Gloria Galán-Marín
Department of Mechanical, Energetic and Materials Engineering,
University of Extremadura,
Avda. de Elvas s/n; 06006 Badajoz, Spain
e-mail: gloriagm@unex.es

Domingo López-Rodríguez
e-mail: dlopez@ctima.uma.es

Enrique Mérida-Casermeiro
e-mail: merida@ctima.uma.es

Department of Applied Mathematics,
University of Malaga,
Campus de Teatinos s/n; 29071 Malaga, Spain

A New Multivalued Neural Network for Isomorphism Identification of Kinematic Chains

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. In this paper, we design a novel multivalued neural network that enables a simplified formulation of the graph isomorphism problem. In order to improve the performance of the model, an additional constraint on the degree of paired vertices is imposed. The resulting discrete neural algorithm converges rapidly under any set of initial conditions and does not need parameter tuning. Simulation results show that the proposed multivalued neural network performs better than other recently presented approaches. [DOI: 10.1115/1.3330427]

1 Introduction

Isomorphism identification between graphs is an important problem in many science and engineering applications but also computationally expensive. In the process of mechanical design, graph theory has been widely applied to represent structures of mechanisms and identify isomorphism of kinematic chains. Detecting possible structural isomorphism between two given chains is one of the major problems encountered in intelligent computer aided design (CAD) for the design of kinematic chains. As recently pointed out by Cubillo and Wan [1], most published algorithms still leave a lot to be desired in different aspects, such as visual inspection, simplifying procedure of identification and adapting automatic computation.

To achieve reliable isomorphism identification algorithms for intelligent CAD mechanisms, novel evolutionary approaches have been recently proposed [2,3]. However, with ant algorithm the solution tends to be unstable while solving the small-scale problem since in this case it is difficult to obtain appropriate parameters [3]. Some spectral methods, that possess the advantages of adapting automatic computation, have been recently presented to identify isomorphic chains. In 2001, the He–Zhang algorithm [4,5], a new eigensystem approach, was proposed. This algorithm was improved in 2005 [6]. In 2002, Chang et al. [7] presented a spectral method for mechanism kinematic chain isomorphism identification. In 2005, Cubillo and Wan [1] pointed out some fundamental errors in the theory presented by Chang et al. [7] and developed another procedure to identify isomorphic chains. However, these works [1,7] do not clearly specify the inadequacies and the possible modes of failure of the eigenvector approach. In 2006, Sunkari and Schmidt [8] critically reviewed some spectral methods, provided a correct proof and presented an eigenvector approach. Our simulation results show that this method implies a high computational cost and cannot be useful for kinematic chains with more than 14 links.

An alternative direction for kinematic chain isomorphism detection has been recently presented based on neural networks [9,10]. Neural networks allow fast parallel computation, which may be needed when we deal with large kinematic chains. Large kinematic chains are applied in robotics and are a useful model for studying biological macromolecules. Synthesis of molecular structures plays a very important role in predicting molecular properties, discovering new materials and designing novel drugs. Molecular simulation has much in common with the study of robotics. It is increasingly believed by scientists [11] that the practical and viable approach to the design and fabrication of artificial nanodevices and machines is to use proteins, which are commonly modeled as large kinematic chains.

Kong et al. [9] presented a neural model for kinematic chain isomorphism detection based on analog Hopfield's neural network [12]. In 2007, Galán-Marín et al. [10] highlighted some of the problems on the use of this network for the graph isomorphism problem. They proposed a binary discrete neural network for this problem [10] based on the competitive Hopfield model (CHOM). The lack of computational effectiveness of both the CHOM network [10] and the eigenvector approach [8] to solve kinematic chain isomorphism problems with more than 14 links led us to design a new neural algorithm. In this paper, the neural network multivalued recurrent model (MREM) [13] is applied to solve the graph isomorphism problem. In order to improve the performance of the model, one modification to the energy function has been considered in which an additional constraint on the degree of paired vertices is imposed. The effectiveness of the resultant network does not seem to be decreased as the size of the graph is increased.

2 Architecture of the Proposed MREM Network

The proposed MREM is characterized by the neuron outputs taking value in a discrete set, denoted by $\mathcal{M}=\{m_1,m_2,\ldots,m_L\}$. The vector V whose components are the corresponding neuron outputs $V=(v_1,v_2,\ldots,v_n)$ is called state vector. If v_i is the state of neuron i, then $v_i \in \mathcal{M}$. Associated to each state vector, an energy function similar to Hopfield [12] can be defined as

$$E(V) = -\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} w_{i,j} f(v_i,v_j) + \sum_{i=1}^{n} \theta_i(v_i) \tag{1}$$

where $W=(w_{i,j})$ is the synaptic weight matrix, expressing the connection strength between neurons, $f:\mathcal{M}\times\mathcal{M}\rightarrow\mathbb{R}$ is the so-called similarity function, and $\theta_i:\mathcal{M}\rightarrow\mathbb{R}$ is the generalization of the biases $\theta_i \in \mathbb{R}$ present in Hopfield's model.

The aim of the network is to minimize the energy function in Eq. (1), i.e., to achieve a stable state corresponding to a local (global, when possible) minimum of the energy function, which is usually identified with the objective function of the problem to solve. Many computational dynamics can be defined for this model, that is, several neuron updating schemes are available provided the versatility of the network. This means that more than

Contributed by the AI/Knowledge Based Systems of ASME for publication in the JOURNAL OF COMPUTING AND INFORMATION SCIENCE IN ENGINEERING. Manuscript received February 22, 2008; final manuscript received October 6, 2009; published online March 10, 2010. Assoc. Editor: J. Shah.

one neuron can be updated at the same time, in parallel. This is achieved by defining the input (synaptic potential) for neurons p and u_p as the opposite of the energy increase when neuron p is updated, that is, $u_p=-(\Delta E)_p$. If $u_p>0$, then the associated update reduces the value of the energy function. Otherwise, since no improvement is made by the update, it is not done.

2.1 Mapping the Kinematic Chain Isomorphism Problem on to the MREM Network. 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. Two graphs are said to be isomorphic if there exists a one-to-one equivalence relation between their vertices and edges that preserve the incidence. It follows that two isomorphic graphs must have the same number of vertices and the same number of edges and the degrees of the corresponding vertices must be equal to one another. As demonstrated in Ref. [8], the graphs represented by the adjacency matrices A and B are isomorphic, if and only if $B=PAP^T$, where P is an orthogonal permutation matrix such that $P^T=P^{-1}$. As applied in Ref. [3], a solution of the graph isomorphism problem can be represented as a permutation of the rows and columns of the adjacency matrix $A_{(n\times n)}$.

Let us consider a MREM network where $\mathcal{M}=\{1,2,\ldots,n\}$, that is, only state vectors V representing permutations of the numbers $\{1,2,\ldots,n\}$ are the feasible states. This means that V is an abbreviate notation for the permutation matrix $P=(p_{i,j})$ such that $p_{i,j}=1$ if, and only if, $v_i=j$, otherwise it is 0. With this notation, the permuted matrix will be $A'=(a_{vi,vj})$. Given two graphs with adjacency matrices $A_{(n\times n)}$ and $B_{(n\times n)}$, the energy function to be minimized can be expressed as

$$E(V)=\frac{1}{2}\sum_i\sum_j (a_{v_i,v_j}-b_{i,j})^2=-\sum_i\sum_j (a_{v_i,v_j}b_{i,j})+\text{constant}$$

This function measures the differences between the permuted matrix A' and B. It achieves its global minimum $E=0$ when $A'=B$, that is, A and B are isomorphic. If we skip the constant term and define the synaptic weights $w_{i,j}=2b_{i,j}$, the similarity function $f(x,y)=a_{x,y}$ and $\theta_i(x)=0$ for all i, we obtain the identification between the energy function of MREM, Eq. (1), and the objective function of the problem. With this identification, computational dynamics can be developed to solve the problem. We have considered the updating of two neurons on every step, interchanging their outputs. Suppose that neurons p and q are marked for updating, that is, $v'_p=v_p(t+1)=v_q(t)$ and $v'_q=v_q(t+1)=v_p(t)$ (where t denotes discrete time), and $v'_i=v_i(t+1)=v_i(t)=v_i$ for $i\notin\{p,q\}$. The synaptic potential associated to this update is $u=-(\Delta E)_{p,q}$.

$$u=E(V)-E(V')=-\frac{1}{2}\sum_i\sum_j \Delta_{i,j} \tag{2}$$

where $\Delta_{i,j}=w_{ij}(f(v_i,v_j)-f(v'_i,v'_j))=2b_{ij}(a_{v_i,v_j}-a_{v'_i,v'_j})$. It is easy to observe that $\Delta_{x,x}=0$ and $\Delta_{x,y}=\Delta_{y,x}$ since adjacency matrices are symmetric. Particularly for $i,j\notin\{p,q\}$, we obtain $\Delta_{i,j}=0$ since $v'_i=v_i$ and $v'_j=v_j$. For $j=p, i\notin\{p,q\}$ we obtain $\Delta_{p,i}=\Delta_{i,p}=2b_{i,p}(a_{v_i,v_p}-a_{v_i,v_q})$ since $v'_i=v_i$, $v'_p=v_q$. Analogously $\Delta_{q,i}=\Delta_{i,q}=2b_{i,q}(a_{v_i,v_q}-a_{v_i,v_p})$. Observe that $\Delta_{p,q}=2b_{p,q}(a_{v_p,v_q}-a_{v_q,v_p})=0$ due, to the symmetry of A. Then, we can deduce that $\Delta_{q,p}=0$ and $\Delta_{p,p}=\Delta_{q,q}=0$.

With these considerations, Eq. (2) can be expressed by

$$u=-\frac{1}{2}\left(\sum_i (\Delta_{i,p}+\Delta_{i,q})+\sum_i (\Delta_{p,i}+\Delta_{q,i})\right)=-\sum_i (\Delta_{i,p}+\Delta_{i,q}) \tag{3}$$

Therefore, in the proposed algorithm every neuron p computes in parallel the synaptic potential $u_p(q)=-(\Delta E)_{p,q}$ by applying Eq. (3). Then, neuron p computes the maximum potential among all possible changes $\alpha(p)=\max_{q\neq p} u_p(q)$ and the corresponding neuron to be updated at the same time q such that $u_p(q)=\max_{q'\neq p} u_p(q')$. The scheduler selects p_0 and q_0 with $\alpha(p_0)=\max_p \alpha(p)$ and $u_{p_0}(q_0)=\max_q u_{p_0}(q)$, and neurons p_0 and q_0 interchange their output. Then, all the steps are repeated until convergence is detected. Since $\max_{p,q} u_p(q)\geq 0$, the decrease of the value of the energy function is guaranteed through iterations. Thus, the network always achieve a local or global minimum of the energy function. Note that a Hopfield-type network can only ensure that, if we reach the energy value $E=0$, then the two graphs are isomorphic. Then, a criterion must be applied to conclude that two graphs are nonisomorphic. As in Refs. [9,10] we consider that if the network does not reach the value $E=0$ after $N_{\max}$ iterations, this corresponds to two chains that are not isomorphic.

2.2 Mapping Additional Constraints on to the MREM Network. In order to improve the performance of the described MREM network, one modification to the energy function has been considered. We base this modification on some additional constraints that must be verified in the optimal final solution. In a graph G, let us denote $d_i^{(G)}$ the degree of the ith node. If two graphs, A and B, are isomorphic, then there is a one-to-one correspondence between the degrees of the corresponding vertices in both graphs. This means that there exists a permutation, denoted as a state vector $V=(v_1,v_2,\ldots,v_n)$, such that $d_{v_i}^{(A)}=d_i^{(B)}$ for all i. This information can be included in the resolution of the problem. It suffices to impose the minimization of the expression

$$T(V)=\frac{1}{2}\sum_i (d_{v_i}^{(A)}-d_i^{(B)})^2=-\sum_i d_i^{(B)}d_{v_i}^{(A)}+\text{constant}$$

Thus, a new version of the energy function is obtained

$$E^*(V)=E(V)+T(V)=-\sum_i\sum_j b_{i,j}a_{v_i,v_j}-\sum_i d_i^{(B)}d_{v_i}^{(A)} \tag{4}$$

By defining $\theta_i(v_i)=d_i^{(B)}d_{v_i}^{(A)}$, we identify Eq. (4) to that of the energy function of the MREM model, Eq. (1). As in the previous section, we can compute the synaptic potential associated to the interchange of values of neurons p and q.

$$u=-(\Delta E^*)_{p,q}-(\Delta E)_{p,q}-(\Delta T)_{p,q}$$

From the previous section, we know that $-(\Delta E)_{p,q}=-\Sigma_i(\Delta_{i,p}+\Delta_{i,q})$. In addition since $v'_i=v_i$, $\forall i\notin\{p,q\}$, $v'_p=v_q$, and $v'_q=v_p$, we obtain

$$-\Delta T=T(V)-T(V')=-\sum_i d_i^{(B)}d_{v_i}^{(A)}+\sum_i d_i^{(B)}d_{v'_i}^{(A)}$$
$$=-(d_p^{(B)}+d_q^{(B)})(d_{v_p}^{(A)}-d_{v_q}^{(A)})$$

Thus, the synaptic potential for the MREM model with additional constraints is

$$u=-\sum_i (\Delta_{i,p}+\Delta_{i,q})-(d_p^{(B)}+d_q^{(B)})(d_{v_p}^{A}-d_{v_q}^{A}) \tag{5}$$

Algorithm 1: MREM implementation

```
begin
  t ← 0
  Select random feasible state vector V=(v_x, ..., v_n)
  convergence=FALSE
  while not convergence do
    convergence=TRUE
    for p ∈ {1, ..., n} do
      for q ∈ {1, ..., p−1, p+1, ..., n} do
        Compute u_p(q) from Eq. (3) and (5)
      end
      α(p)=max_{q≠p} u_p(q)
    end
    Select p_0 such that α(p_0)=max_p α(p)
    if α(p_0)>0 then
      Select q_0 such that u_{p_0}(q_0)=α(p_0)
      v_{p_0}(t+1)=v_{q_0}(t); v_{q_0}(t+1)=v_{p_0}(t)
      v_i(t+1)=v_i(t), i ∉ {p_0, q_0}
      convergence=FALSE
    end
    t ← t+1
  end
end
```

In Algorithm 1, we present the implementation for the MREM model used in this work, both for the simple and for the modified algorithm.

3 Results and Discussion

In this section we present results given by the proposed MREM network and by the modified MREM network in which an additional constraint on the degree of paired vertices is imposed. In comparing our results, we have found that there is no description of computation time in the eigenvector approaches reported in mechanical literature [1,4–8]. Then, for comparison of computational costs we have programmed in MATLAB the most recent algorithm presented in 2006 by Sunkari and Schmidt [8] and the CHOM network [10].

As case studies, we consider design examples proposed in the recent bibliography to test methods developed for automatic computation in the kinematic chain isomorphism problem [1,4–8,14] (Figs. 1 and 2). The four algorithms were implemented on a 3 GHz Pentium IV PC with 512 MBytes RAM by MATLAB. Table 1 presents the average and maximum computation time required by each algorithm to solve the five selected isomorphic test problems. The results were obtained for a total of 1000 independent runs of each algorithm. Numerical results show that the MREM algorithm is much superior to both the CHOM model [10] and Sunkari's eigenvector approach [8] in terms of computation time for all the test isomorphic problems. Table 1 also show that an improvement is made with the modified MREM network.

Table 2 presents the computation time required by each algorithm to solve the selected nonisomorphic test problems. As pointed in Sec. 2.1, a criterion must be adopted for a Hopfield-type network to detect nonisomorphic graphs. Thus, for both the CHOM and the MREM models, it is considered that if the network does not reach the value $E=0$ after $N_{\max}=100$ iterations, this corresponds to a pair of graphs that are not isomorphic. For this reason, it is not necessary to present for nonisomorphic test cases the maximum and average computation time. We only show the computation time required by the CHOM and MREM networks to perform 100 independent runs in order to ensure that we have nonisomorphic graphs. In the same way, for Sunkari's algorithm we show the computation time needed to check the permutation matrices in order to confirm that two graphs are not isomorphic.

The simulation results show that both the MREM and the CHOM models take seconds to converge to a global minimum for the selected problems. On the other hand, it can be observed that Sunkari's eigenvector approach is superior to both CHOM and

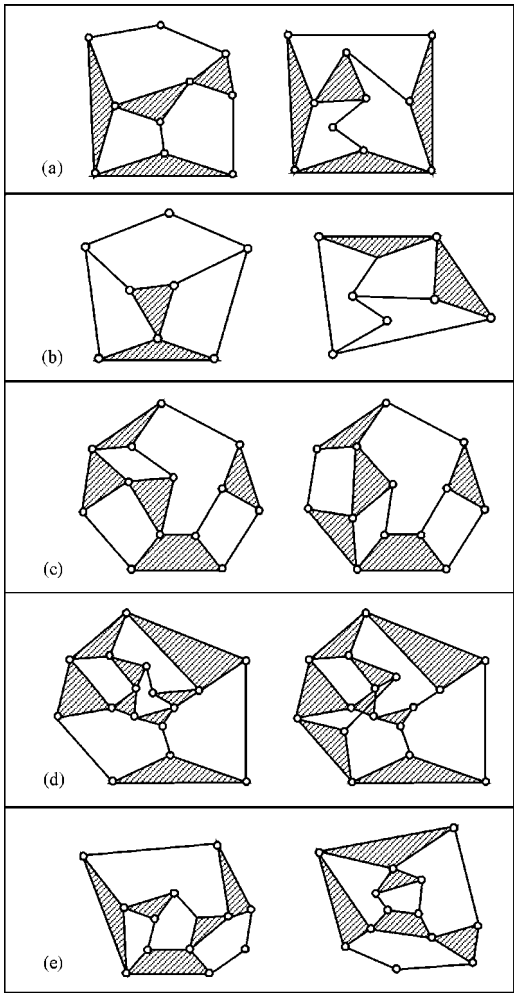

Fig. 1 Different pairs of isomorphic and nonisomorphic kinematic chains

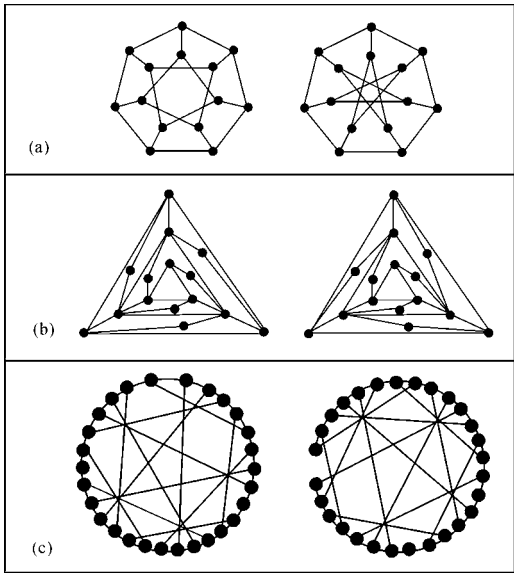

Fig. 2 Different pairs of isomorphic and nonisomorphic graphs

Table 1 Comparison of the average and maximum computation time needed for solving the isomorphic test problems using the eigenvector approach of Sunkari and Schmidt, the CHOM network, the MREM network, and the modified MREM network

	Sunkari's approach		CHOM		MREM		Modified MREM	
Graphs	Avg. time	Max. time	Avg. time	Max. time	Avg. time	Max. time	Avg. time	Max. time
Figure 1(*a*) (eight vertices)	4.75 s	8.37 s	6.9 s	27.4 s	0.02 s	0.12 s	0.01 s	0.09 s
Figure 1(*b*) (eight vertices)	2.17 s	3.69 s	2.3 s	9.8 s	0.01 s	0.1 s	0.01 s	0.06 s
Figure 1(*c*) (ten vertices)	0.12 s	0.21 s	11.4 s	47.3 s	0.02 s	0.13 s	0.01 s	0.08 s
Figure 2(*a*) (14 vertices)	>24 h	>24 h	87.1 s	470.2 s	0.03 s	0.82 s	0.01 s	1.08 s
Figure 2(*c*) (28 vertices)	>24 h	>24 h	>24 h	>24 h	0.07 s	37.76 s	0.01 s	14.95 s

Table 2 Comparison of the computation time needed for solving the nonisomorphic test problems using the eigenvector approach of Sunkari and Schmidt, the CHOM network, the MREM network, and the modified MREM network

	Sunkari's approach	CHOM	MREM	Modified MREM
Figure 1(*e*) (ten vertices)	0.03 s	47.72 s	0.08 s	0.11 s
Figure 1(*d*) (12 vertices)	0.02 s	93.67 s	1 s	1 s
Figure 2(*b*) (15 vertices)	>24 h	217.41 s	1.17 s	1.21 s

MREM models in terms of the computation time for small sized nonisomorphic problems with 12 vertices or less. Note that in the neural networks 100 runs must be performed, which represents an increase in the algorithm running time. Nevertheless, with Sunkari's eigenvector approach the exponentially increasing computation time prohibits us from solving the nonisomorphic example with 15 vertices shown in Fig. 2(*b*) while the MREM network takes only 1.17 s to solve this problem.

4 Conclusion

In this paper we design a new multivalued neural network for isomorphism identification of kinematic chains, mapping additional constraints to improve its performance. This approach is specially suitable for automatic computation since it rapidly provides solutions without a burden on the parameter tuning. Note that with some recent approaches based on ant algorithm [2,3] it is difficult for some cases to find appropriate parameters. Simulation results for nonisomorphic and isomorphic graphs with 15 vertices or more show that the exponentially increasing computation time prohibits us from solving the graph isomorphism problem by applying the eigenvector approach [8]. In contrast, the proposed multivalued network solves in seconds all the isomorphic and nonisomorphic test problems. In fact, only an average time of 0.04 s is needed on a conventional PC to solve a graph isomorphism problem with 28 vertices while both the eigenvector approach [8] and the CHOM network [10] take more than 24 h to solve the same problem.

On the other hand, the weak point of the proposed neural model is that neither of the two presented neural algorithms guarantees global minima convergence. The same deficiency appears for all optimization algorithms, such as novel evolutionary approaches [2,3], that is, a global optimal solution is not theoretically guaranteed. Therefore, it is not possible for optimization techniques to provide theoretical basis for the case of nonisomorphic chains.

References

[1] Cubillo, J. P., and Wan, J. B., 2005, "Comments on Mechanism Kinematic Chain Isomorphism Identification Using Adjacent Matrices," Mech. Mach. Theory, **40**(2), pp. 131–139.

[2] Xiao, R. B., Tao, Z. W., and Liu, Y., 2005, "Isomorphism Identification of Kinematic Chains Using Novel Evolutionary Approaches," ASME J. Comput. Inf. Sci. Eng., **5**(1), pp. 18–24.

[3] Yang, P., Pei, Z., Liao, N., and Yang, B., 2007, "Isomorphism Identification for Epicyclic Gear Mechanism Based on Mapping Property and Ant Algorithm," Eng. Comput., **21**, pp. 237–246.

[4] He, P. R., Zhang, W. J., and Li, Q., 2001, "A Quadratic Form-Based Approach to Identification of Kinematic Chains in Structural Analysis and Synthesis of Mechanisms," *Proceedings of the 2001 ASME Design Engineering Technical Conferences*, Pittsburgh, PA, Paper No. DETC2001/DAC-21067.

[5] He, P. R., Zhang, W. J., Li, Q., and Wu, F., 2003, "A New Method for Detection of Graph Isomorphism Based on the Quadratic Form," ASME J. Mech. Des., **125**(3), pp. 640–642.

[6] He, P. R., Zhang, W. J., and Li, Q., 2005, "Some Further Development on the Eigensystem Approach for Graph. Isomorphism Detection," J. Franklin Inst., **342**, pp. 657–673.

[7] Chang, Z. Y., Zhang, C., Yang, Y. H., and Wang, Y., 2002, "A New Method to Mechanism Kinematic Chain Isomor-Phism Identification," Mech. Mach. Theory, **37**(4), pp. 411–417.

[8] Sunkari, R. P., and Schmidt, L. C., 2006, "Reliability and Efficiency of the Existing Spectral Methods for Isomorphism Detection," ASME J. Mech. Des., **128**(6), pp. 1246–1252.

[9] Kong, F. G., Li, Q., and Zhang, W. J., 1999, "An Artificial Neural Network Approach to Mechanism Kinematic Chain Isomorphism Identification," Mech. Mach. Theory, **34**(2), pp. 271–283.

[10] Galán-Marín, G., Mérida-Casermeiro, E., and López-Rodríguez, D., 2007, "Improving Neural Networks for Mechanism Kinematic Chain Isomorphism," Neural Process. Lett., **26**, pp. 133–143.

[11] Kazerounian, K., Latif, K., Rodriguez, K., and Al-varado, C., 2005, "Nano-Kinematics for Analysis of Protein Molecules," ASME J. Mech. Des., **127**(4), pp. 699–711.

[12] Hopfield, J. J., and Tank, D. W., 1985, "Neural Computation of Decisions in Optimization Problems," Biol. Cybern., **52**, pp. 141–152.

[13] Mérida-Casermeiro, E., and Muñoz-Pérez, J., 2002, "MREM: An Associative Autonomous Recurrent Network," Int. J. Fuzzy Syst., **12**, pp. 163–173.

[14] Shin, J. K., and Krishnamurty, S., 1994, "On Identification and Canonical Numbering of Pin-Jointed Kinematic Chains," ASME J. Mech. Des., **116**(1), pp. 182–188.