

Improving Neural Networks for Mechanism Kinematic Chain Isomorphism Identification

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Abstract Detection of isomorphism among kinematic chains is essential in mechanical design, but difficult and computationally expensive. It has been shown that both traditional methods and previously presented neural networks still have a lot to be desired in aspects such as simplifying procedure of identification and adapting automatic computation. Therefore, a new algorithm based on a competitive Hopfield network is developed for automatic computation in the kinematic chain isomorphism problem. The neural approach provides directly interpretable solutions and does not demand tuning of parameters. We have tested the algorithm by solving problems reported in the recent mechanical literature. Simulation results show the effectiveness of the network that rapidly identifies isomorphic kinematic chains.

Keywords Kinematic chains · Synthesis of mechanism · Graph isomorphism · Discrete Hopfield model · Binary neural network

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1 Introduction

Synthesis is a procedure by which a product (a mechanism for example) is developed to meet the desired needs. From the view point of mechanical design, synthesis of kinematic chains is very important for the invention and innovation of mechanisms. A kinematic chain designates several links movably connected together by joints called kinematic pairs to transmit motion. A link is defined as a machine part or a component of a mechanism, assumed to be rigid.

Synthesis of kinematic chains usually involves the generation of a complete list of kinematic chains followed by a time-consuming procedure for the elimination of isomorphs. Undetected isomorphic chains result in duplicate solutions an unnecessary effort. Falsely identified isomorphism eliminates possible candidates for new mechanisms. Therefore, detection of isomorphism among kinematic chains is essential at the conceptual stage of mechanical design. Yet isomorphism detection is not easy and is computationally expensive.

To date, a lot of work for detection of isomorphic chains has been reported. However, Tischler et al. [1] concluded that, in the general case, the traditional methods for detecting kinematic chain isomorphism have not been found to be an efficient solution of this problem. Most of these algorithms proved to be too convoluted and cumbersome to use in practice and cannot work for the chains with the number of links greater than 12 [2]. Therefore, as it has been recently pointed out [3], most published algorithms still have a lot to be desired in different aspects, such as simplifying procedure of identification and adapting automatic computation.

In characteristic and other polynomial methods the kinematic chain is represented by a graph and the approaches are based on the adjacency matrix of the graph [4]. These are computerized methods, usually less convoluted and can work for the chains with the number of links greater than 12. Unfortunately, the reliability of these algorithms to solve the kinematic chain isomorphism problem was in question, as several counter-examples were found [4,5]. Therefore, novel methods have been recently presented that posses the advantages of using standard matrix theory and adapting automatic computation [3,6,7]. All these algorithms to identify isomorphic chains are based on a combination of eigenvalues and eigenvectors of the adjacency matrix of the graph.

An alternative direction for kinematic chain isomorphism detection based on the analog Hopfield model was also investigated by Kong et al. [8]. Although this approach can theoretically work for any number of links, the authors point out [9] that they have observed potential structures of chains which can make this approach fail. Wilson and Pawley [10] highlighted some of the problems on the use of the analog Hopfield model. One of them is the need to tune the parameters in the energy function. Besides, due to its continuous change in the state variable it has been shown that its convergence is slow [11].

The graph isomorphism problem is an NP-complete problem according to the computational complexity theory. Recently presented novel neural approaches based on the discrete Hopfield model have been shown to provide powerful algorithms for some NP-complete problems [12–14]. These networks provide fast and accurate solutions without the fine-tuning of parameters required in analog Hopfield models like the one proposed by Kong et al. [8]. Moreover, it has been shown that discrete neurons are more efficient than continuous neurons in terms of computation time and quality of the obtained solutions [14,15]. Therefore, in this paper we propose a discrete competitive Hopfield approach to identify the isomorphism of the mechanism kinematic chain. It is shown that this neural network provides fast solutions for the design examples found in the recent literature using other techniques [3,6–8].

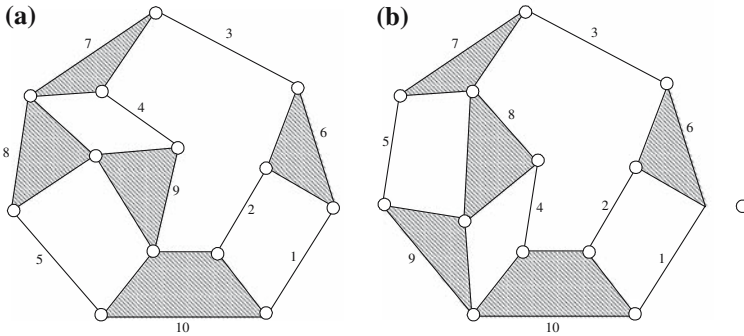


Fig. 1 A pair of 10-links isomorphic kinematic chains

Besides, the algorithm provides directly interpretable solutions and does not demand tuning of parameters.

2 Formulation of the Mechanism Kinematic Chain Isomorphism Problem

A mechanism kinematic chain is an assembly of links and kinematic pairs or joints. Two kinematic chains are said to be isomorphic if there is a one-to-one correspondence between the links of one chain and those of the second chain such that two links of a chain are jointed by a kinematic pair, if and only if the corresponding links of the other chain are jointed by a kinematic pair.

Graph theory has been widely adopted for the representation of mechanisms because it is mathematically rigorous, visually intuitive and easily adaptable to computation. A mechanism kinematic chain can be uniquely represented by a graph whose vertices correspond to the links of the chain and whose edges correspond to the joints of the chain. The adjacency matrix of a mechanism kinematic chain $A = [a_{ij}]$ is defined as:

$$\begin{aligned}
 a_{ij}(i \neq j) &= 1, \text{ if links } i \text{ and } j \text{ are adjacent} \\
 a_{ij}(i \neq j) &= 0, \text{ if links } i \text{ and } j \text{ are not adjacent} \\
 a_{ij}(i = j) &= 0.
 \end{aligned}$$

Figure 1 shows two isomorphic kinematic chains both with 10 links and Fig. 2 represents the adjacency matrices for these chains.

If the kinematic chains represented by the adjacency matrices A and B are isomorphic, then these matrices can become equal by means of interchanging rows and columns of one of them at the same time. Therefore, as demonstrated in [3, 8], if A and B are adjacent matrices of two isomorphic chains then $B = VAV^{-1}$, where V is an orthogonal permutation matrix such that $V^t = V^{-1}$. Because this operation matrix V reflects the row and column exchanges, it has the feature that on each column and row there is only one element for 1 and all the others for 0. Figure 3 represents two different outputs obtained by applying our binary neural network to the chains shown in Fig. 1. Since these solutions correspond to orthogonal permutation matrices V , their existence shows that the kinematic chains are isomorphic.

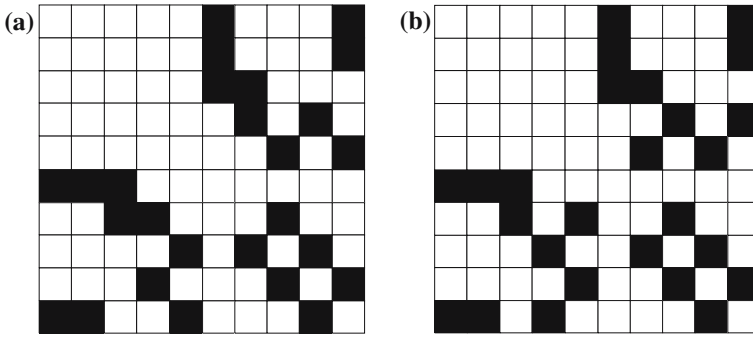


Fig. 2 The adjacency matrices of the two chains shown in Fig. 1. Black and white squares represent 1 and 0 values, respectively

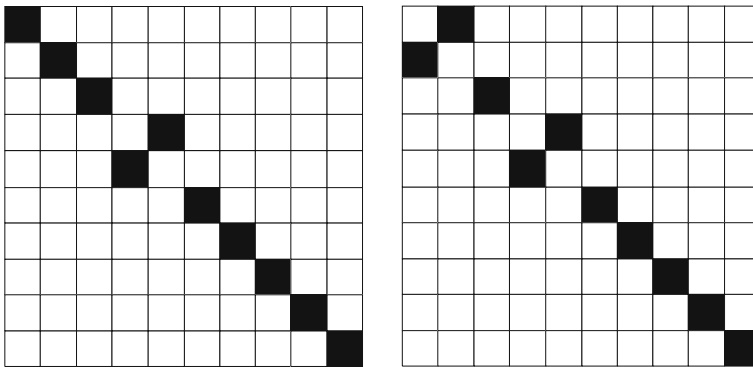


Fig. 3 Two different solutions V obtained by our binary neural network for the isomorphic chains shown in Fig. 1. Black and white squares indicate 1 and 0 outputs, respectively

3 The Existing Neural Network for the Mechanism Kinematic Chain Isomorphism Problem

In this section we describe the existing analog Hopfield network for identifying isomorphic chains since the energy function applied in our discrete model is inspired from the one proposed by Kong et al. [8]. We also indicate the deficiencies of the neural network that can make this approach fail for some structures of chains as pointed out by the authors [9].

In the analog Hopfield network [8], a solution for the mechanism kinematic chain isomorphism problem is described by a neuron matrix $V = (v_{ij})_{n \times n}$ which corresponds to the orthogonal permutation matrix defined in Sect. 2. Given two chains with adjacency matrices $A = (a_{ij})_{n \times n}$ and $B = (b_{xy})_{n \times n}$, the energy function in this model is:

$$\begin{aligned}
 E = & \frac{A}{2} \sum_i \sum_x \sum_{y \neq x} v_{ix} v_{ij} + \frac{B}{2} \sum_i \sum_{j \neq y} \sum_x v_{ix} v_{jx} \\
 & + \frac{C}{2} \left(\sum_i \sum_x v_{ix} - n \right)^2 + \frac{D}{2} \sum_x \sum_y \sum_i \sum_j |a_{ij} - b_{xy}| v_{ix} v_{jy} \tag{1}
 \end{aligned}$$

A valid neuron output V corresponding to an orthogonal permutation matrix requires that one and only one neuron per row and column must have the output $v_{ij} = 1$ and all the other outputs must be $v_{ij} = 0$. Then, the first term in (1) is of row constraint and the second term is of column constraint. The third term ensures the number of mapping between the graphs of the chains to be n times. The fourth term is the objective function to be optimized and it reaches a minimum only when the two chains are isomorphic. Observe that in (1) four positive parameters must be fine-tuned.

The dynamic equation of the network is:

$$\frac{du_{xi}}{dt} = -\frac{u_{xi}}{\tau} - A \sum_{y \neq x} v_{iy} - B \sum_{j \neq i} v_{jx} - C \left(\sum_j \sum_y v_{jy} - n \right) - D \sum_j \sum_y |a_{ij} - b_{xy}| v_{jy}$$

where τ is the characteristic time constant that has to be determined. The numerical form of the described dynamic equation introduces a new constant Δ :

$$u_{xi}^{n+1} = u_{xi}^n + \left(\frac{\Delta}{\tau} \right) \frac{du_{xi}^n}{dt}$$

Besides, each neuron applies the continuous sigmoid input–output function whose slope u_o must also be determined. Therefore, it is concluded that the seven parameters A, B, C, D, τ, u_o and Δ must be tuned in this model. This is a difficult task since some of these values are very sensitive to network change [8].

Note that at each iteration of the network, a neuron matrix must be built with “zero” and “one” elements. However, as Kong et al. point out [8], the exact zero and one values are not possible to reach because continuous neurons are applied. Then, the output neuron matrix V is sometimes difficult to interpret since only gives approximate values. Hence, it is concluded this network is not very suitable for automatic computation. Moreover, convergence is slow with continuous neurons. It has been shown that analog Hopfield networks like this usually take hours to produce accurate solutions [11]. In contrast, we propose a binary Hopfield model that converges rapidly and provides directly interpretable solutions without a burden on the parameter tuning.

4 The Proposed Neural Algorithm for the Mechanism Kinematic Chain Isomorphism Problem

In this section we apply a competitive Hopfield network [12, 13] for identifying isomorphic chains which implements novel dynamics that are inspired from the discrete Hopfield model. The proposed network consists of a single layer of N binary interconnected neurons. Let us consider now that the network is partitioned into n disjoint groups, where each group is composed of m neurons, such that $N = n \times m$.

If k represents discrete time, the output state of the i th neuron in the x th group is denoted by $v_{xi}(k) \in \{0, 1\}$, its input by $u_{xi}(k)$ and its bias by θ_{xi} , for $x = 1, \dots, n, i = 1, \dots, m$. The interconnection strength between neurons xi and yj is denoted by $\omega_{xi,yj}$, for $x, y = 1, \dots, n; i, j = 1, \dots, m$, where symmetric weights $\omega_{xi,yj} = \omega_{yj,xi}$ are considered. The neural network is characterised by the Hopfield’s energy function

$$E(k) = -\frac{1}{2} \sum_{x=1}^n \sum_{i=1}^m \sum_{y=1}^n \sum_{j=1}^m \omega_{xi,yj} v_{xi}(k) v_{yj}(k) + \sum_{x=1}^n \sum_{i=1}^m \theta_{xi} v_{xi}(k) \tag{2}$$

and the inputs of the neurons are computed by the updating rule

$$u_{xi}(k) = \sum_{y=1}^n \sum_{j=1}^m \omega_{xi,yj} v_{yj}(k) - \theta_{xi} \tag{3}$$

Since the network is partitioned into disjoint groups of neurons we can introduce the notion of group update. Thus, instead of selecting a single neuron for update as in the standard discrete Hopfield model, we select a complete group of neurons. We shall say that the network M is a *Competitive Hopfield Model (CHOM)* if one and only one neuron per group has 1 as its output at every time k .

Theorem *Let M be a CHOM in which only one group x , for $x = 1, \dots, n$, is selected for updating at time k . Let x_o be the neuron in group x with the output 1 at time k and x_c the candidate neuron in group x that will have the output 1 at time $k + 1$. Then, the energy difference resulting is:*

$$\Delta E_x(k) = E(k + 1) - E(k) = u_{x_o}(k) - u_{x_c}(k) - \frac{1}{2}(\omega_{x_o,x_o} + \omega_{x_c,x_c} - 2\omega_{x_c,x_o})$$

Thus, if the dynamics of the CHOM are given by

$$v_{xi}(k + 1) = \begin{cases} 1 & \text{if } u_{xi}(k) - K_{x_o,xi} = \max_{j=1\dots m} \{u_{xj}(k) - K_{x_o,xj}\} \\ 0 & \text{otherwise} \end{cases} \tag{4}$$

where $K_{x_o,xj} = -\frac{1}{2}(\omega_{x_o,x_o} + \omega_{xj,xj} - 2\omega_{x_o,xj})$ for $j = 1, \dots, m$, then convergence of the energy function to a local/global minimum is guaranteed.

Proof See Appendix. □

As proposed by Kong et al. [8], in the mechanism kinematic chain isomorphism problem a valid solution can be represented by a neuron state $V_{n \times n}$ in which one and only one neuron per row and per column must be “on”. Then, the n groups for the CHOM can be constructed such that every group is a row or a column of the network. Since we choose groups of rows, then the first term (row constraint) can be removed from the energy function (1) proposed by Kong et al. [8]. Besides, since there are always n activated neurons, the third term in (1) can also be eliminated. Therefore, given two kinematic chains with adjacency matrices $A = (a_{ij})_{n \times n}$ and $B = (b_{xy})_{n \times n}$, if we write the term of column constraint in a more computationally efficient way, the resulting simplified energy function for our model is:

$$E = \frac{1}{2} \sum_j \left(\sum_k v_{kj} - 1 \right)^2 + \frac{1}{2} \sum_x \sum_y \sum_i \sum_j |a_{ij} - b_{xy}| v_{ix} v_{jy} \tag{5}$$

In order to obtain the connections weights $\omega_{xi,yj}$ and the biases θ_{xi} of the neural network, we will compare the energy function (5) and the Hopfield’s energy function (2). By substituting these values in the updating rule (3) we have that the input of every neuron is given by:

$$u_{ix} = 1 - v_{ix} - \sum_{r \neq i} v_{rx} - \sum_j \sum_y |a_{ij} - b_{xy}| v_{jy} \tag{6}$$

Note that the weak point for a Hopfield-type network is the local minima problem. In the model proposed by Kong et al. [8] the following criterion is considered: if the network

does not yield a stable neuron matrix after 1,000 iterations, this corresponds to two chains that are not isomorphic. Obviously this criterion does not show that the two chains are not isomorphic, because if the network is trapped in a local minimum then we cannot detect two isomorphic chains. A Hopfield-type network can only ensure that, if we reach the energy value $E = 0$, then the two kinematic chains are isomorphic.

In this paper we apply a binary neural model with a high convergence speed that allows to perform very rapid simulations of the network. If we implement complicated dynamics in order to escape from local minima, the computation time is highly increased. It has been observed that the fastest identification of isomorphism is obtained by performing runs from different initial states. Simulation results show that this simple strategy is a very efficient and reliable approach for mechanism kinematic chain isomorphism identification. The following procedure describes the proposed neural algorithm based on the *CHOM*:

1. Set an initial state of the neuron matrix $V_{n \times n}$ by randomly setting the output of one neuron in each row to be 1 and all the other neurons in the row to be 0.
2. Evaluate the initial value of the energy function E given by Eq. 5.
3. Select a row i of V .
4. Compute the inputs of the neurons in the row i , u_{ij} , by Eq. 6, for $j = 1, \dots, n$.
5. Select the activated neuron io in the row i and select the neuron ic with the maximum value of $\{u_{ij} - K_{io,ij}\}$ per row i .
6. If $\max\{u_{ij} - K_{io,ij}\} \neq u_{io}$, then $v_{ic} = 1$, $v_{io} = 0$ and $\Delta E = u_{io} - u_{ic} + K_{io,ic}$; else $\Delta E = 0$ since no updating is made.
7. Repeat from step (3) until the number of iterations $NI = NI_{\max}$ or $E = 0$.
8. Repeat from step (1) until the number of initial states $NS = NS_{\max}$ or $E = 0$.

On step 3 we select a row randomly or easier, we follow $i = 1, \dots, n$. On step 5, if there are different neurons in row i with the maximum value of u , the algorithm must randomly select one of them. However, for simplicity, it selects the first neuron in the row with the maximum value of u .

5 Simulation Results

We consider in this section examples presented in the most recent approaches developed for automatic computation in the kinematic chain isomorphism problem. In comparing our results, we have found in the literature that in all these reported algorithms there is no description of computation time. In order to illustrate the effectiveness of the analog Hopfield network, Kong et al. [8] tested their algorithm for two counter-examples known for other methods. They solved the pair of 10-links isomorphic kinematic chains shown in Fig. 1 and the pair of 12-links non-isomorphic chains shown in Fig. 4c.

Chang et al. [6] presented a new method based on eigenvectors and eigenvalues of the adjacency matrix. In 2005 Cubillo et al. [3] pointed out some fundamental errors in the theory presented by Chang et al. [6] and developed a new procedure to identify isomorphic chains. They tested their algorithm for the pair of eight-links isomorphic chains shown in Fig. 4a and for the pair of eight-links isomorphic chains shown in Fig. 4b. The most complete eigensystem algorithm for chain isomorphism detection was presented by He et al. [7]. They showed that the adjacency matrix is not sufficient in the eigensystem approach to ensure isomorphism and developed the adjusted adjacency matrix. They solved the two pairs of non-isomorphic chains shown in Fig. 4c (12 links) and d (10 links). They also applied their method to the pair of non-isomorphic graphs with 15 vertices shown in Fig. 5 and to the pair of isomorphic

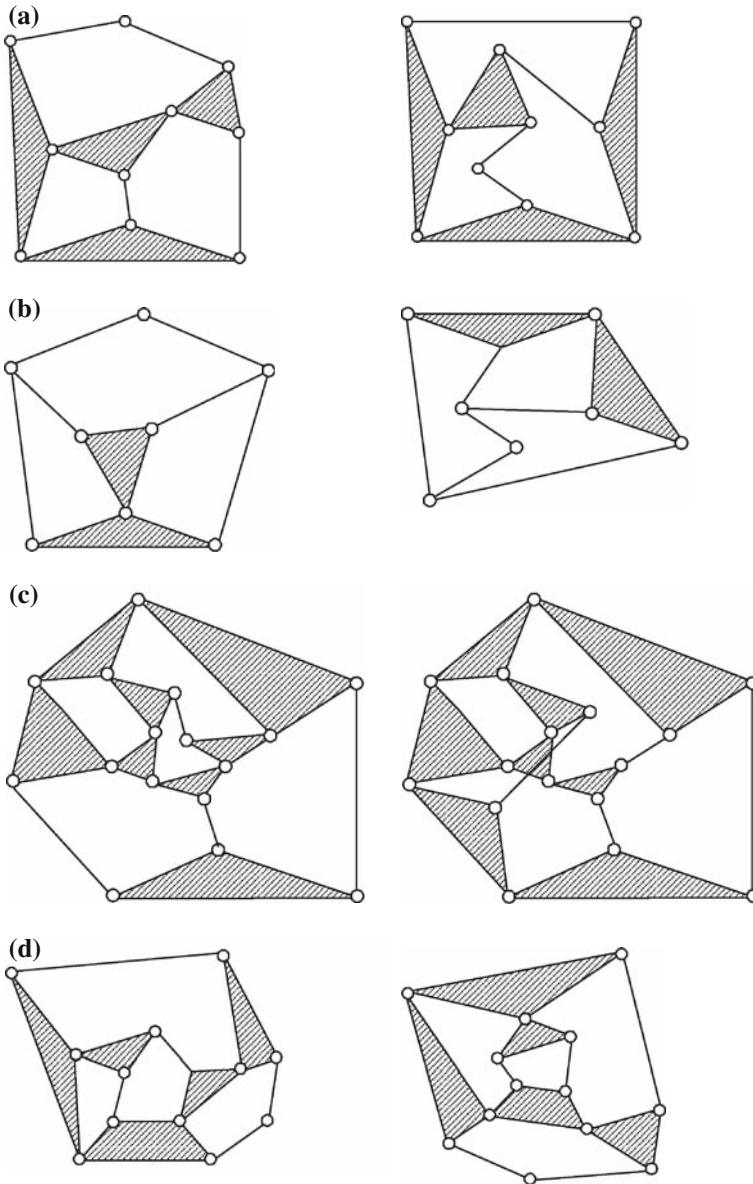


Fig. 4 Different pairs of isomorphic and non-isomorphic kinematic chains

graphs with fourteen vertices shown in Fig. 6. We have tested our neural network solving successfully all the described examples taken from the recent bibliography.

All experiments were run on a conventional 3 GHz Pentium IV PC with 512 MBytes RAM by Matlab. For every one of the seven selected test problems, the results were obtained for a total of 1,000 runs of the neural algorithm described in Sect. 4. Simulation results show that with only 10 iterations of the proposed discrete neural network we can detect a local minimum in order to select a new random initial state. Thus, it is always considered $NI_{\max} = 10$ for all experiments. For the maximum number of initial states we consider that if the network

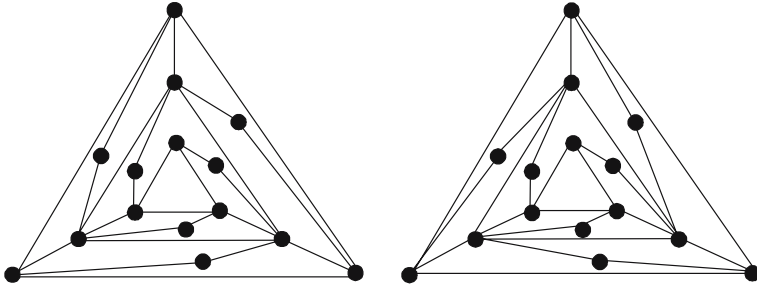


Fig. 5 Two non-isomorphic graphs with 15 vertices

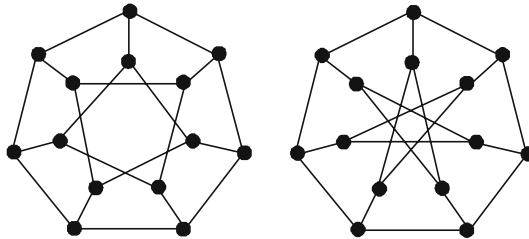


Fig. 6 Two isomorphic graphs with 14 vertices

Table 1 Simulation results obtained for the isomorphic test problems using the proposed discrete neural algorithm

| | Fig. 4a (8 vertices) | Fig. 4b (8 vertices) | Fig. 1 (10 vertices) | Fig. 6 (14 vertices) |
|----------------------------|-------------------------|-------------------------|-------------------------|-------------------------|
| Av. No. of initial states | 35 | 12 | 25 | 53 |
| Av. computation time (s) | 6.9 | 2.3 | 11.4 | 87.1 |
| Max. No. of initial states | 139 | 51 | 103 | 286 |
| Max. computation time (s) | 27.4 | 9.8 | 47.3 | 470.2 |

Av., average; No., number; Max., maximum

does not reach the value $E = 0$ after a number of random initial states $NS_{max} = 1,000$ this corresponds to two chains that are not isomorphic.

For the pair of 10-links isomorphic chains proposed by Kong et al. [8] shown in Fig. 1, the value $E = 0$ is reached after an average number of initial states equal to 25, where an average time of 11.4 s is needed. Two different outputs of the proposed binary network that directly provide the required orthogonal permutation matrices are shown in Fig. 3. Note that for an analog Hopfield model like the one proposed by Kong et al. [8], the average computation time is of hours, while our discrete neural algorithm only takes seconds to find a solution.

For the test examples shown in Figs. 4c, d and 5 the maximum number of initial states $NS_{max} = 1,000$ was reached and the condition $E = 0$ was not satisfied. It indicates that they are non-isomorphic graphs. For all the considered isomorphic test problems, Table 1 shows the average number of random initial states that the network needs to provide a correct solution, that is, to reach the value $E = 0$ and the corresponding computation time in seconds. The table also presents the most unfavourable circumstance, that is, the maximum number of random initial states that the network needs to reach the value $E = 0$ and

the corresponding computation time in seconds. These simulation results obtained for the isomorphic test problems show that this a fast strategy even on a conventional PC.

6 Conclusion

A lot of methods have been proposed for the kinematic chain isomorphism problem. However, the tool is still needed in building intelligent systems for product design and manufacturing. Therefore, a new discrete neural approach has been developed specially suitable for automatic computation since it provides directly interpretable solutions and does not demand tuning of parameters. We have successfully tested the examples solved by other approaches developed for identifying isomorphic chains published in the recent bibliography. The presented results illustrate the effectiveness of the discrete neural algorithm. Moreover, an advantage of the proposed neural network is that, though it can be implemented on a conventional PC, it can also be implemented in parallel, significantly increasing the convergence speed and reducing the computation times presented in Table 1. It may be needed when the number of vertices in a graph is very large. Besides, our network is much superior to the previously proposed analog neural network for identifying isomorphic chains in terms of the computation time and the interpretation of solutions.

Cubillo et al. [3] pointed out that recently methods based on eigenvalues and eigenvectors of the adjacency matrix [3,6,7] can identify faster non-isomorphic chains than isomorphic chains. Then, these are algorithms usually applied to quickly check out non-isomorphic chains. In contrast, the presented neural network can identify faster isomorphic chains than non-isomorphic chains. A Hopfield network can sometimes be trapped in a local minimum and then it is not always possible to guarantee that the two chains are not isomorphic. Thus we can consider neural algorithms and methods based on eigenvalues and eigenvectors as complementary techniques.

To solve the local minima problem, the practical method proposed in this paper is selecting different random initial states and running the fast neural algorithm until it reaches $E = 0$ which confirms the isomorphism. An alternative method to help the *CHOM* network to escape from local minima was recently presented by Wang et al. [16]. They have improved this network by incorporating stochastic hill-climbing dynamics. Simulation runs show that this algorithm obtains better solutions for some problems [16,17], though the computation time is increased. Also, the method is more complex to implement. If the mechanical designer effort is of concern, then the simple proposed neural algorithm is a good choice to quickly identify the isomorphism of the mechanism kinematic chain.

Appendix

Let us suppose that at time k the neuron xo is the only one that is “on” in group x and that neuron xc is the candidate neuron in group x that is going to be “on” at time $k + 1$. Hence, we have that if $c \neq o$ then $\Delta v_{xo}(k) = -1$; $\Delta v_{xc}(k) = 1$; $\Delta v_{xi}(k) = 0, \forall i = 1, \dots, m, i \neq o, c$. By substituting these values we have that the difference in the energy that would result if only the states of the neurons in the group x is altered is

$$\begin{aligned} \Delta E_x(k) &= - \sum_{i=1}^m \Delta v_{xi} \left[u_{xi}(k) + \sum_{y=1}^n \sum_{j=1}^m \frac{\omega_{xi,yj}}{2} \Delta v_{yj}(k) \right] \\ &= u_{xo}(k) - u_{xc}(k) - \frac{1}{2}(\omega_{xo,xo} + \omega_{xc,xc} - 2\omega_{xc,xo}) = u_{xo}(k) - [u_{xc}(k) - K_{xo,xc}] \end{aligned}$$

Therefore, if the neuron with the maximum value of $\{u_{xi}(k) - K_{xo,xi}\}$ per group x is always selected as the candidate neuron xc , then the energy descent, $\Delta E(k)_x \leq 0$, is guaranteed since the condition

$$u_{xc}(k) - K_{xo,xc} \geq u_{xo}(k) - K_{xo,xo} = u_{xo}(k)$$

is satisfied. Moreover, the absolute value of the energy decrease $|\Delta E_x(k)|$ is the maximum possible at every time k . Observe that, since E is bounded from above, then the energy function will converge in step k_e . In this equilibrium value it is verified in every group x of neurons that

$$u_{xo}(k_e) = \max_{j=1,\dots,m} \{u_{xj}(k_e) - K_{xo,xj}\}$$

If we activate any other neuron $xc \neq xo$ in any group x in this stable state of E , we will have $\Delta E_x(k_e) > 0$ if $u_{xc}(k_e) - K_{xo,xc} < u_{xo}(k_e)$ and $\Delta E_x(k_e) = 0$ if $u_{xc}(k_e) - K_{xo,xc} = u_{xo}(k_e)$. Therefore, the network is in a state corresponding to a local/global minimum of E .

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