



Gradient free optimization of neuroscience models at different scales with L2L

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Motivation

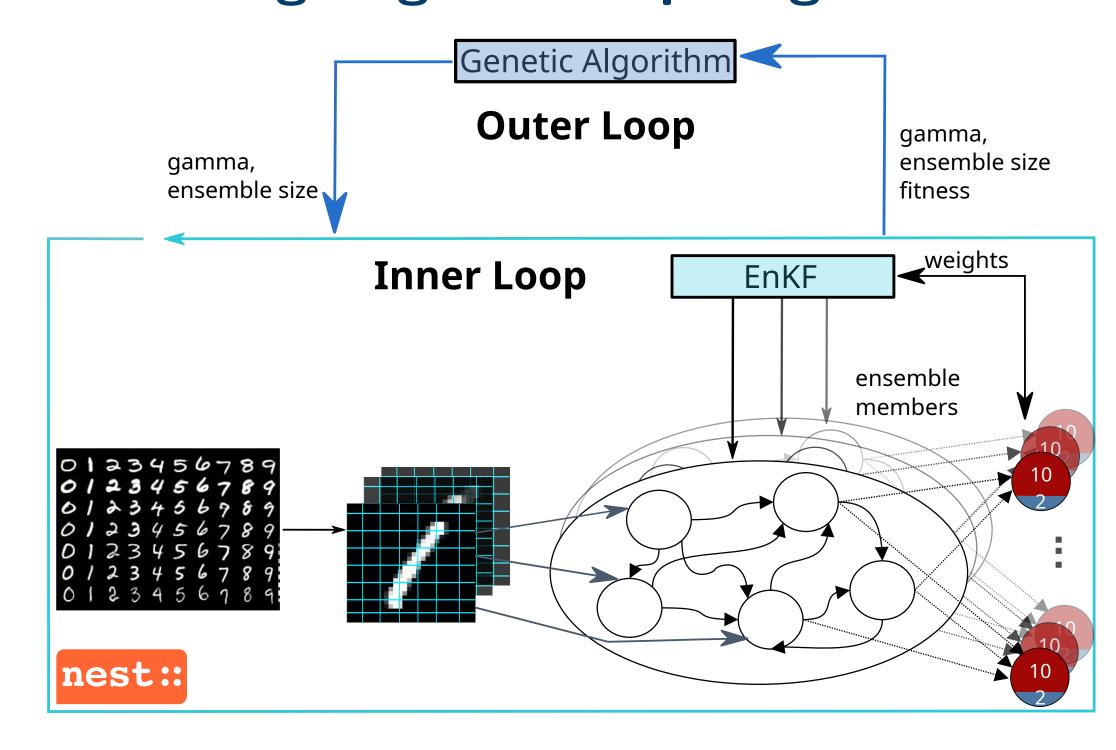
Problem:

- 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:

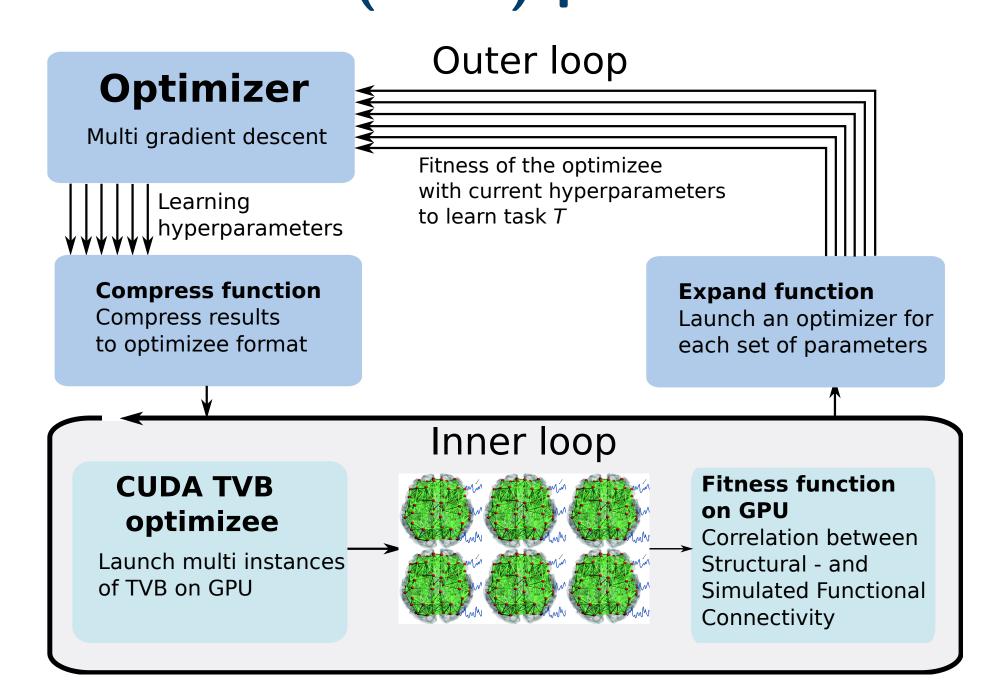
- High throughput hyper-parameter optimization at scale using Machine Learning
- 2 Parallelization on high performance computing systems (HPCs)
- Handling of complex problems with arbitrary tools and algorithms

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

The Virtual Brain (TVB) parameter sweeps

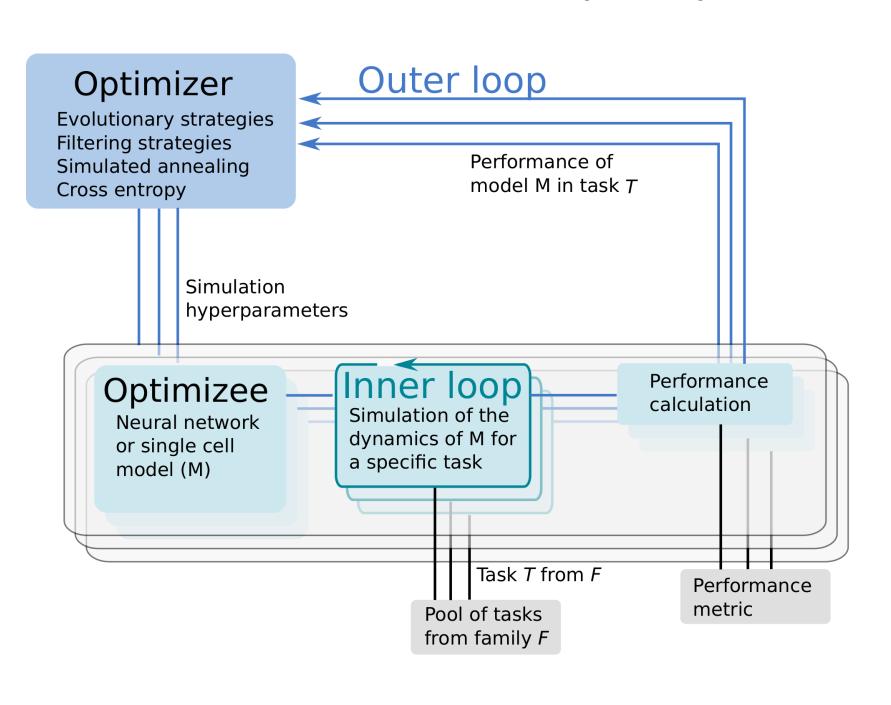


- TVB [5]: whole brain simulation using neural mass models and detailed connectomes
- Parameter fitting to match patient EEG/fMRI
- TVB Python optimizee available
- TVB CUDA multi-instance optimization (see figure)
- Recommended usage of RateML to easily build TVB model

Acknowledgments

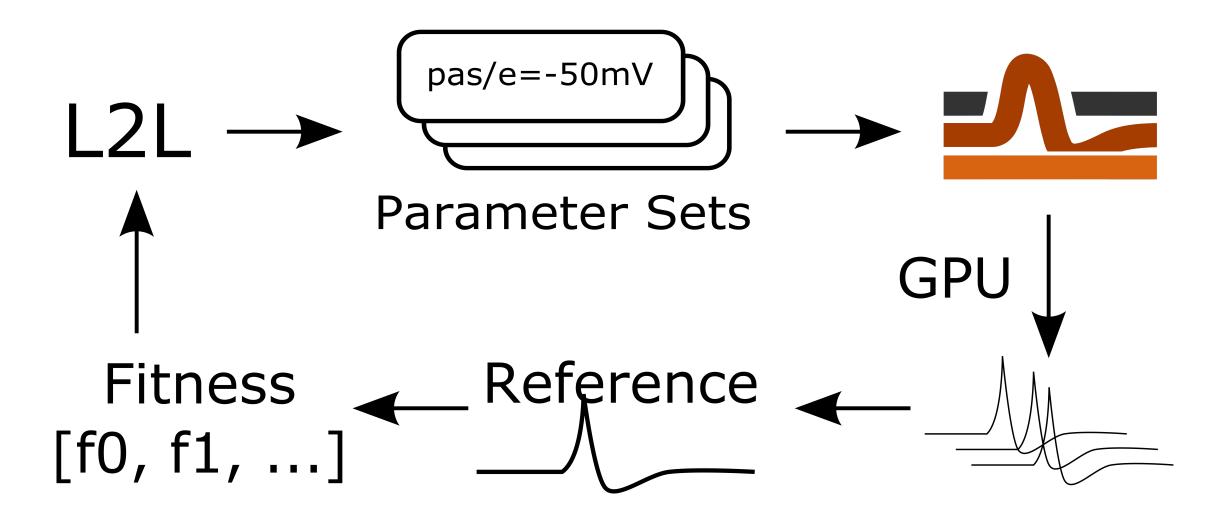
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Learning to Learn (L2L) framework



- 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

Arbor: Single cell parameter optimization

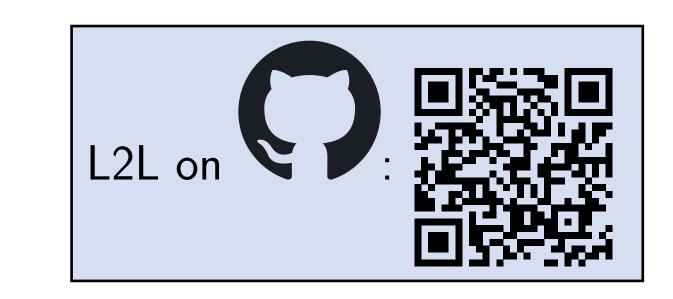


- Network simulations of morphologically-detailed neurons [4] Built for modern, accelerated HPC using C++20 and Python
- For a given model, i.e. morphology and assignment of ion channels, find parameters to match empirically obtained voltage traces
- Working prototype for distributed optimization using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

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



References

- [1] Sebastian Thrun and Lorien Pratt. *Learning to learn*. Springer Science & Business Media, 2012.
- Alper Yegenoglu et al. "Exploring Parameter and Hyper-Parameter Spaces of Neuroscience Models on High Performance Computers With Learning to Learn". In: *Frontiers in Computational Neuroscience* 16 (2022).
- [3] Jan Hahne et al. NEST 3.0. Version 3.0. June 2021. DOI: 10.5281/zenodo.4739103. URL: https://doi.org/10.5281/zenodo.
- 4739103.
 N. Abi Akar et al. "Arbor A Morphologically-Detailed Neural Network Simulation Library for Contemporary High-Performance Computing Architectures". In: 2019 27th Euromicro International Conference on Parallel, Distributed and Network-Based Processing (PDP). Feb. 2019,
- pp. 274–282. DOI: 10.1109/EMPDP.2019.8671560.

 Paula Sanzleon et al. "The virtual brain: A simulator of primate brain network dynamics". In: Frontiers in Neuroinformatics 7.MAY (2013).
- ISSN: 16625196. DOI: 10.3389/fninf.2013.00010.

 Seth Tisue and Uri Wilensky. "Netlogo: A simple environment for modeling complexity". In: *International conference on complex systems*. Vol. 21. Boston, MA. 2004, pp. 16–21.