Gradient free optimization of neuroscience models at different scales with L2L

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Motivation

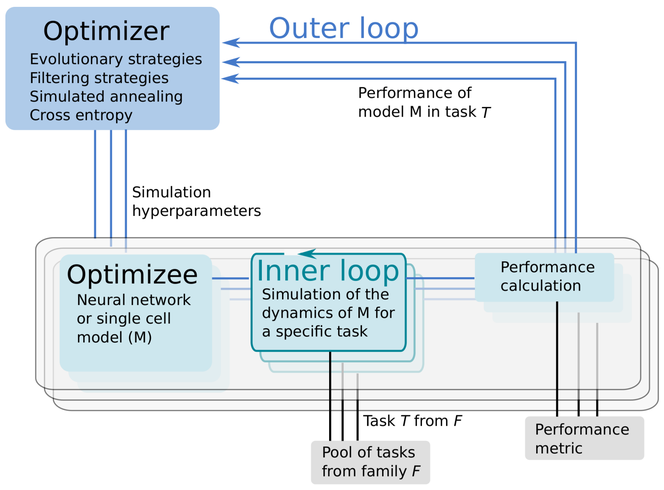
Problem:

- Neuroscience models have high number of degrees of freedom
- Only specific parameter regions are of interest
- Finding these regions efficiently requires development of complex tools and strategies

Goal:

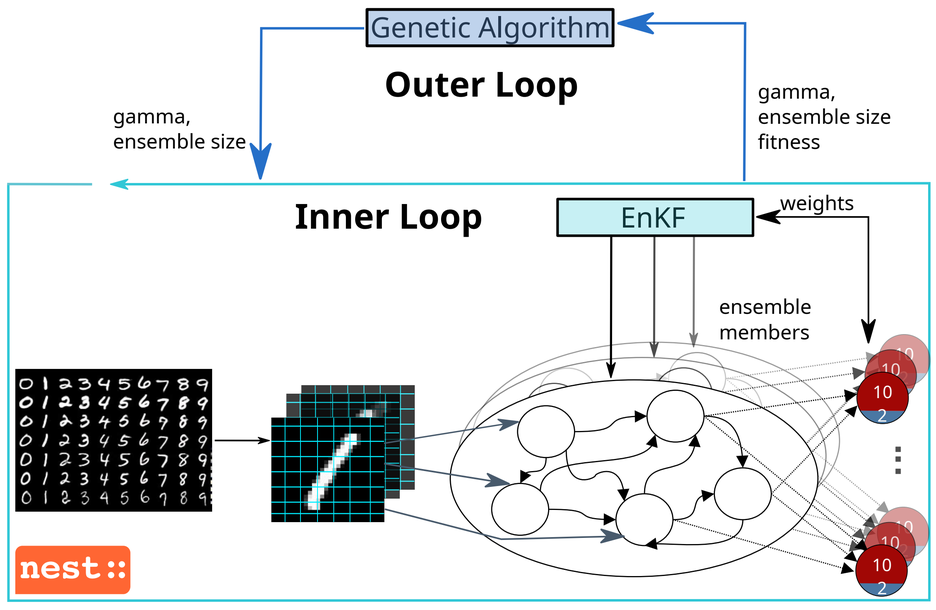
1. High throughput hyper-parameter optimization at scale using Machine Learning
2. Parallelization on high performance computing systems (HPCs)
3. Handling of complex problems with arbitrary tools and algorithms

Learning to Learn (L2L) framework



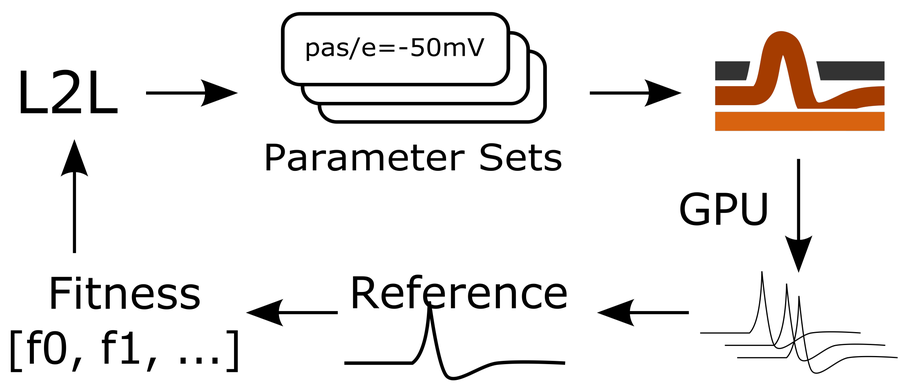
- Implements the concept of meta-learning [1, 2]
- Generalization on new data sets via experience
- Parameter space exploration
- Variety of gradient-free metaheuristics
- Easily parallelizable on HPC systems and applicable to different scientific fields

NEST: Tuning large scale spiking networks



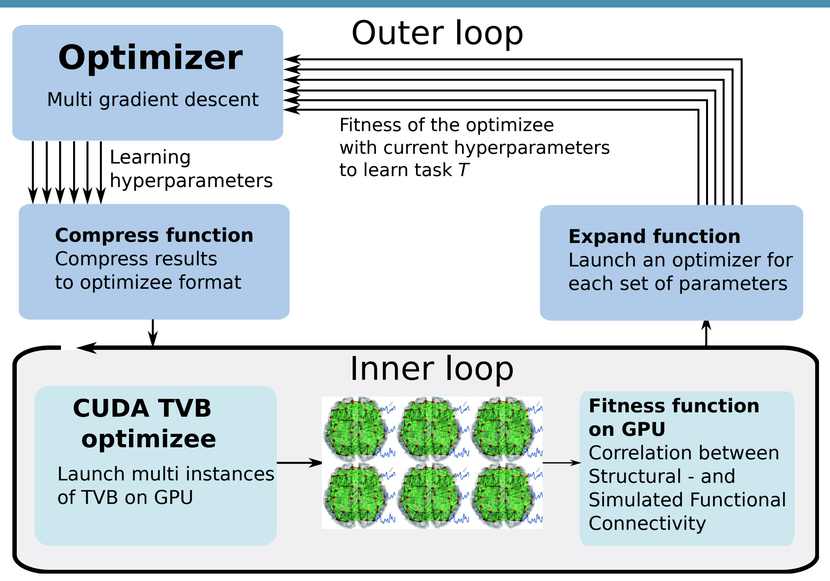
- Two loop parameter optimization scheme of spiking reservoir
- Implemented in NEST [3] on HPC systems
- Reservoir classifies digits
- Ensemble Kalman filter (Enkf) optimizes weights of n individuals
- Genetic algorithm optimizes hyper-parameters γ and ensemble size

Arbor: Single cell parameter optimization



- Network simulations of morphologically-detailed neurons [4] Built for modern, accelerated HPC using C++20 and Python
- For a given model, i.e. morphology and assignment of ion channels, find parameters to match empirically obtained voltage traces
- Working prototype for distributed optimization
- Proof of concept for multi-instance optimization leveraging Arbor's GPU support → simultaneous evaluation of a large population of individuals

The Virtual Brain (TVB) parameter sweeps



- TVB [5]: whole brain simulation using neural mass models and detailed connectomes
- Parameter fitting to match patient EEG/fMRI
- TVB Python optimizee available
- TVB CUDA multi-instance optimization (see figure)
- Recommended usage of RateML to easily build TVB model

NetLogo-Nest: Ant colony optimization

- Multi-agent simulation in NetLogo [6]
- Ants (red, green) explore and forage for food (green, brown leaves)
- Drop pheromones (blue, white) for communication
- Steered by a Spiking Neural Network
- Optimization of weights and delays
- 32 individuals optimized in parallel, 15 ants

L2L on :

Acknowledgments

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