

Replicated Computations Results (RCR) Report for “Statistical Abstraction for Multi-scale Spatio-temporal Systems”

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“Statistical abstraction for multi-scale spatio-temporal systems” proposes a methodology that supports analysis of large-scaled spatio-temporal systems. These are represented via a set of agents whose behaviour depends on a perceived field. The proposed approach is based on a novel simulation strategy based on a statistical abstraction of the agents. The abstraction makes use of Gaussian Processes, a powerful class of non-parametric regression techniques from Bayesian Machine Learning, to estimate the agent’s behaviour given the environmental input. The authors use two biological case studies to show how the proposed technique can be used to speed up simulations and provide further insights into model behaviour. This replicated computation results report focuses on the scripts used in the paper to perform such analysis. The required software was straightforward to install and use. All the experimental results from the paper have been reproduced.

CCS Concepts: • **Applied computing** → **Systems biology**;

Additional Key Words and Phrases: RCR report, multi-scale systems, spatio-temporal, agent-based, statistical abstraction, coarsening

ACM Reference format:

Michele Loreti. 2019. Replicated Computations Results (RCR) Report for “Statistical Abstraction for Multi-scale Spatio-temporal Systems”. *ACM Trans. Model. Comput. Simul.* 29, 4, Article 23 (December 2019), 2 pages. <https://doi.org/10.1145/3341094>

1 INTRODUCTION

In Reference [1] a methodology that aims to support analysis of large-scaled spatio-temporal systems is proposed. The authors consider a framework where multiple identical agents are distributed in space over an external field. The agents perceive the field locally and perform internal stochastic computations to determine their subsequent behaviour, such that their actions are influenced by their environment. Agents can also act locally upon the external field, enabling the latter to become a medium for signals between agents. The proposed methodology allows to replace expensive stochastic parts of the model with input-output maps estimated via a machine learning procedure. The authors focus on a particular macro-scale behaviour as output from the model, and devise a statistical abstraction of the system to produce a simpler system that preserves the macro-scale behaviour. The necessary input-output relation is estimated by learning a parameters-to-behaviours regression map using Gaussian Processes (GPs), a powerful class of non-parametric Bayesian regression models. To illustrate the application of the proposed abstraction,

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1049-3301/2019/12-ART23 \$15.00

<https://doi.org/10.1145/3341094>

the authors consider two case studies: a model of *Escherichia coli chemotaxis* and a model of *Dictyostelium discoideum aggregation*.

Detailed instructions on how to replicate the results of the experiments have been made available by the authors at the following link: <http://bit.ly/2WMoi2E>. The code needed for abstracting and simulating the two case studies is made available in two *Git* repositories referenced in the link above. The results obtained from the replicated computations were compatible with the ones presented in the paper. For these reasons “Artifacts Evaluated Functional,” “Artifacts Available,” and “Results Replicated” badges can be applied to Reference [1].

2 REPLICATION OF COMPUTATION RESULTS

To replicate the results reported in Reference [1], *Python* (version 3.5 or later) is needed together with the following packages:

- *Numpy*, a package for scientific computing;
- *SciPy*, a library providing user-friendly and efficient numerical routines;
- *Matplotlib*, a plotting library.

Additionally, to run *Ecoli* experiments, one has to also install *pyGPs* (a Python Library for Gaussian Process Regression and Classification), *StochPy* (a package for stochastic modelling). The package *GPFlow*, to build Gaussian processes, is needed to run *Discoideum* experiments. All these tools are released with an *open source licence* and can be easily installed.

If all the system requirements are satisfied, the installation process is straightforward and it just consists in following the detailed instructions provided by the authors. All the computations have been performed on a standard PC equipped with a 3.5GHz *Intel Core i7* and 16GB of RAM.

The authors first apply the proposed approach to the case study of *Chemotaxis in E. coli*. All the scripts to run the experiments (together with the results presented in the paper) are available via a *Git* repository.¹ All the experiments can be easily reproduced by following the detailed instructions provided by the authors. The obtained results are all compatible with the ones presented in the paper. However, to obtain them, around three days have been necessary to complete the simulations.

In the second case study, a model of *Dictyostelium discoideum aggregation* is studied. Different from the *Ecoli* scenario, in *Discoideum*, model agents can influence their immediate environment. This enables inter-agent interactions with the environment layer, which acts as a conduit for signalling. As done for the other case study, the authors have set up a *Git* repository with all the scripts and data.² The authors conducted their experiments on a 64-core server reporting an execution time of about four hours. The same experiments, on a standard PC, required about seven days. The obtained results are all compatible with the ones presented in the paper.

ACKNOWLEDGMENTS

The author would like to thank all the authors of Reference [1], and in particular Michalis Michaelides, for providing access to the appropriate scripts to replicate the experiments described in their paper.

REFERENCES

- [1] Jane Hillston, Michalis Michaelides, and Guido Sanguinetti. 2019. Statistical abstraction for multi-scale spatio-temporal systems. *Trans, Mod, Comput, Simul*, (2019). To appear.

Received June 2019; accepted June 2019

¹<https://bitbucket.org/webdrone/ecoli/src/master/>.

²<https://bitbucket.org/webdrone/ddiscoideum/src/master/>.