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Large Scale Simulations of a Neural Network Model for the Graph Bisection Problem on Geometrically Connected Graphs^{*}

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Abstract

In this work some preliminary numerical results obtained by large scale simulations of the sequential dynamics of a neural network model for the graph bisection problem on random geometrically connected graphs are presented. It can be concluded that the sequential dynamic is a low cost, effective and very fast local minima optimization heuristic for the Graph Bisection Problem.

Keywords: Graph Bisection Problem, Neural Networks, Geometrically Connected Graphs

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1 Extended Abstract

The Graph Bisection Problem (GBP), which arises in various areas of computer science, like parallel computing and circuit layout, can be defined as follows: given a finite, undirected and connected graph $G = (V, E)$, where V is the set of vertices with $|V| = n$ an even natural number and $E \subseteq V \times V$ is the set of edges, find two subsets of vertices V_1 and V_2 (the bisection of V)

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that verify: $|V_1| = |V_2| = \frac{n}{2}$ and $V_1 \cap V_2 = \emptyset$ such that the cardinality of the set $\{(i, j) \in E / i \in V_1 \text{ and } j \in V_2\}$ is minimal. This set is called the cut set and the cardinality of the optimal cut set is called the bisection width. The GBP is a NP-Complete combinatorial optimization problem, see refs. [3, 13], and several heuristics have been proposed to solve it, see for instance refs. [1, 2, 7, 10 – 12, 14 – 16].

A symmetrical neural network with sequential dynamics, see refs. [4, 6, 9], is a discrete in time and space dynamical system defined by:

- A symmetrical connectivity matrix $W = (w_{ij})_{i,j=1}^n$ that represents the interaction weights between neurons i and $j \forall i, j = 1, \dots, n$.
- A threshold vector $b = (b_i)_{i=1}^n$, where b_i is the threshold of neuron $i \forall i = 1, \dots, n$.
- A local transition function associated with the sequential dynamics: at each time step t an unique neuron, for example the k -th one, changes its state according to:

$$\begin{aligned} x(0) &\in \{0, 1\}^n \\ x(t+1) &= (x_1(t), \dots, x_{k-1}(t), x_k(t+1), x_{k+1}(t), \dots, x_n(t)) \quad (1) \\ x_k(t+1) &= \mathbb{1} \left(\sum_{j=1}^n w_{kj} x_j(t) - b_k \right) \end{aligned}$$

where $\mathbb{1}$ is the Heaviside function defined by: $\mathbb{1}(u) = 1$ iff $u \geq 0$ and 0 otherwise.

In refs. [4, 6, 9] it was proved that if the connectivity matrix W is symmetrical with non negative diagonal the sequential dynamics converges only to fixed points which are also local minima of the quadratic Lyapunov functional $E : \{0, 1\}^n \rightarrow \Re$ defined by:

$$E(x(t)) = -\frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n w_{ij} x_i(t) x_j(t) + \sum_{i=1}^n b_i x_i(t) \quad (2)$$

Therefore, the sequential dynamics is a local minima optimization heuristic for the Lyapunov functional E , see ref. [4 – 6, 9]. To obtain a neural network model for the GBP a change of variables must be made:

$$x_i \in \{0, 1\} \longleftarrow y_i \in \{-1, 1\} \quad y_i = 2x_i - 1 \iff x_i = \frac{y_i + 1}{2} \quad \forall i = 1, \dots, n$$

With this new variables: $y_i = 1$ iff $i \in V_1$ and $y_i = -1$ iff $i \in V_2$. If the graph architecture is represented by a symmetrical connectivity matrix $W =$

$(w_{ij})_{i,j=1}^n$ with no loops, i.e.: $w_{ii} = 0$, then:

$$w_{ij}y_iy_j = \begin{cases} 0 & \text{iff } w_{ij} = 0 \\ 1 & \text{iff } i, j \in V_1 \text{ (or } V_2) \\ -1 & \text{iff } i \in V_1 \text{ and } j \in V_2 \text{ (or } i \in V_2 \text{ and } j \in V_1) \end{cases} \quad (3)$$

In order to fulfil the cardinality constraint: $|V_1| = |V_2| = \frac{n}{2}$ (n is an even number) it must be imposed the condition: $\sum_{i=1}^n y_i = 0$. Therefore, the following constrained combinatorial optimization problem (P) is equivalent to the GBP:

$$(P) \quad \underset{y \in \{-1, 1\}^n}{\text{Min}} \quad G(y) \doteq -\frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n w_{ij}y_iy_j \quad \text{such that: } \sum_{i=1}^n y_i = 0$$

A relaxation of (P) can be obtained by the application of the standard quadratic penalization technique. An unconstrained combinatorial optimization problem (P_α) for the GBP is, see ref. [8]:

$$(P_\alpha) \quad \underset{y \in \{-1, 1\}^n}{\text{Min}} \quad G_\alpha(y) \doteq -\frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n v_{ij}(\alpha)y_iy_j \quad (4)$$

Where $\alpha \geq 0$ is the penalization parameter, $v_{ij}(\alpha) = w_{ij} - \alpha [1 - \delta(i, j)]$ $\forall i, j = 1, \dots, n$ and $\delta(i, j) = 1$ iff $i = j$ and 0 otherwise $\forall i, j = 1, \dots, n$. The problem (P_α) is equivalent (in a weak sense due to the existence of the parameter α) to the GBP.

A neural network with sequential dynamics can be associated to the variables $y \in \{-1, 1\}^n$, the connectivity matrix $V(\alpha) = (v_{ij}(\alpha))_{i,j=1}^n$ and the Lyapunov functional G_α defined in (P_α), see ref. [8]. The sequential dynamics:

$$\begin{aligned} y(0) &\in \{-1, 1\}^n \\ y(t+1) &= (y_1(t), \dots, y_{k-1}(t), y_k(t+1), y_{k+1}(t), \dots, y_n(t)) \\ y_k(t+1) &= \text{sign} \left(\sum_{j=1}^n v_{kj}(\alpha)y_j(t) \right) \end{aligned} \quad (5)$$

converges only to fixed points which are also local minima of G_α . The equations (5) define a local minima optimization heuristic for the functional G_α .

The methodology for the large scale simulations was the following:

- (i) The size of the neural network model was fixed to $n = 8192$ and 16384 .
- (ii) For each neural network size the simulations were performed for the penalization parameter $\alpha = 0.5, 0.6, 0.7, 0.8, 0.9$ and 1.0 .
- (iii) Given a neural network size n and penalization parameter α , n random geometrically connected graphs with connectivity radius $r = 0.1, 0.15, 0.2, 0.25$ and 0.3 were generated.
- (iv) After all the above parameters were fixed, n random initial conditions $y(0)$ were generated.
- (v) For each $y(0)$ the sequential dynamics (5) was applied.

To analyze the performance of the sequential dynamics (5) as an optimization heuristic, the following quantities were computed:

- (i) **Delta Cut Prom:** Given n, α, r , it corresponds to the averaged over all the random geometrically connected graphs and over all the random initial conditions of the difference between the final and the initial cut, i.e. for t large enough:

$$\Delta\text{Cut Prom} = \left[\left| \{(i, j) \in E : y_i(t) \neq y_j(t)\} \right| - \left| \{(i, j) \in E : y_i(0) \neq y_j(0)\} \right| \right]_{ave} \quad (6)$$

- (ii) **Delta Cut Min and Max:** Given n, α, p , it correspond to the worse and best performance of the neural network sequential dynamics, computed over all the random geometrically connected graphs and initial conditions. They will be denoted by **Delta Cut Min** and **Delta Cut Max**, respectively.
- (iii) **Delta Cut Prom Standard:** Corresponds to **Delta Cut Prom** normalized by n . It will be denoted by **Delta Cut Prom Std**.

Only the results for $\alpha = 1.0$ will be presented because the small variations for other values of α . Due to the lack of space, the results for $n = 8192$ will be shown.

- (a) The transient time is $O(n)$
- (b) For $n = 8192$, **Delta Cut Min** is approximately 5% lower than the **Delta Cut Prom** while **Delta Cut Max** is approx. 4% higher than the **Delta Cut Prom**.
- (c) For $n = 8192$, **Delta Cut Prom Std** is a **linear function** of the **Connectivity Radius** r (with correlation coefficient equals to 0.97) :

$$\Delta\text{Cut Prom Std} = 152.78 - 1939.75 \times r \quad (7)$$

2 Conclusions

The sequential dynamics of a symmetrical neural network model for the GBP on geometrically connected graphs was studied numerically by large scale simulations . The numerical study allow us to claim that the sequential dynamics can be used as a local search heuristic on the base of the following numerical properties:

- (i) Low cost: it is very simple to implement.
- (ii) Very fast: it converges in $O(n)$, where n is the size of the neural network.
- (iii) Effective: it produces a linear improvement of the Δ **Cut Prom Std** as a function of the connectivity radius, equation (7) .

3 Future Work

The preliminary results presented in this paper must still be complemented with a theoretical and numerical study of the sequential and parallel dynamics of the neural network model for the GBP on geometrically connected graphs. This study will allow us to improve the theoretical results that have been obtained and to prove the properties that have been determined numerically by large scale simulations. The specific objectives of this further study will be the following:

- (i) To obtain Lyapunov functionals for the sequential and parallel dynamics on random geometrically connected graphs, allowing to prove linear transient time for the dynamics.
- (ii) To determine the classes of the dynamical attractors and its valleys of attraction for the sequential and parallel dynamics on random geometrically connected graphs.
- (iii) To prove analytically the linear improvement property, equation (7) .
- (iv) To design a two-stages heuristic for the GBP. For the first stage of this hybrid heuristic the neural network dynamics is proposed and for the second stage a local minima improvement technique like Simulated Annealing is suggested.

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