Scaling up the self-optimization model by means of on-the-fly computation of weights

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Abstract—The Self-Optimization (SO) model is a useful computational model for investigating self-organization in “soft” Artificial life (ALife) as it has been shown to be general enough to model various complex adaptive systems. So far, existing work has been done on relatively small network sizes, precluding the investigation of novel phenomena that might emerge from the complexity arising from large numbers of nodes interacting in interconnected networks. This work introduces a novel implementation of the SO model that scales as $O(N^3)$ with respect to the number of nodes $N$, and demonstrates the applicability of the SO model to networks with system sizes several orders of magnitude higher than previously was investigated. Removing the prohibitive computational cost of the naive $O(N^3)$ algorithm, our on-the-fly computation paves the way for investigating substantially larger system sizes, allowing for more variety and complexity in future studies.

Index Terms—self-organization, self-optimization, Hopfield neural network, Hebbian learning, large-scale systems

I. INTRODUCTION

Self-organization is the process by which stable structures, or patterns, emerge spontaneously as a result of nonlinear interaction between a large number of components. Self-organization is observed in all matter on any scale, from the nanoscale of quantum particles to the macroscale of galaxies [1], and in particular life forms are known to be highly self-organized dynamic molecular systems [2], [3]. Consequently, self-organization has played a major role in soft (simulated), hard (robotic), and wet (chemical and biochemical) domains of Artificial life (ALife) [4]. Adaptive networks are networks whose states interact with each other, are highly coupled, and keep changing due to the system’s own dynamics, producing emergent behavior that would not be seen in other forms of networks [5]. As such, adaptive networks have been used to describe the self-organization of various systems, ranging from systems like the brain or the nervous system (due to the interaction between neurons that produces behavioral and cognitive patterns [3]), to social and engineered complex systems [5].

Of particular interest for the current paper is the Self-Optimization\(^1\) (SO) model [6], [8]. The SO model demonstrates how a system (an adaptive network) that augments its behavior with an associative memory of its own attractors is capable of solving constraint optimization problems by spontaneous (without an external reward signal) self-organization. The SO model has been shown to be general enough to model various complex adaptive systems, from gene regulation networks [9] and nematode worms [10], [11], to selfish agents [12] and sociopolitical networks [13], [14] (more references are given in Table I).

Aside of its domain-generality, what makes the SO model particularly interesting is that it is simple to implement and understand, yet with sufficient complexity to exhibit a multitude of effects relevant, evidently, for various fields. It remains to be answered, however, how practical is the model? The original model [6], [8] was used on networks with non-directed connections constrained to symmetric weights with a discrete state. Since then several studies showed that the SO model can be generalized to asymmetric weight matrices and continuous-state [15], multiple directed connections [10], and continuous-time [7].

In this work, we continue this effort of generalization by showing that the SO model is also scalable to large systems, which is crucial to support arguments in the literature that the model can provide insights into biological and social systems that consist of thousands, tens of thousands, or more elements. We do so by deriving a novel implementation that reduces the scaling from $O(N^3)$ of the straightforward implementation of the mathematical model to $O(N^2)$ through rearranging the terms. Consequently, an analysis of networks with sizes that would otherwise have incurred prohibitive computational requirements becomes accessible.

The rest of the paper is structured as follows: Section II introduces the model and its regular straightforward computational implementation. Section III describes the proposed novel implementation. In Section IV we will present computation results for our work and in Section V we will draw the conclusions of this work.
II. BACKGROUND

A. Theoretical model

The self-optimization (SO) model is a model introduced by [6], [8], that combines two well-known dynamical behaviors of recurrent neural networks: constraint satisfaction, that can be understood as an energy minimization process, and autoassociative memory that forms as a result of associatively modifiable recurrent connections in the network. This combination results in a significant improvement in the ability of the neural network to find configurations that satisfy constraints, and thus performs effective optimization.

At the basis of the model is a Hopfield neural network [16]. The Hopfield network is a representation of a physical system with \( N \) nodes (or “neurons”), where each node can be in one of two possible states, either \( s = 1 \) or \( s = -1 \). At any given time, the state of the system is defined by a vector \( \mathbf{S}(t) = \{s_1(t), ..., s_N(t)\} \). Overall there are \( 2^N \) possible states of the system. The connections between the nodes are defined by a weight matrix, \( \mathbf{W} \), of size \( N \times N \), where \( w_{ij} = 0 \) means that there is no connection present between nodes \( i \) and \( j \). The dynamics of the system is chosen to be asynchronous, that is at each time step \( t \), a node \( i \) is chosen at random and updated using the following rule

\[
s_i(t+1) = \theta \left[ \sum_{j} w_{ij} s_j(t) \right],
\]

where \( w_{ij} \) are elements of the weight matrix \( \mathbf{W} \), and \( \theta \) is a Heaviside threshold function (taking values -1 for negative arguments and +1 otherwise). When the connection strengths are symmetric (i.e. \( w_{ij} = w_{ji} \)), the Hopfield model admits a Hamiltonian description, and an energy function can be defined

\[
E(\mathbf{W}) = -\frac{1}{2} \sum_{ij} w_{ij} s_i(t) s_j(t).
\]

Given a fixed weight matrix \( \mathbf{W} \) that represents the constraints of a constraint optimization problem (e.g. in Fig. 1), a random initial state \( \mathbf{S} \), and the dynamics described by update rule (1), the system will converge towards some local minimum in the attractor landscape described by (2), which are locally optimal solutions to that problem given by the weight matrix \( \mathbf{W} \). If the system is initialized to another random state, it will again converge, but perhaps to another local minimum as shown in Fig. 2a.

The learning phase consists of updating the weights according to an associative rule in a form of Hebbian learning [17]

\[
w_{ij}(t+1) = w_{ij}(t) + \alpha s_i(t) s_j(t), \quad \alpha > 0
\]

where \( \alpha > 0 \) is a learning rate constant. The system is repeatedly allowed to converge to a local attractor. After performing \( T \) steps the state is reset to a new random state. In total the procedure is run for \( R \) resets. The energy of the system is always computed with regards to the initial weight matrix, but the state update depends on the learned weight matrix.

Fig. 1. A symmetric modular connectivity weight matrix for a system of size \( N = 100 \) with 20 modules of size \( k = 5 \), intramodule weights set at random to either 1 or -1, and intermodule weights set at random to either 0.1 or -0.1. For details on various constraint problems see [18].

Given a suitable parameter \( \alpha \), the system will go through a self-organization such that regardless of the initial state of the system, it converges to a lower energy state (a global attractor) as shown by the arrow in Fig. 2b, despite never having visited that attractor before.

When we change the perspective on convergence of the state under the update rule (1), as illustrated in Fig. 2, and instead we plot only the energy at the end of convergence for a set of random initial states it allows us to look at the distribution of the attractor energies with and without learning (Fig. 3).

The repeated energy minimization and slow accumulation of changes to the connections modifies the network to constitute an associative memory of its own attractor states. But in this case, the accumulation of weights also changes the sizes of basins of attraction, such that some attractor basins are enlarged at the expense of others, eventually resulting in a positive feedback that significantly improves the system’s ability to find configurations that resolve the constraints of the original weight matrix to a globally minimal energy state [6].

In next section we discuss the computational implementation of the SO model.

B. Computational implementation

A review of the SO literature shows that large networks are generally not studied (Table I). Given the possibility for novel phenomena to emerge from the complexity possible when large numbers of nodes interact in interconnected networks, it is pertinent to ask why that limitation to relatively small network sizes persists? Since the implementation details in these articles are usually not discussed\(^2\), it is fair to assume that their authors implement a straightforward direct computation as shown in Algorithm 1.

\(^2\)Among all the references in Table I, only [19] provided the code, and according to it they perform the straightforward computation of (3).
Fig. 2. Dynamics of the SO model. (a) Without learning. This is equivalent to the dynamics of a regular Hopfield network, where the system will converge to various minima according to the initial state. (b) With learning, (3), $\alpha = 1 \times 10^{-6}$. On both plots, the energy is computed using (2) for the chosen initial weight matrix in Fig. 1, and the state at each step is updated asynchronously according to (1). The plots show the individual traces of energy for 100 different initial random states in grey, the energy mean for 1000 different initial random states in dark blue, and its standard deviation in light blue.

**TABLE I**

| N          | Reference                      |
|------------|--------------------------------|
| 30         | Watson et al. (2010) [9]       |
| 36         | Mills et al. (2011) [20]       |
| 66         | Froese et al. (2014) [13]      |
| 70         | Froese et al. (2018) [14]      |
| 10,36,100  | Woodward et al. (2015) [21]    |
| 100        | Watson et al. (2009) [8], Davies et al. (2011) [22], Zarco et al. (2018) [15] |
| 100,120    | Watson et al. (2011) [12]      |
| 100,40,100,120 | Mills et al. (2011) [23]     |
| 32,128     | Fernando et al. (2013) [24]    |
| 150        | Watson et al. (2011) [6]       |
| 200        | Watson et al. (2011) [18]      |
| 279        | Morales et al. (2020) [11]     |
| 280        | Morales et al. (2020) [25]     |
| 282        | Morales et al. (2019) [10]     |
| 400        | Power et al. (2015) [26], Shipurov et al. (2021) [19] |

*Continuous state

**Algorithm 1:** Direct implementation of learning stage in the SO model

```
1 for $0 < r \leq R$ do
2     Generate random state $S$
3 for $0 < t \leq T$ do
4     Choose random index $0 < i_t \leq N$
5     Compute binary state $s_{i_t}$ $\triangleright$ Eq. (1)
6     Compute $dW$ and $W$ $\triangleright$ Eq. (3)
7 end
8 end
```

This is fine, however, much of the computational effort in Algorithm 1 is dominated by the need to update the weight matrix $W$ at each learning step according to (3) which subsequently is required for the state update (1). Since the weight matrix has $N^2$ elements and there are $\propto N$ steps per reset, the weight matrix update scales as $O(N^3)$. With a simple addition to be performed, it is primarily memory bandwidth constrained. This significantly limits the size one can investigate in a research project.

In next section we present a novel implementation that reduces this dependence on the size of the system to $O(N^2)$.  

### III. NOVEL IMPLEMENTATION

Whether the SO model is scalable or not is a really important consideration that has not been addressed by previous work. However, a straightforward computation of (3) and (2) takes a very long time to compute for large systems because of the $O(N^3)$ dependence on the size of the system.

In order to test the effect of scaling the SO model to substantially higher node counts, a series of mathematically...
transparent but algorithmically significant manipulations were implemented to reduce the time of computation. Here we discuss the dominant reduction of memory accesses from $O(N^3)$ to $O(N^2)$, other minor manipulations are outlined in the Appendix.

The cost of the memory bandwidth constraint can be reduced dramatically based on the observation that for large $N$, the change of the weight matrix $dW$ is mostly constant from step to step with (on average) only a few changes according to (1). If the history of state changes step to step with (on average) only a few changes according to (1), the weight matrix need never be updated explicitly but rather the value of $W$ at time $t$ needed for the state update $s_i$ at time $t$ can be computed on the fly as follows: The row $W[i,:]$ is computed as the sum of $W[i,:]$ at the last time that state $s_i$ was updated, and $(t-t')dW[i,:]$ at time $t$. Since this sum ignores the state changes since $t'$, these changes are then applied through $(t-t')$ individual changes to $W[i,:]$ to correct for this omission (see Algorithm 2).

This procedure is computationally more elaborate, but never needs to adjust more than one row of $W$ for each step. It thus reduces the memory accesses from $O(N^3)$ to $O(N^2)$. In the next section we compare the execution time between the two procedures numerically.

IV. RESULTS

After a proof of principle of the above-mentioned optimized procedure was attained, the algorithm was implemented as a compiled FORTRAN module to be loaded from Julia or Python. This combination retains the flexibility of rapid testing of many different ideas as offered by an interpreted language while benefiting from the speed of execution of a compiled language for the most time critical parts. We checked that the “on-the-fly” implementation and the regular direct implementation return identical states, energies, and weight matrices for the true run time of a benchmark instead of the mean or median, since it provides the smallest error [27]. We first made a comparison for a typical run of 1000 resets (see Fig. 3 for reference) between the direct and the on-the-fly implementation. For comparison, the non-learning stage is also shown.

Figure 4 shows that, indeed, not only is the novel implementation faster than the regular one, but it scales differently. That said, already for $N > 2000$ the execution time becomes prohibitive for continuing our comparison. For this reason, in order to investigate how the procedures compare for even larger systems we continued the comparison with a reduced number of 10 resets as shown in Fig. 5.
Algorithm 2: "On-the-fly" implementation of learning stage in the SO model

for $0 < r \leq R$ do
  1. Generate random state $S$
  2. Initialize state-to-time map
     \[ t'(i) = 1 \ldots N \] = 1
  3. Allocate time-to-state map
     \[ i'(t) = 1 \ldots T \]
  4. Allocate state change history
     \[ s'(t) = 1 \ldots T \]
  5. for $0 < t \leq T$ do
     6. Choose random index $0 < i_t \leq N$
     7. Compute the constant change
        \[ W[i_t,:) = W[i_t,:] + (t - t'(i_t))dW[i_t,:] \]
     8. Correct for the state changes since $t'(i_t)$:
     9. for $t'(i_t) \leq t'' < t$ do
        10. \[ W[i_t, i'(t'')] = W[i_t, i'(t'')] + (s_t, s'(t'') - dW[i_t, i'(t'')]) (t - t'') \]
     11. end
     12. Store the step $t'(i_t) = t$
     13. Store the index $i'(t) = i_t$
     14. Compute binary state $s_{i_t}$ \( \triangleright \) Eq. (1)
     15. Store the state change $s'(t) = s_{i_t}$
     16. end
     17. Accumulate remaining corrections at $t = T$
     18. for $0 < i \leq N$ do
     19. Compute the constant change
        \[ W[i,:) = W[i,:) + (t - t'(i))dW[i,:] \]
     20. Correct for the state changes since $t'(i)$:
     21. for $t'(i) \leq t'' < t$ do
        22. \[ W[i, i'(t'')] = W[i, i'(t'')] + (s_t, s'(t'') - dW[i, i'(t'')]) (t - t'') \]
     23. end
     24. end
 25. end

Section IV-B shows the results of a simulation for a system of size \( N = 10000 \).

B. Simulation results for \( N = 10000 \)

To investigate the scalability of the SO model, similar computations to that in Sec. II-A were performed for larger systems and similar behavior was observed. For brevity, we only show results for \( N = 10000 \). The weight matrix \( W \) (Fig. 6) has symmetric modular connectivity with modules of size \( k = 400 \), with intramodule weights set at random to either 1 or -1, and intermodule weights set at random to either 0.1 or -0.1. Note that the size of the individual modules in this initial large scale test is equivalent to biggest total system size tested in previous work! (see Table I).

As it can be seen from Fig. 7, the behavior obtained from the SO model for substantially enlarged systems is similar to the small systems that were previously tested.

V. CONCLUSIONS

This work provides a novel implementation of a by-now classic model of complex adaptive systems developed in the field of artificial life, the SO model that reduces the memory access from \( O(N^3) \) to \( O(N^2) \). This substantial reduction in computational effort enables the investigation of dramatically larger systems. We demonstrated the applicability of the SO model to a network that is two orders larger than was used in previous studies. Having the possibility to compute large scale
systems opens up a door to new research investigations (e.g. more complex connectivity of the weight matrix with several modular scales).

It is important to note that here we have updated the weights of the system at every step of the simulation. Similar dynamics can be achieved by making a weight update only at the reset of the system. This might make the system less biologically plausible, but considerably faster, opening the option to compute even larger systems than shown in this work.

It should be noted as well that although we have used a discrete state in Algorithm 2, it is relatively straightforward to generalize the algorithm to a continuous state as well. In this case, the implementation A in the Appendix would not be applicable, and implementation B would have to be modified slightly since $s_x^2 \neq 1$, but that does not affect the salient point of this article, the improvement of the algorithmic scaling.

As was mentioned in Sec. I, the SO model has been demonstrated to be applicable for a wide range of complex adaptive systems. With this new implementation, the future work in these various fields may take a new turn into investigating systems with much higher complexity. Researchers working on adaptive self-organization in neural, gene regulatory, ecological, or social networks, who may have previously overlooked this model because their networks operate at a much larger scale, can now more easily apply the model to their systems of interest. Given the robustness and generality of the model’s self-optimization process, we can expect that actual implementations of this process are awaiting to be discovered in various natural systems.

Looking further into the future, we might wish to address the network topology studied. The current model of Hopfield neural network implies a fully connected network of nodes. This is plausible or even necessary to achieve a biologically relevant level of complexity. Building on the substantial increase in scale of tractable SO problems demonstrated in this article we can remove this requirement of fully connected networks. Since we can now treat networks with modules that exceed the size of entire systems previously treated, the modules themselves can provide a sufficient level of complexity. Given the new source of biological complexity, perhaps full connectivity between all modules is no longer required. The number of connections (i.e. the size of the populated weight matrix) determines the computational cost for evaluating the model. Limiting the number of connections explicitly accounted for leads to a less dramatic increase in computational cost when further increasing the scale of the network with many more, but partially interconnected, modules. Using an approach of this sort we hope to study the behavior of interconnected systems on a truly massive scale.

VI. DATA AVAILABILITY STATEMENT

The model from the main text as well as the code used for the simulation are available at [28].

VII. ACKNOWLEDGMENT

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APPENDIX

In addition to the main optimization outlined in Section III, we performed a series of different mathematical manipulations of the Hopfield update rule, (1), energy computation, (2), and Hebbian learning rule, (3), to further optimize the SO procedure to decrease its computational time. These are used in [28] and described below.

A. Integer computation of W

By dividing (3) by $\alpha$, we can rewrite it to

$$\eta w_{ij} (t+1) = \eta w_{ij} (t) + s_i (t) s_j (t), \quad \eta = \frac{1}{\alpha}. \quad (4)$$

Assuming $\alpha$ is typically much smaller than one, $\eta$ can be chosen to be a large integer number. We can therefore scale $W$ by multiplying it by $\eta$ before the simulation starts. This in turn allows us to set the type of $W$ to 64-bit integer and the type of $dW = ss^T$ to 8-bit integer, which decreases the computation time since floating-point operations typically take longer to execute than integer operations.

B. Computation of energy from the previous step

Since at each step $t$ only one discrete state $s_x$ is updated we can rewrite (2) as

$$E = - \frac{1}{2} \left[ \sum_{i \neq x}^{N} \sum_{j \neq x}^{N} w_{ij} s_i s_j + s_i \sum_{j \neq x}^{N} w_{ix} s_j \right] + s_j \sum_{i \neq x}^{N} w_{ix} s_i + s_i w_{xx} \quad (5)$$

$$= - \frac{1}{2} \left[ \sum_{i \neq x}^{N} \sum_{j \neq x}^{N} w_{ij} s_i s_j + 2s_x \sum_{i \neq x}^{N} w_{ix} s_i + w_{xx} \right] \quad (6)$$

since $s_x^2 = 1$ always, and $w_{xx} = w_{ix}$ since $W$ is symmetric. Energy change between each step is

$$\Delta E = E(t-1) - E(t). \quad (7)$$

Rearranging (7) and substituting (6) we get

$$E(t) = E(t-1) +$$

$$\frac{1}{2} \left[ \sum_{i \neq x}^{N} \sum_{j \neq x}^{N} w_{ij} s_i^{t-1} s_j^{t-1} + 2s_x^{t-1} \sum_{i \neq x}^{N} w_{ix} s_i^{t-1} + w_{xx} \right]$$

$$- \left[ \sum_{i \neq x}^{N} \sum_{j \neq x}^{N} w_{ij} s_i s_j + 2s_x \sum_{i \neq x}^{N} w_{ix} s_i + w_{xx} \right]$$

$$= E(t-1) + (s_x^{t-1} - s_x^t) \sum_{i \neq x}^{N} w_{ix} s_i.$$
where the double sum elements are canceled out since $s_{t+1:s} \neq s_t$ do not change from $t-1$ to $t$, and therefore the time label from them were removed for clearness. We can thus rewrite (2) as

$$E(t) = E(t-1) + \left( s_{t-1}^T s_t - s_t^T s_{t+1} \right) \sum_{i=1}^{N} w_{ix}s_i - s_i^T w_{x}.$$  

(8)

With this optimization, we can compute the energy once using (2) and then compute energy every other step using (8).

C. Row and column update of W

The straightforward computation (1) can be slightly optimized if we compute the entire matrix $dW = \cos\theta^T$ at the first step of each reset, and then just update one row and one column in $dW$ with $dW[ i, :] = dW[ :, i] = \cos\theta$. This can further be optimized by noting the fact that W is symmetric, so in principle, we only need to update the upper triangular half of $dW$ (and consequently W) and then copy that part to the lower triangular half at the end (as used in [28]).

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