Hyper-parameter space exploration of neuroscience models on high performance computers with the Learning to Learn framework

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Motivation

Problem:

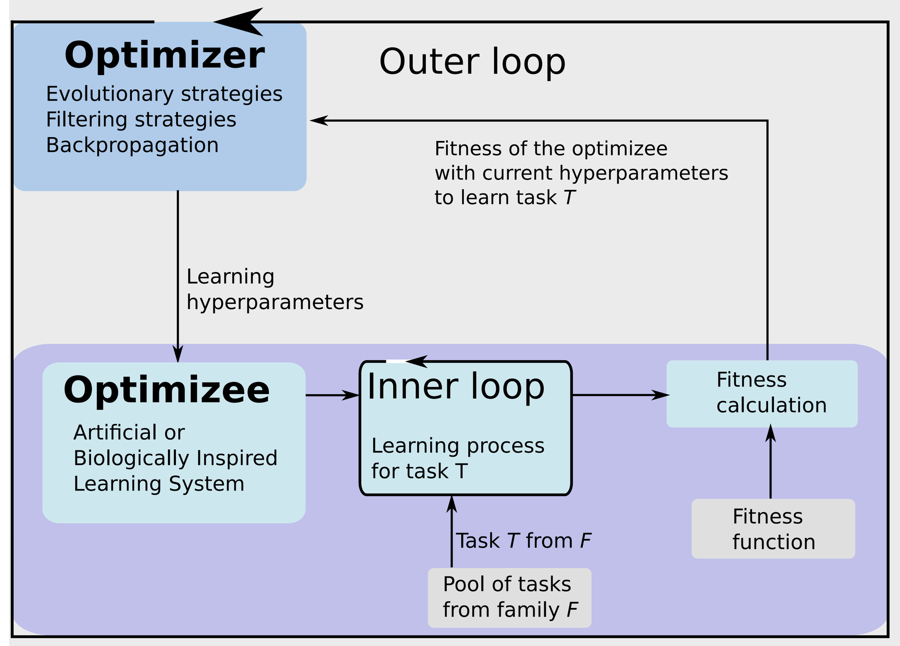
- Neuroscience models have high number of degrees of freedom
- Only specific parameter regions are of interest
- Finding these regions efficiently requires development of complex tools and strategies

Goal:

1. High throughput hyper-parameter optimization at scale using Machine Learning
2. Parallelization on multi-node HPCs
3. Handling of complex problems with arbitrary tools and algorithms

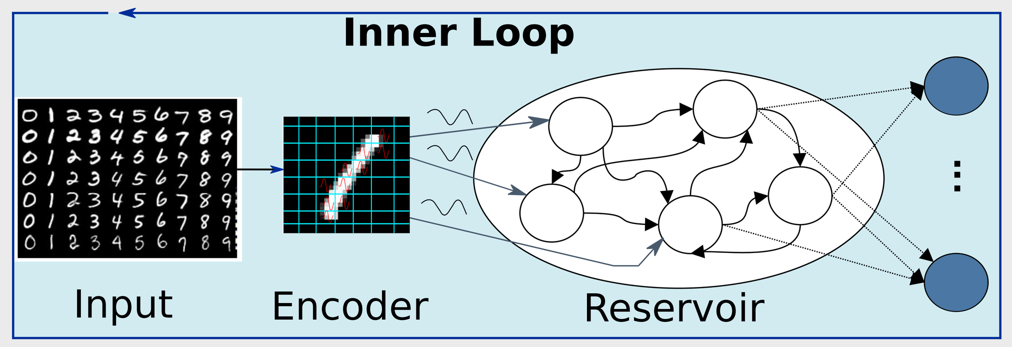
Focus: Showcasing different neuroscience models optimized with the **Learning to Learn (L2L)** framework

Introduction: Learning to Learn (L2L)



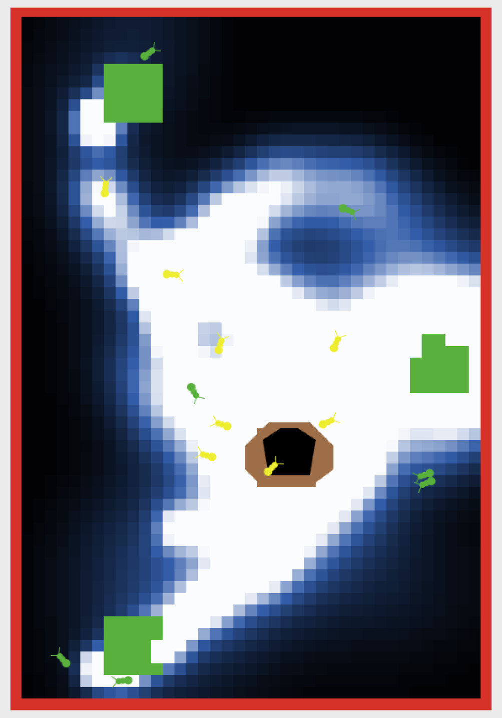
- Concept formalized by Thrun and Pratt [1]
- Generalization on new data sets via experience
- Parameter space exploration
- Two loop structure
- Different optimization algorithms
- Easily parallelizable on HPC installations

NEST: Tuning large scale spiking networks



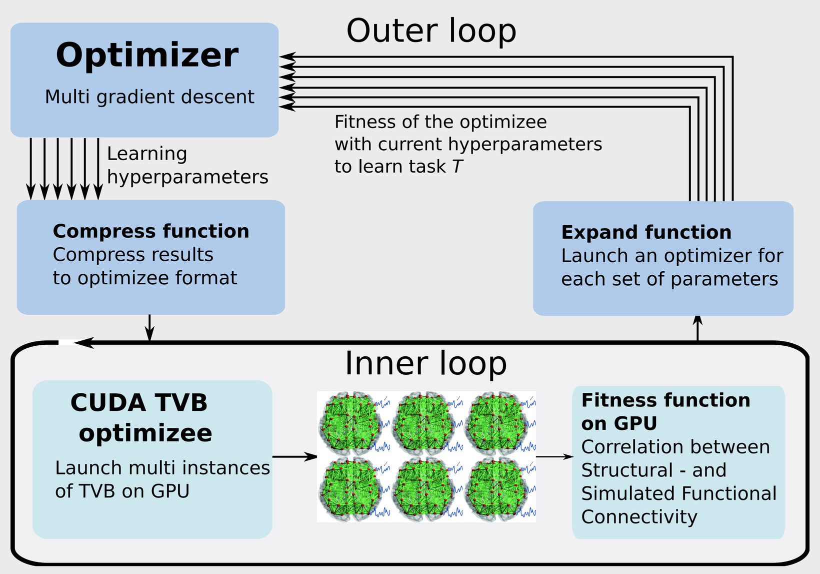
- Flexible parameter exploration of spiking networks using NEST on HPC
- Leverages the internal parallelization capabilities of NEST
- UC1: Optimization of connectivity using metrics of expected dynamics
- UC2: Optimization of plasticity rules to generate new models with specific structural-functional constraints
- UC3: Optimize networks to perform a specific task e.g. classification (top figure)

NetLogo-Nest: Ant Colony Optimization



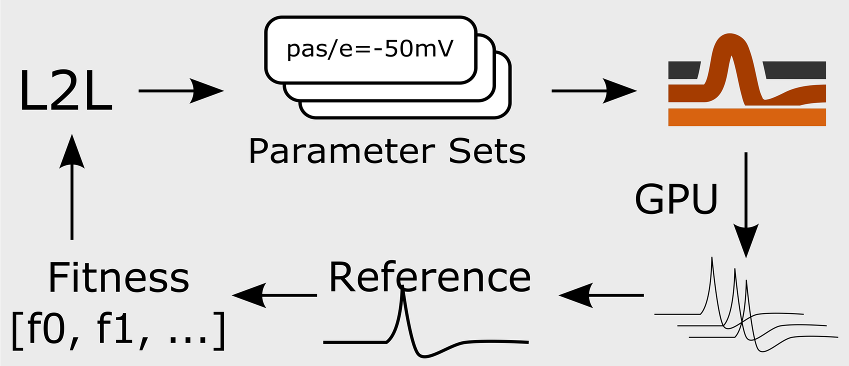
- Multi-agent simulation in NetLogo [2]
- NEST [3], SpikingLab [4] as back-end
- Ants explore food and avoid collisions
- Drop pheromones for communication
- Steered by a Spiking Neural Network
- Optimization of the weights and delays
- ≈100 individuals optimized in parallel, 15 ants

The Virtual Brain (TVB): Parameter exploration



- 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 (left figure)
- Recommended usage of RateML to easily build TVB models

Arbor: Single Cell Parameter Optimization



- Arbor: Network simulations of morphologically-detailed neurons [6]
  Built for modern, accelerated HPC using C++20 and Python
- Python interface connects L2L and Arbor
- Use-case: 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 using single individuals
- Proof of concept for multi-instance optimization leveraging Arbor's GPU support → simultaneous evaluation of a large population of individuals

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