| Thermodynamic Analytics Toolkit (TATi) - Roadmap i |  |  |  |  |  |
|--|--|--|--|--|--|
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
| Thermodynamic Analytics Toolkit (TATi) - Roadmap   |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |

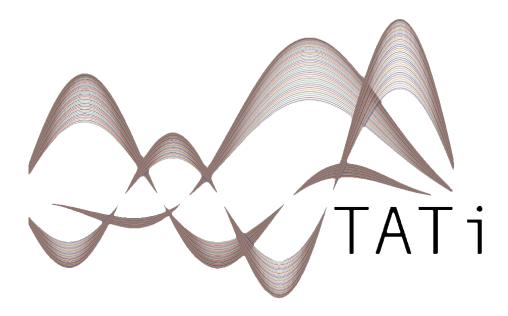
## COLLABORATORS

|            | TITLE: Thermodynamic Anal  | ytics Toolkit (TATi) - |           |
|------------|--|------------------------|-----------|
| ACTION     | NAME   | DATE                   | SIGNATURE |
| WRITTEN BY | sampling methods<br>based on Langevin<br>Dynamics and<br>Hamiltonian | 2018-08-17             |           |

| REVISION HISTORY  |            |             |      |  |  |  |  |
|-------------------|------------|-------------|------|--|--|--|--|
| NUMBER            | DATE       | DESCRIPTION | NAME |  |  |  |  |
| v0.9.1-0-g994aa50 | 2018-08-17 |             | S    |  |  |  |  |

## **Contents**

1 Roadmap 1



## 2018-08-17 thermodynamicanalyticstoolkit: v0.9.1-0-g994aa50

TATi is a software suite written in Python based on tensorflow's Python API. It brings advanced sampling methods (GLA1 and GLA2, BAOAB, HMC) to *neural network training*. Its **tools** allow to assess the loss manifold's topology that depends on the employed neural network and the dataset. Moreover, its **simulation** module makes applying present sampling Python codes in the context of neural networks easy and straight-forward. The goal of the software is to enable the user to analyze and adapt the network employed for a specific classification problem to best fit her or his needs.

TATi has received financial support from a seed funding grant and through a Rutherford fellowship from the Alan Turing Institute in London (R-SIS-003, R-RUT-001) and EPSRC grant no. EP/P006175/1 (Data Driven Coarse Graining using Space-Time Diffusion Maps, B. Leimkuhler PI).

Frederik Heber

## 1 Roadmap

TATi is a work in progress and always open for enhancements be it from the side of its core programmers or from collaborators. The following items are on the current roadmap in no specific order and subject to change:

- Remodeling of the general python interface (**not** simulation)
- Allowing arbitrary option changes in simulation.set\_options()
- Taking over parameters to enlarged neural networks as best as possible
- Fixing CCAdL and possibly allowing for more covariance-controlling thermostats
- · Adding support for network topologies other than fully connected feed-forward, i.e. multi-layer perceptrons