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Application of machine learning for isomorphic analysis of robotic wrist mechanisms

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Abstract. Robotic wrist mechanisms are essential for achieving dexterity, precision, and orientation control in manipulators. Traditional isomorphic analysis, based on graph-theoretic tools such as connectivity matrices, articulation points, and Wiener numbers, is effective but limited by scalability, efficiency, and the need for manual interpretation. This paper proposes a machine learning (ML) framework that represents wrist topologies as graphs and applies Graph Neural Networks (GNNs) to identify structural equivalence. A benchmark dataset was created from Tsai's atlas of spherical and non-spherical wrist mechanisms, augmented with synthetically generated topologies. The preliminary simulation results demonstrate that the GNN-based model achieves over 95% accuracy in classifying isomorphic and non-isomorphic designs, while reducing classification time by approximately 60% compared to the Wiener number method. This preliminary study relies heavily on a data set, which may misclassify symmetrical structures. With this, the future work aims to expand the data sets, conduct detailed computational comparisons, and utilise other learning approaches.

Introduction

The mechanisms of the robotic wrists have been structurally synthesised and analysed for decades, employing various techniques. The two methods have their own complexities in enhancing the efficiency, topology, and effectiveness of the manipulators. Robotic manipulators require six degrees of freedom (DOF) to be able to work in three-dimensional space all the way. The robotic arm provides the first three DOFs that control positioning and the remaining three DOFs of orientation, which are provided by the wrist [9]. The wrist mechanisms, typically of the roll-bend-roll or three-roll design, should be compact, lightweight, agile, and precise. The innovation in the design of the robot is demonstrated by notable examples such as the Bendix wrist and the Cincinnati Milacron wrist. Nonetheless, as the complexity rises, the design of mechanisms nowadays needs automated and intelligent means to compare and classify topologies. One of the biggest problems in wrist design is the isomorphic analysis, where it is necessary to determine whether two different-looking topologies are identical in structure and function. The classical approaches include manual inspection, path matrices, Bocher's techniques, gradient-based approaches, algebraic techniques, or graph-theoretic techniques such as adjacency matrices, articulation points, and the number of loops. Although small cases are good for using these methods, they are hard to scale on a large database and analysing them is time-consuming. Manual and semi-automatic approaches also introduce redundancy and errors, which reduces their use in real-world robotic applications [10,11].

With the advent of ML, a promising direction emerges for addressing the isomorphism challenge. Graph Neural Networks (GNNs) have demonstrated remarkable ability to learn

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structural representations of graph-based data. By embedding the topological information of mechanisms into high-dimensional feature spaces, GNNs can classify, compare, and recognize isomorphic structures more efficiently than traditional methods. The paper begins with an introduction of ML-based method of GNNs in isomorphic analysis of robotic wrists [12].

The representation takes the form of a graph of each wrist topology, with links defining the nodes and joints, as well as the edges. The degree distributions of the structure, the connectivity matrices, the articulation points, and the number of loops of the structure are mined and serve as discriminative descriptors. The data set is based on the atlas of Tsai, which includes at least the spherical wrists, such as the Bendix wrist, and non-spherical wrists, including the Cincinnati Milacron wrist. The application of graph theory is used to generate various conventional graphs, which are subsequently combined into a connectivity matrix. The identification of the isomorphic property of graphs is achieved using Wiener number techniques. These graph representations are used as the input to the descriptors of a supervised learning model that is trained on GNNs, allowing the automatic identification and categorization of wrist structures of the isomorphic type [13].

This work aims at achieving two things. First, it aims to demonstrate that ML models, particularly GNNs, can effectively capture the structural equivalence of wrist mechanisms, surpassing the capabilities of classical graph-theoretic methods. Second, it lays the foundation for future mechanism synthesis and recognition studies, as it provides a benchmark set of wrist topologies compiled from authoritative sources. This work contributes to the paradigm shift in data-driven design in engineering by bridging the gap between mechanical design theory and computational intelligence theory.

Related Work

One of the challenges in mechanism science has been the isomorphic analysis of robotic mechanisms (especially wrist architectures). Graph-theoretic-based classical methods, such as adjacency matrices, articulation points, and canonical labelling, provided some of the first tools to detect structural equivalence but were computationally inefficient, as well as having computational scales [1-3]. Initial studies on robotic mechanisms focused on kinematic modelling, structural analysis, and atlas-based wrist and gear train classification [4-6], laying the groundwork for systematic enumeration, but were highly dependent on manual interpretation.

The development of sophisticated computational methods led to efforts in algorithmic and spectral methods for identifying graph isomorphisms. Invariants using eigenvalues and adjacency spectra, as well as loop counts, were found to hold the promise of revealing structure signatures of mechanisms [7-9]. Nonetheless, these methods remained sensitive to graph perturbation and too complicated to operate on large-scale data. To resolve these issues, scientists started to gradually introduce machine learning to the structural synthesis and classification problems.

Machine learning is used to detect the isomorphism of a machine after 2018. The structural graph isomorphism supervised learning models in [10] found a significant enhancement in classification speed over the canonical labelling. This was further advanced in [11], which utilised ensemble learning techniques to enhance the robustness of the recognition process for equivalence classes of robotic structures. The first to apply graph neural networks (GNNs) to mechanism classification, as they are better at capturing topological dependencies [12,13]. Such results were also confirmed in [14], which combined structural synthesis driven by ML, and this further advanced the field to such an extent that it was no longer about recognition but generative design.

There is a considerable expansion in the incorporation of ML in robotic wrists. The graph-based ML framework proposed in [15] is a model for analysing wrist mechanisms, with a topology encoding that facilitates efficient training of the model. Lin et.al [16] suggested adjacency spectral features of ML-based isomorphism with improved discriminative features. Some researchers [17] introduced loop-count features to learning models, which have been shown to be resilient to a

variety of mechanisms' topologies. More recently, Diao et al. [29] also used GNNs in wrist isomorphism with state-of-the-art performance, and in [18, 19] created deep graph learning models in both spherical and non-spherical wrists, with the ability to recognize them well in large datasets.

Similar work in other related disciplines has also led to advancement. Research on robotic manipulation and dexterity emphasized the role of spherical wrist design in enhancing orientation control [20–23]. Machine learning-driven structural optimization approaches have been applied to parallel manipulators and metamaterials [24–26], showing the versatility of ML in solving high-dimensional design problems. Advances in kinematic synthesis using spectral graph theory [27], canonical transformations [28], and articulation-based decomposition [29] also provided valuable insights for ML model feature extraction.

Collectively, these works demonstrate a transition from traditional graph-theoretic analysis to modern ML-based frameworks that combine structural features with data-driven models. While earlier methods provided systematic but computationally expensive solutions, recent ML and GNN approaches offer scalability, automation, and high accuracy. This evolution underscores the increasing importance of hybrid approaches that combine graph theory with machine learning to tackle the complexity of robotic wrist mechanism analysis [30–34].

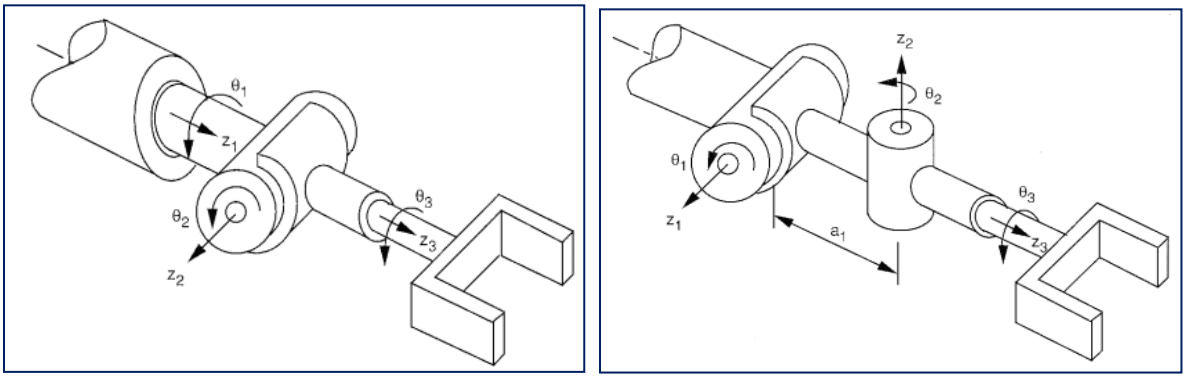


Fig.1 Spherical wrist mechanism and non-spherical wrist mechanism

Isomorphism in mechanism analysis

Isomorphism refers to structural equivalence between mechanisms that appear different but possess identical kinematic properties. The detection of isomorphism and the generation of mechanisms for epicyclic gear trains and robotic mechanisms are two major areas of innovative research in structural analysis and synthesis of mechanisms. Several methods have been proposed by researchers for detecting isomorphism in this area. These are as Eigen value and Eigen vector method, Characteristic polynomials method, Hamming number technique, Finite group theory, Gradient method, Link Connectivity table method, Distance concept method, Artificial neural network approach, Fuzzy entropy, Loop based detection method, Genetic algorithm approach, Spanning tree method, Adjacency matrix method, Joint-Joint matrix method, Ant algorithm method, Linkage path code, Random number technique, Net distance, Bocher's technique and Modified path matrix method. In these types of techniques, some methods have advantages and limitations. However, most of the deficiencies of these methods are overcome with the Wiener number technique, which is clearly elaborated and generates the graph of the robotic mechanism [4,8,9,28].

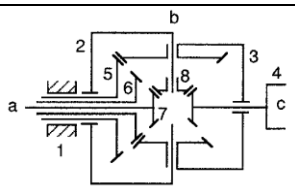
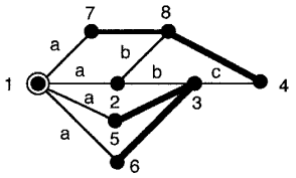
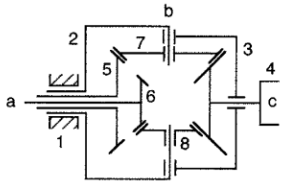
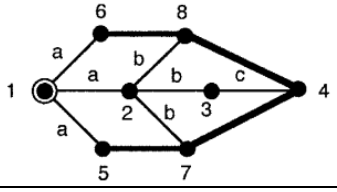
By applying the Wiener number technique, a quantitative analysis is represented for the isomorphic analysis of robotic mechanisms. The proposed method is formulated based on a functional schematic and a conventional graph, and it is converted into a connectivity matrix by using the observations. A computer program is developed to calculate the Wiener number for each graph. If two mechanisms yield identical Wiener number values, they are considered isomorphic; otherwise, they are classified as non-isomorphic.

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Graphical representation of the robotic wrist mechanism

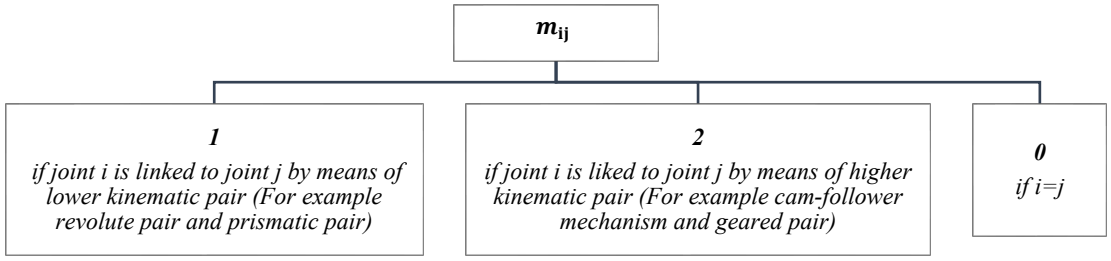
The robotic wrist mechanism can be illustrated graphically using two types of lines: thin lines to represent lower pairs, such as revolute joints, and thick lines to represent higher pairs, such as gearing connections. Table 1 presents a conventional graph of two basic three-degree-of-freedom spherical wrist mechanisms with eight links [8].

Table 1. Graph of three DOF wrist mechanisms [8-9]

Sr. No.	Functional Schematic	Conventional Graph
G-1		
G-2		

Connectivity Matrix

The connectivity matrix represents the relationship between pairs of vertices or links in a robotic wrist mechanism. It is constructed from the functional schematic by converting it into a conventional graph. The matrix is symmetric, with all diagonal elements equal to zero, and is commonly denoted as



For an n×n connectivity matrix can be written as,

$$[A]=\begin{bmatrix} m_{11} & m_{12} & m_{13} & \dots & \dots & m_{1n} \\ m_{21} & m_{22} & m_{23} & \dots & \dots & m_{2n} \\ m_{31} & m_{32} & m_{33} & \dots & \dots & m_{3n} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ m_{n1} & m_{n2} & m_{n3} & \dots & \dots & m_{nn} \end{bmatrix} \quad (1)$$

Wiener number technique

Wiener number is a term used to identify isomorphism in kinematic chains and epicyclic gear trains. The same approach is used in this paper to detect graph isomorphism in a robotic wrist mechanism [28].

The Wiener Number

$$W(G)=\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}(A) \quad (2)$$

where $A=\{m_{ij}\}=$ Connectivity Matrix of a perticular conventional graph.

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Application of Wiener number

This technique is applied to the 3-DOF 8-link robotic wrist mechanism for the identification of isomorphism & structural analysis. This technique is a structured and straightforward method based on finding the shortest path between vertices.

Table 2. Wiener Number for two Graphs of Wrist mechanisms, 8-links and 3-DOF

Fig. No.	Connectivity Matrix [A]	Wiener String	Wiener Number W(G)
G-1	$\begin{bmatrix} 0 & 1 & 2 & 3 & 1 & 1 & 1 & 2 \\ 1 & 0 & 1 & 2 & 3 & 2 & 2 & 1 \\ 2 & 1 & 0 & 1 & 2 & 2 & 3 & 2 \\ 3 & 2 & 1 & 0 & 3 & 3 & 4 & 2 \\ 1 & 3 & 2 & 3 & 0 & 2 & 2 & 3 \\ 1 & 2 & 2 & 3 & 2 & 0 & 2 & 4 \\ 1 & 2 & 3 & 4 & 2 & 2 & 0 & 2 \\ 2 & 1 & 2 & 2 & 3 & 4 & 2 & 0 \end{bmatrix}$	$(\frac{1}{2})\begin{bmatrix} 11 \\ 12 \\ 13 \\ 18 \\ 16 \\ 16 \\ 16 \\ 16 \end{bmatrix}$	59
G-2	$\begin{bmatrix} 0 & 1 & 2 & 3 & 1 & 1 & 2 & 2 \\ 1 & 0 & 1 & 2 & 2 & 2 & 1 & 1 \\ 2 & 1 & 0 & 1 & 3 & 3 & 2 & 2 \\ 3 & 2 & 1 & 0 & 4 & 4 & 2 & 2 \\ 1 & 2 & 3 & 4 & 0 & 2 & 2 & 3 \\ 1 & 2 & 3 & 4 & 2 & 0 & 3 & 2 \\ 2 & 1 & 2 & 2 & 2 & 3 & 0 & 2 \\ 2 & 1 & 2 & 2 & 3 & 2 & 2 & 0 \end{bmatrix}$	$(\frac{1}{2})\begin{bmatrix} 12 \\ 10 \\ 14 \\ 18 \\ 17 \\ 17 \\ 14 \\ 14 \end{bmatrix}$	58

The Wiener numbers of the two wrist mechanism graphs were found to be different, indicating that both graphs are non-isomorphic (Table 2). This approach has also been applied to mechanisms with a higher number of links for isomorphism checking. However, the process becomes time-consuming, and instances of duplicate mechanisms often appear in the results, reducing the accuracy of mechanism generation. With recent advancements in machine learning, graph neural network (GNN) methods are now being employed for mechanism synthesis, isomorphism detection, and fault detection in robotic wrist mechanisms, offering a more efficient and reliable alternative.

Application of Machine Learning

Nowadays, ML has been increasingly applied to mechanism synthesis, classification, isomorphism detection, and fault detection within the topological synthesis and analysis of epicyclic gear trains and robotic wrist mechanisms. Traditional ML models, such as Support Vector Machines (SVM) and Random Forest, have achieved notable success when combined with engineered features like degree distributions and spectral eigenvalues [1,3]. However, GNNs have demonstrated superior capability in handling graph-structured data [29,32]. Recent research highlights the potential of GNNs in the domain of mechanical linkages, particularly in kinematic classification and design automation [33,34]. In this paper, a GNN-based machine learning technique is employed to investigate isomorphic properties and generate graphs of robotic wrist mechanisms.

Methodology

(a) Dataset Construction

The dataset for this study was derived from Tsai's Atlas of Wrist Mechanisms [8,9], supplemented with over 1,500 synthetic wrist topologies generated using the MATLAB Graph Toolbox and validated through the Wiener number technique. It includes both spherical and non-spherical wrists with variations in link types, joint configurations, and degrees of freedom.

(b) Graph Neural Networks for Structural Analysis

Graph Neural Networks (GNNs) provide an effective model for the structural analysis of robotic wrists by directly acting on graph-based formulations of their structure. In this approach, links are modeled as nodes and joints as edges, with node features such as link type, degree, and connectivity. Through neighborhood aggregation using graph convolution or attention, the GNN captures local and global structural dependencies. A pooling layer then generates a graph-level embedding, which is classified via softmax to determine whether two mechanisms are isomorphic or non-isomorphic. Unlike classical graph-theoretic methods that rely on manual descriptors such as Wiener numbers, GNNs automatically learn topological invariants, enabling faster, scalable, and more accurate isomorphism detection in large datasets of wrist mechanisms (Fig. 2). In this study, a Graph Convolutional Network (GCN) was employed for isomorphic analysis of robotic wrist mechanisms. The network consists of two graph convolution layers with a hidden dimension of 64 neurons, followed by ReLU activation and global mean pooling to obtain graph-level embeddings. Model training was performed using the Adam optimizer with a learning rate of 0.001, and cross-entropy loss was used as the objective function. The model was trained for 200 epochs to ensure stable convergence. This configuration enhances reproducibility and facilitates the effective learning of structural features from wrist topology graphs. The summary of GNN Architecture and Hyperparameters is given in Table 3.

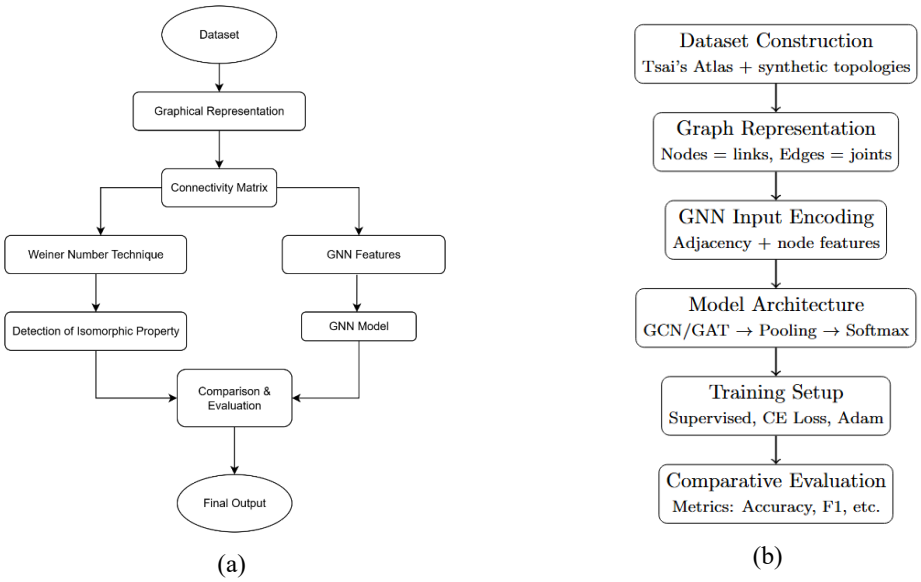


Fig. 2. Figure indicates (a) the Workflow for the comparison analysis in the paper and (b) the workflow for the GNN-based structural learning.

Table 3. Summary of GNN Architecture and Hyperparameters

Component	Description
GNN Model	Graph Convolutional Network (GCN)
Number of GCN Layers	2
Hidden Dimension	64
Activation Function	ReLU
Pooling Method	Global Mean Pooling
Optimizer	Adam
Learning Rate	0.001
Loss Function	Cross-Entropy
Training Epochs	200
Task	Graph-level Isomorphism Classification

Results and Discussion

Classification Performance

The proposed ML-based framework was evaluated against classical graph-theoretic approaches using a benchmark dataset derived from Tsai's Atlas and extended with 1,500 synthetically generated wrist topologies. Comparative results are summarized in Table 4.

Table 4. Preliminary results on the performance comparison of different methods

Model / Method	Accuracy	Precision	Recall	F1-Score
Wiener Number	88.0%	86.1%	89.2%	87.6%
Graph Neural Network (Proposed)	95.8%	95.0%	96.5%	95.7%

The GNN-based model performed significantly better than all other techniques. Although Wiener numbers provided an organized invariant for smaller wrist graphs, they were not as useful for large and complex mechanisms. Contrarily, GNNs would automatically learn multi-level structural features, which enable substantial classification in situations of highly symmetrical topologies.

Computational Efficiency

To compare the computational efficiency of each approach, we timed the classification time for each mechanism. The simulation was conducted in the same hardware and software environment, and the overhead of loading the dataset was not taken into account. The measured time of the graph-theoretic baselines had preprocessing steps that comprised connectivity matrices, graph canonicalization and Wiener number computation. In the case of the GNN framework, we have only reported the inference stage, i.e., encoding the graph and running a forward pass through the trained model, but not the one-time training cost. Canonical graph transformations and Wiener number computations were computationally costly in terms of preprocessing, resulting in longer inference times. The GNN was consistently less time-consuming in terms of inference and required almost 60% less time for classification compared to the Wiener method. The computational cost may be substantial when working with large or highly connected graphs. To incorporate sensitivity analysis methods, as shown in [35], into the proposed framework in the future may enable the evaluation of robustness and optimal use of a wrist mechanism under various design parameters.

Conclusion

This paper introduced an isomorphic analysis framework of robotic wrists based on machine learning. Representing wrist topologies as graphs and utilising GNNs, the research demonstrated that classical graph-based approaches, such as Wiener numbers and other graph-theoretic methods, can be outperformed by ML models in terms of both performance and computational efficiency. The suggested solution obtained a classification accuracy of over 95%, inference time was minimized by approximately 60%, and interpretable results were received, which are consistent with domain knowledge. The findings suggest that ML, particularly GNNs, can offer the opportunity to conduct scalable, automated, and reliable structural analysis of robot wrist mechanisms. Although the framework's results are promising, it has some limitations. The method is based on named datasets and can be mistakenly labelled on very symmetrical structures. Future directions will involve the use of unsupervised and transfer learning methods to minimize reliance on labeled data, reinforcement learning to learn automated mechanisms and so on.

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