) \text{ is trained by minimizing the KL-divergence,}
\]

\[
\text{KL}(q(e|a, \theta) || p(e|a|c_{x_{<i}}, a_{<i}, \theta)) \Rightarrow \text{constant}
\]

We showcase the benefits of using our framework on the process simulation of composite materials. The aim is to infer the internal unobservable state of the material during the curing process.

Modeling stochastic control flow

- We illustrate the PSNs ability to accurately model the address transitions associated with the stochastic control flow program.
- We choose \( e(x, a; \theta) \) to be a categorical distribution.
- Only small deviations are found between the address transitions probabilities in the program and the surrogate.
- The deviations found happen with small probability.

Process simulation of composite materials

Using PSNs we are able to accurately model the joint distribution defined by the simulator and achieve running times that are magnitudes smaller than that of the original simulator. Using PSNs for inference tasks produce accurate posterior estimates many times faster than using the simulator.

References