Data-driven efficient surrogate-assisted evolutionary method for multi-objective optimization of high-dimensional neural dynamical systems

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Overview: Biophysical modeling of hippocampal networks at full scale

Parallel, efficient, flexible data storage for large-scale network models

Realistic 3D anatomy and topographical gradients of functional and connectivity properties

Towards a general framework for modeling large-scale biophysical neuronal networks: a full-scale computational model of the rat dentate gyrus

Raikov... Soltesz, 2021.

https://www.biorxiv.org/content/10.1101/2021.11.02.466940v1
Surrogate-assisted optimization overview
Gaussian Process Regression for Surrogate Modeling

Gaussian processes provide methods for regression modeling by defining a conditional probability distribution over a number of functions that represent a given collection of points.

![Gaussian Process Regression Diagram](image)
Surrogate-Assisted Optimization With Evolutionary Algorithms

https://www.strong.io/blog/evolutionary-optimization
Objective: find the minimal value(s) of the function

$$z = 3(1 - x)^2 e^{-x^2 - (y+1)^2} - 10\left(\frac{x}{5} - x^3 - y^5\right) e^{-x^2 - y^2} - \frac{1}{3} e^{-(x+1)^2 - y^2}.$$
Objective: find the minimal value(s) of the function

\[ z = 3(1 - x)^2 e^{-x^2 - (y+1)^2} - 10\left(\frac{x}{5} - x^3 - y^5\right) e^{-x^2 - y^2} - \frac{1}{3} e^{-(x+1)^2 - y^2}. \]

B)

<table>
<thead>
<tr>
<th></th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>True minimum</td>
<td>0.3061</td>
<td>-1.5306</td>
<td>-6.3898</td>
</tr>
<tr>
<td>Surrogate minimum</td>
<td>0.1</td>
<td>-1.5632</td>
<td>-6.3001</td>
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</tbody>
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Surrogate optimization of biophysical neuron models based on the Pinsky-Rinzel model formalism

\[
C_m V'_s = -I_{\text{Leak}}(V_s) - I_{\text{Na}}(V_s, h) - I_{K-\text{DR}}(V_s, n) \\
+ (g_c/p)(V_d - V_s) + I_s/p
\]

\[
C_m V'_d = -I_{\text{Leak}}(V_d) - I_{\text{Ca}}(V_d, s) - I_{K-\text{AHP}}(V_d, q) \\
- I_{K-C}(V_d, Ca, c) - I_{\text{Syn}}/(1 - p) \\
+ (g_c/(1 - p))(V_s - V_d) \\
+ I_d/(1 - p)
\]

(1)


Surrogate optimization of Pinsky-Rinzel models of neurons in the dentate gyrus: Mossy Cell

- Input resistance [MOhm]
- Membrane time constant [ms]
- Spike threshold [mV]

**Frequency-current relationship**
- Frequency [Hz]
- Injected current [nA]

**ISI adaptation**
- ISI ratio last/first
- Injected current [nA]

**Comparison of locally optimal solutions**
- Various parameters including rn_error, tau_error, fi_error, spike_amplitude_error, ISI_adaptation_error
Surrogate optimization of a model of a network of the dentate gyrus (1)

Optimization targets:
- GC selectivity (SNR)
- GC firing rate
- GC fraction active
- MC selectivity (SNR)
- MC firing rate
- MC fraction active
- IN firing rates: AAC, BC, HICAP, HIPP, IS, MOPP, NGFC

Dentate Gyrus Output to CA3
Surrogate optimization of a model of a network of the dentate gyrus (2)

Reconstruction of hippocampal volume

Model of dentate gyrus volume with layer-specific somata distribution

Multi-objective genetic algorithm

Evaluation

Principal neuron

Interneuron

Target synapse for optimization

Subset of connections extracted from Full Scale Network

Full Scale Network
Surrogate optimization of a model of a network of the dentate gyrus (3)

Results collected: 1004
Total walltime: 12.42 hours
Mean time per call: 1.3 hours
Std. dev. of time per call: 0.19 hours
Mean calls per worker: 7.8 [min 7 max 9]
Number of processes: 28544 (1024 nodes; 223 processes per worker)
Number of workers: 127

Distributed work queue based on mpi4py
https://github.com/iraikov/distwq
Surrogate optimization of a model of a network of the dentate gyrus (4)
Surrogate optimization of a model of a network of the dentate gyrus (5)
Summary

Computationally expensive model

Distributed evaluation

Worker #1

Worker #2

Worker #N

Surrogate model

Evolutionary optimization

Evaluation

Selection

Mutation

Crossover

Software Availability
https://github.com/iraikov/dmosopt
Distributed surrogate assisted optimization toolbox:

https://github.com/iraikov/dmoso-opt

NIH BRAIN 1U19NS104590-01
Towards a Complete Description of the Circuitry Underlying Sharp Wave-Mediated Memory Replay

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