Code user manual for stochastic framework for evolving grain staitistics

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June 12, 2022

1 Introduction

This document is an user manual on the code for *stochastic framework for evolving grain staitistics*, which is introduced in the paper (x). The input to the framework is a joint probability distribution $F(A, S, t = 0)$ of grain area and number of sides, and the output is its time evolution $F(A, S, t)$. In this framework, we employ a stochastic method to evolve the statistics of the two descriptors using a reduce order grain topology transformation model (TTM). The construction of the TTM relies on a data-driven approach using a fully connected deep neural network. Topology transformations recorded in phase-field isotropic grain growth simulations are used as training data. The overal algorithm is summarized in Algorithm 1, and detailed information is also available in the paper and `comment` in each file.

The overall structure of the code is as follow.

1. `MC_main.py`

   A main driver that runs the simulation

2. `MC_NeuralNetworks.py`

   A library file. It has necessary functions and Pytorch neural net class.

3. `NetworkParameter/*.pth`

   A set of neural network parameter trained from the phase field simulation result

To run this code, one should install some open source libraries. Required libraries are summarize in Table 1. The code can be executed by the following command line.

```
python3 MC_main.py
```

Name	Description	Website	License
Pytorch	Python machine learning framework	`https://pytorch.org`	BSD
Numpy	Python scientific computing	`https://numpy.org`	BSD
mathplotlib	Python 2D plotting library	`https://matplotlib.org`	PSF

Table 1: Open source tool used in this code

Algorithm 1 A Monte Carlo simulation to evolve grain statistics

Input: a) Initial grain statistics $F(A, S, t = 0)$; b) trained TTMs $\mathcal{F}_1, \ldots, \mathcal{F}_9$ for topology transformation probabilities; c) time step size Δt; d) final time T; and e) number of rep grains N.
Initialize the random states (A_i, S_i) $(i = 1, \ldots, N)$ of N rep grains using $F(A, S, t = 0)$
for ($i = 0$ to N) **do**
    Construct the states $\{(a_{\alpha i}, s_{\alpha i}) : \alpha = 1, \ldots, S_i\}$ of the neighbors of grain i using the initial distribution $F(A, S, 0)$
    Form the adjacency list $\boldsymbol{D}$. ▷ Initialize neighbor information
end for
t=0
while (t < T) **do**
    $i = 1$
    while $(i \leq N)$ **do**
        Let $A = A_i$, $S = S_i$, and $\alpha = 1, \ldots, S_i$
        Form the adjacency matrix $\boldsymbol{C}$ from the i-th row of $\boldsymbol{D}$
        Calculate $v_\alpha = \pi(s_\alpha/3 - 2)/a_\alpha$ and $V = \pi(S/3 - 2)/A$
        Let $\boldsymbol{x} = (a_1/A, \ldots, a_S/A, V, v_1, \ldots, v_S, \boldsymbol{C})$
        $\boldsymbol{p} = \mathcal{F}_S(\boldsymbol{x})$
        Threshold $\boldsymbol{p}$ to obtain the topology change ΔS
        if $(\Delta S = 0)$ **then**
            continue
        else if $(\Delta S = 1)$ **then**
            Add a new random labels to $\boldsymbol{d}_i$
        else if $(\Delta S = -1)$ **then**
            Delete one neighbor grain from $\boldsymbol{d}_i$ that has minimum v_α
        else if $(\Delta S \leq -3)$ **then**
            Delete the ith rep grain and $\boldsymbol{d}_i$. Generate a new random rep grain using $F(A, S, t)$.
            Construct the random neighbors to $\boldsymbol{d}_i$.
        end if
        $S_i \leftarrow S_i + \Delta S$
        $A_i \leftarrow A_i + (\pi/3)(S_i - 6)\Delta t$
        $i \leftarrow i + 1$
    end while
    $t \leftarrow t + \Delta t$
    Calculate $F(A, S, t)$ from the current rep grain states $\{(A_i, S_i) : i = 1, \ldots, \mathrm{N}\}$
end while
Output: $\{F(A, S, t) : 0 \leq t \leq T\}$