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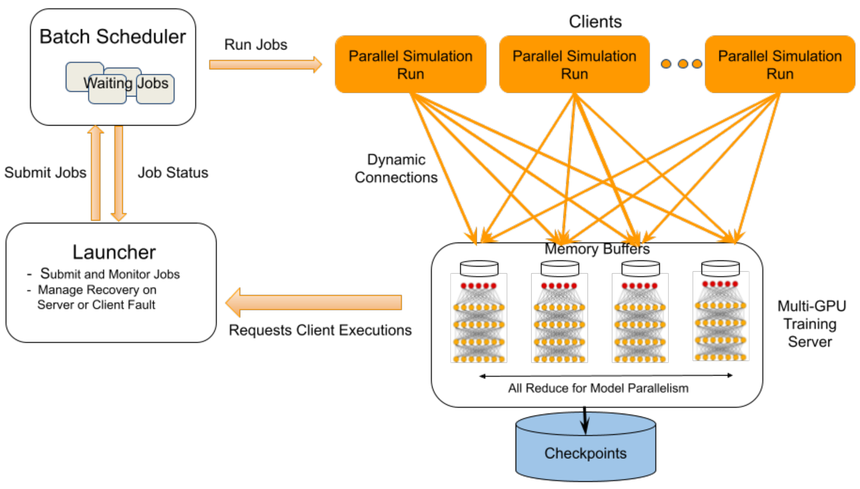
Loss-driven sampling for online NN training with large scale simulations

Sofya Dymchenko*
Bruno Raffin

Context

We want to advance applications of DL to sciences by **improving online training** techniques. DataMove team contributed with **DeepMelissa framework** for large-scale deep surrogate training on supercomputers.



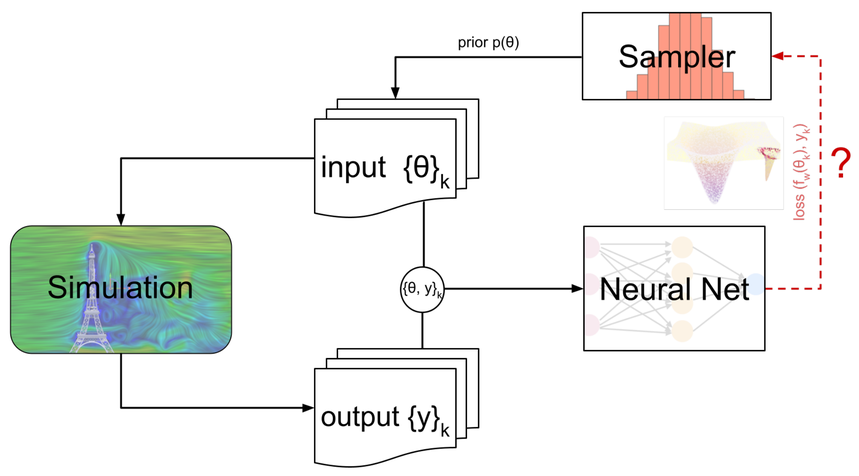
Motivation

★ **Avoidance of I/O bottleneck**: with file-free processing high-dimensional data is given "on-the-fly".

★ **Infinite data stream**: no limitations for generalization.

☆ **Ability to control data stream**: choice of data to sample can be explicit rather than random. Training can be more data-efficient. But how to choose?

Problem statement



Simulation: program that returns outputs by given inputs, *e.g.* initial state of water flow in tube and t-state.

Neural network: any NN that uses data from simulation, *e.g.* a surrogate that imitates simulation.

Sampler: takes inputs from defined prior distribution, *e.g.* uniform distribution. Can we do better?

Method

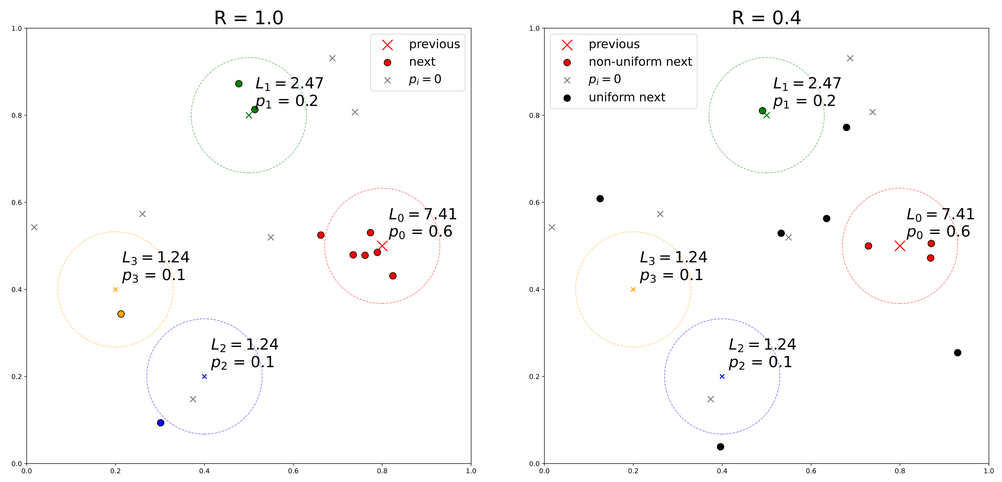
Hypothesis

High loss $\implies$ difficult sample to learn
$\implies$ region* needs to be fed to neural network

Adaptive sampling

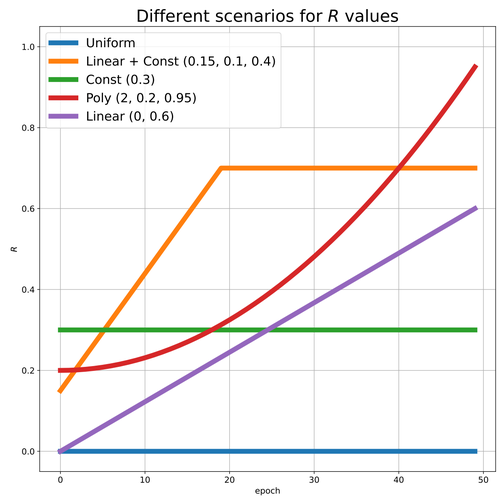
First batch is sampled uniformly. Loop-process:

1) NN provides **loss values statistic** per batch-point
2) Select points w.r.t. **distribution** calculated as **normalised loss**
3) Next batch is sampled from their **Gaussian neighbourhoods**



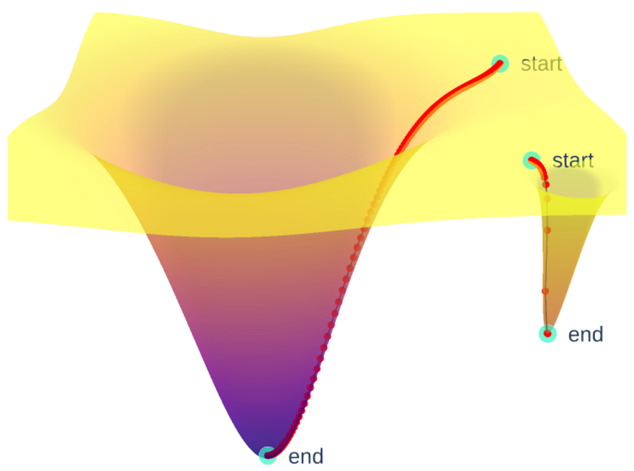
R-value

The value R is **a ratio** (percentage) **of points** to be sampled for next epoch in a **loss-driven** manner. It is a trade-off between "exploring hard points" and "remembering/learning easy points".



Experiments

The **simulation** gives closest minima by running **gradient descent** on the fixed surface. Current fixed surface is two imbalanced pits.



Input (x, y)
NN
sim
Output (x^*, y^*)

*We assume roughly that region of inputs is close to region of outputs.
Formalization:
Let f be a simulation program.

$$f(\theta) = y_\theta$$

where $\theta = \{\theta^{(0)}, \dots, \theta^{(d_{in}-1)}\} \in \mathbb{R}^m$ is a set of simulation input parameters coming from prior, and $y_\theta = \{y^{(0)}, \dots, y^{(t)}\} \in \mathbb{R}^{d_{out} \times t}$ is a simulation output sample, and $t \in [0, T], T \in \mathbb{R}^+$.
Roughly, in toy example $\theta = y^{(0)}$ and $f(\theta) = y^{(1)}$.
Surrogate f_w is a neural network which learns data generated by f.

$$f_w(\theta) = \hat{y}_\theta$$

The goal is:

$$\text{dist}(f_w(\theta), f(\theta)) \to_w 0$$

Probability distributions:
Prior $p(\theta)$
Likelihood $p(y|\theta)$
Posterior $p(\theta|y)$
Main struggle with simulations — they are not probabilistic and there is no direct access to its outputs.

Toy experiment variations
- predict trajectory: output is $\{(x, y)\}_k$
- less surjective simulation surface: different inputs give different outputs (imagine long pit)
- several extreme saddle points: mimics molecular exploration problem

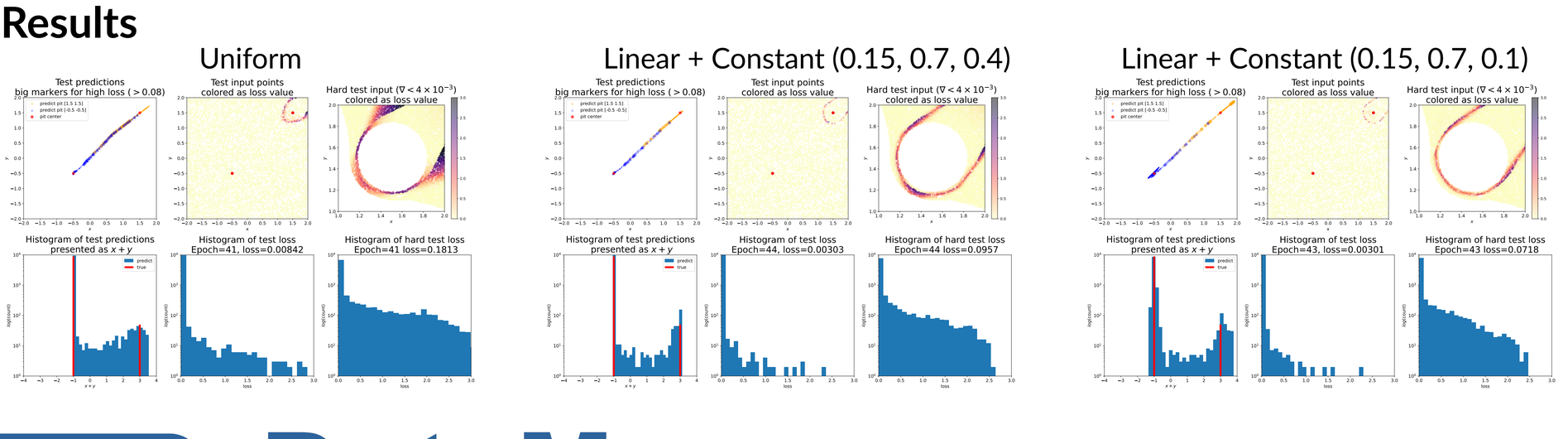
Related works:
- RAR algorithm
- Evo algorithm

Future studies:
- trajectory prediction, t -> t+1
- experiments for not toy examples (physics inspired, i.e. room heat, turbulent flows, lorenz system)
- Bayesian Experimental Optimal Design for implicit models for finding a sequence of new input parameters to run simulation with.
- Simulation Based Inference techniques for learning likelihood/posterior of simulation data space.
- explore Reinforcement Learning models for "exploring and exploiting" data space.

DNN: linear 2x64, ReLU, linear 64x32, LeakyReLU, linear 32x16, LeakyReLU, linear 16x8, ReLU, linear 8x2 (2954 par-s).

Loss: HuberLoss (MSE+MAE)

Results

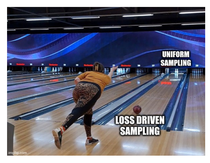


Conclusion

★ Overall **speed-up** in convergence

★ Significantly **increased** prediction accuracy for "hard area"

★



DataMove
Mouvement de données pour le calcul haute performance

Laboratoire d'Informatique de Grenoble

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