

Ontology-Based Parkinson's Disease Monitoring and Alerting with PHKG-GNNs

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In the realm of Parkinson's Disease (PD) research, the integration of wearable sensor data with personal health records (PHR) has emerged as a pivotal avenue for patient alerting and monitoring. The complex domain of PD patient care was delved into, with a specific emphasis on harnessing the potential of wearable sensors to capture, represent and semantically analyze crucial movement data and knowledge. The primary objective is to enhance the assessment of PD patients by establishing a robust foundation for personalized health insights through the development of Personal Health Knowledge Graphs (PHKGs) and the employment of personal health Graph Neural Networks (PHGNNs) that utilize PHKGs. The objective is to formalize the representation of related integrated data, unified sensor and PHR data in higher levels of abstraction, i.e., in a PHKG, to facilitate interoperability and support rule-based high-level event recognition such as patient's missing dose or falling. This is an extension of researchers' previous related work, presents the Wear4PDmove ontology in detail and evaluates the ontology within the development of an experimental PHKG. Furthermore, the integration and evaluation of PHKG within the implementation of a Graph Neural Network (GNN) are focused on. The importance of integrating PD-related data for monitoring and alerting patients with appropriate notifications are emphasized. These notifications offer health experts precise and timely information for the continuous evaluation of personal health-related events, ultimately contributing to enhanced patient care and well-informed medical decision-making. Finally, a novel approach for integrating personal health KGs and GNNs for PD monitoring and alerting solutions is proposed.

Keywords: ontology ; knowledge graphs ; Graph Neural Networks ; Parkinson's Disease

1. Introduction

In the landscape of Parkinson's Disease (PD) research, the fusion of wearable sensor data with personal health records (PHR) has emerged as a pivotal avenue, promising to enhance patient monitoring and alerting capabilities.

The intricate domain of PD patient care was delved into, with a specific emphasis on harnessing the potential of wearable sensors to capture, represent, and semantically analyze PD patient's movement data and domain knowledge. The primary objective is to elevate the assessment of PD patients by establishing a robust foundation for personalized health insights through the development of Personal Health Knowledge Graphs (PHKGs) ^[1]. Additionally, a personal health Graph Neural Network (PHGNN) is developed leveraging the PHKG to formalize the representation of related sensors and PHR integrated/unified data at a higher level of abstraction ^[2]. This is an extension of researchers' previous related work ^[3], provides a detailed exploration of the Wear4PDmove ontology and evaluates its integration within the development of an experimental PHKG ^[3].

The challenge lies in seamlessly integrating off-the-shelf wearable sensor data with PHRs to create a comprehensive and interoperable framework for effective PD patient monitoring and alerting ^[4]. This requires addressing complexities in data representation, interoperability, and high-level event recognition. The main target of the approach is to propose a holistic solution for personalized PD patient monitoring and alerting in terms of the Wear4PDmove ontology applied over a novel experimental PHKG framework, which is appropriately integrated with PHGNNs.

The motivation stems from the need to enhance the monitoring, assessment and alerting of PD patients by creating an advanced knowledge representation and reasoning (KRR) system. Integrating off-the-shelf wearable sensor data and PHRs into a PHKG along with PHGNNs ^[5] aligns with the growing demand for sophisticated and personalized healthcare solutions.

2. Background Knowledge

This part presents key concepts spanning symbolic artificial intelligence (AI) and ontological frameworks, Knowledge Graphs (KG), PHKG, and Neurosymbolic AI [6]. Symbolic AI, epitomized by ontologies, forms the cornerstone of logical reasoning and knowledge representation, laying the groundwork for understanding/capturing complex relationships within healthcare data. KGs, through their capacity to organize and contextualize information, offer reasoning capabilities that result in valuable insights. Researchers extend this paradigm to the case of PHKG, interlinking and reasoning with diverse health-related datasets. The emergence of Neurosymbolic AI, coupling KGs with neural networks into GNNs, signifies a novel approach to decoding intricate medical data. This collective exposition establishes the essential backdrop for the subsequent in-depth exploration and contributions in the following sections.

2.1. Symbolic AI and Ontology Engineering

Symbolic AI, encompassing logical reasoning, knowledge representation, and rule-based systems, constitutes a multifaceted approach to artificial intelligence. At its core, logical reasoning forms the basis of AI systems, employing several types of mathematical logic to support deductive reasoning and decision-making mechanisms. Knowledge representation involves the explicit portrayal of information using symbols, rules, and relationships [7]. This structured representation allows systems to comprehend intricate datasets effectively and manipulate them.

Ontologies play a key role in semantic modeling, explaining object behavior and enriching raw sensor data. While progress has been made in developing semantic models for healthcare, there is an ongoing interest in developing models focusing on sensor data related to PD and wearable devices [8].

Considering symbolic AI, the development of rule-based systems is commonplace, where sets of logical rules govern the system's behavior. These rules, derived from data-driven learning strategies, serve as the guiding principles for drawing conclusions from given inputs. Technologies like RDF and OWL, often employed alongside Symbolic AI methodologies, play a crucial role in effective implementation.

2.2. Knowledge Graphs

KG serves as a structured and interconnected representation of information, adopting a graph format to represent real-world entities, their attributes, and their relationships. This semantic framework enhances understanding and facilitates reasoning. KGs feature a graph structure comprising nodes (representing entities) and edges (representing relationships), allowing the depiction of complex inter-entity connections. By incorporating Linked Data (LD) principles, KGs interconnect with external sources of information, thereby enhancing the comprehensiveness of information [9]. Their scalability accommodates vast datasets with efficient traversal and retrieval capabilities.

2.3. PHKG

In the evolving landscape of healthcare informatics, the development and utilization of PHKGs have emerged as instrumental components for advancing personalized medicine. A PHKG represents a structured and interconnected knowledge base that combines diverse personal health data, ranging from clinical records to sensor-derived information, with the aim of fostering a holistic understanding of an individual's health profile [10]. The conceptual underpinning of a PHKG draws from the principles of the Semantic Web (SW) and LD standards, facilitating the creation of a comprehensive framework that transcends traditional health record silos.

2.4. Neurosymbolic AI and GNNs

Neurosymbolic AI is a powerful interdisciplinary approach at the intersection of symbolic reasoning and neural network-based learning, aiming to harness the logical strengths and explicit knowledge representation of symbolic methods and the pattern recognition capabilities of neural networks (NNs). This hybrid model seamlessly integrates symbolic reasoning, often associated with rule-based systems, with subsymbolic learning, utilizing neural networks for effective pattern recognition. One of its distinguishing features is the capability to create interpretable and explainable AI models by leveraging explicit rule-based representations from symbolic components. A key subset, GNNs, excels in processing graph-structured data by capturing intricate dependencies and interactions among entities (nodes) connected by relationships (edges). GNNs use a message-passing mechanism, allowing nodes to iteratively exchange information and aggregate insights, deepening their understanding of the graph's structure.

3. Related Work

In the realm of PD research, a comprehensive understanding relies on the exploration of various domains, including ontologies, PHKGs, and GNNs. This part delves into state-of-the-art research, examining the pivotal role of ontologies in structuring PD-related knowledge, the application of PHKGs for personalized health insights, and the advancements brought by GNNs in analyzing complex medical data. Each sub-section within this segment unfolds the landscape of relevant studies, providing insights into the contributions, methodologies, and findings that have shaped the understanding of PD through ontological frameworks, KGs, and NN approaches.

3.1. Ontologies for PD

An ontology in the health domain serves as a framework for organizing and adding meaning to health-related data and information that is shared across different applications, services, and systems. Such ontologies play a crucial role in representing, integrating, and sharing health-related knowledge in a standardized and widely accepted format that can be understood by both humans, such as doctors and patients, and software agents. Younesi et al. have developed the PD Ontology (PDON) as a standardized vocabulary and definition system for PD and its associated symptoms, treatments, and clinical studies. The ontology has been built using standard ontology development life cycle stages such as requirements gathering, conceptualization, implementation, and evaluation.

The Parkinson's Movement Disorder Ontology (PMDO) is a significant ontology for PD created by movement disorder specialists. The PMDO encompasses three major categories: neurological observations, treatment plans, and tools used to evaluate various aspects of PD. This ontology is a valuable asset for researchers and clinicians to label, share, and consolidate data related to PD and other movement disorders, as it offers a uniform terminology for these conditions.

3.2. PHKGs for PD

Recent studies have investigated the advantages of PHKGs in advancing smart health applications. A representative example is the IoT Semantic Annotations System (IoTSAS), which processes real-time sensor stream data, integrating semantic annotations to deliver immediate health information to citizens, especially concerning air pollution and weather conditions.

Ontologies offer a means to explicitly represent unified knowledge related to sensor and PHR data, supporting knowledge creation through semantic inferencing. While advancements have occurred in semantic models for healthcare monitoring, there remains untapped potential for developing or extending existing models, particularly those focused on rules-based high-level event recognition for PD monitoring and alerting.

3.3. GNNs for PD

GNNs rapidly advance PD research through robust data analysis, handling patient-reported outcomes, imaging data, and EHRs. Integrated into knowledge graphs, GNNs unveil intricate patterns, offering insights into PD's mechanisms. Progress in GNNs for PD diagnosis, particularly Deep Learning models analyzing imaging data, shows potential for detection and prognosis. These advancements aim to enhance patient well-being and alleviate PD-related healthcare burdens, holding promise for future exploration and improved understanding.

- Graph Convolutional Networks (GCNs)

Recent advances in GCNs, particularly in PD diagnosis using Deep Learning models for imaging data scrutiny, are promising in enhancing patient outcomes and reducing the healthcare burden. The Multi-View Graph Convolutional Network (MV-GCN) enhances prediction accuracy in PD-related predictive tasks, utilizing multiple brain graph inputs. Validation with real-world data from the Parkinson's Progression Markers Initiative (PPMI) demonstrates its promising performance in predicting pairwise matching relationships in the context of PD ^[11].

- Graph Attention Networks (GATs)

Notably, GATs excel in managing extensive and intricate graphs, effectively filtering irrelevant data during DP. Advances in GAT applications for PD diagnosis, employing DL models for imaging data analysis, show promise in enhancing accuracy rates and patient outcomes. Studies introduce novel approaches like multimodal GCN (M-GCN) and GAT models for predicting phenotypic measures, showcasing ongoing exploration of graph-based NN models to advance understanding neurological conditions ^[12]. A deep multi-modal fusion model (DMFM) based on GAT is proposed, effectively

incorporating spatial dependencies for spatiotemporal correlation modeling using ConvLSTM and a temporal attention mechanism (TAM), ultimately enhancing prediction accuracy ^[13].

- Graph Recurrent Networks (GRNs)

Recent advances in deploying GRNs for PD diagnosis, particularly using DL models for analyzing time-series imaging data, show promising results with high accuracy rates ^[14]. This suggests the potential to enhance patient outcomes and alleviate the burden of PD on healthcare systems. In summary, GRNs offer a robust tool for processing time-series data in PD research, holding substantial promise for advancing researchers' understanding of this complex condition and improving patient outcomes ^[13].

- Graph Transformer Networks (GTNs)

GTNs demonstrate proficiency in managing complex graph structures, particularly relevant in handling intricate data sources like EHRs and imaging data. This enables GTNs to capture the intricate interconnections between various data elements, providing a comprehensive perspective on disease progression and patient outcomes. Recent advancements in applying GTNs to PD diagnosis and treatment involve the use of DL models for analyzing imaging data and predicting disease progression ^[14].

- Graph Autoencoders (GAEs)

GAEs also serve as valuable tools for dimensional reduction, addressing challenges posed by high-dimensional datasets in PD research, especially in imaging data, and facilitating the identification of latent patterns and relationships. Significant progress has been achieved in employing GAEs for PD diagnosis and therapeutic interventions, utilizing DL models for analyzing imaging data and predicting disease progression ^[15].

- Graph Generative Networks (GGNs)

By combining graph-based representations and generative models, GGNs offer a powerful tool for unraveling the intricate relationship between PD symptoms and disease pathology, paving the way for more effective and personalized PD treatments. In the realm of medical image analysis ^[16], GGNs play a crucial role in data augmentation, addressing limitations in labeled images by employing a generative framework with a generator network crafting synthetic data and a discriminator network distinguishing between real and synthetic data.

- Graph Reinforcement Learning Networks (GRLNs)

The integration of graph-based representations with reinforcement learning enhances the precision of treatment choices for PD patients, resulting in improved outcomes. Notable applications of deep reinforcement learning networks in the medical field include predicting brain tumor locations using a deep Q-network (DQN), a method for medical image semantic segmentation, and a recommendation system for antihypertensive medications for patients with hypertension and type 2 diabetes ^[17].

4. The Wear4PDmove Ontology

The proposed ontology represents knowledge related to the monitoring of PD patients' movement and to the integration of such data with PHR data towards supporting real-time recognition of events such as a missing dose event, eventually triggering the appropriate alerting. Wear4PDmove is an ontology that reuses and extends other ontologies, including DAHCC, SOSA, SAREF, and PMDO (**Figure 1**). The imported ontologies extend the capabilities of Wear4PDmove ontology by providing the necessary concepts and relationships to model real-world data and knowledge related to PD patients' monitoring and alerting.

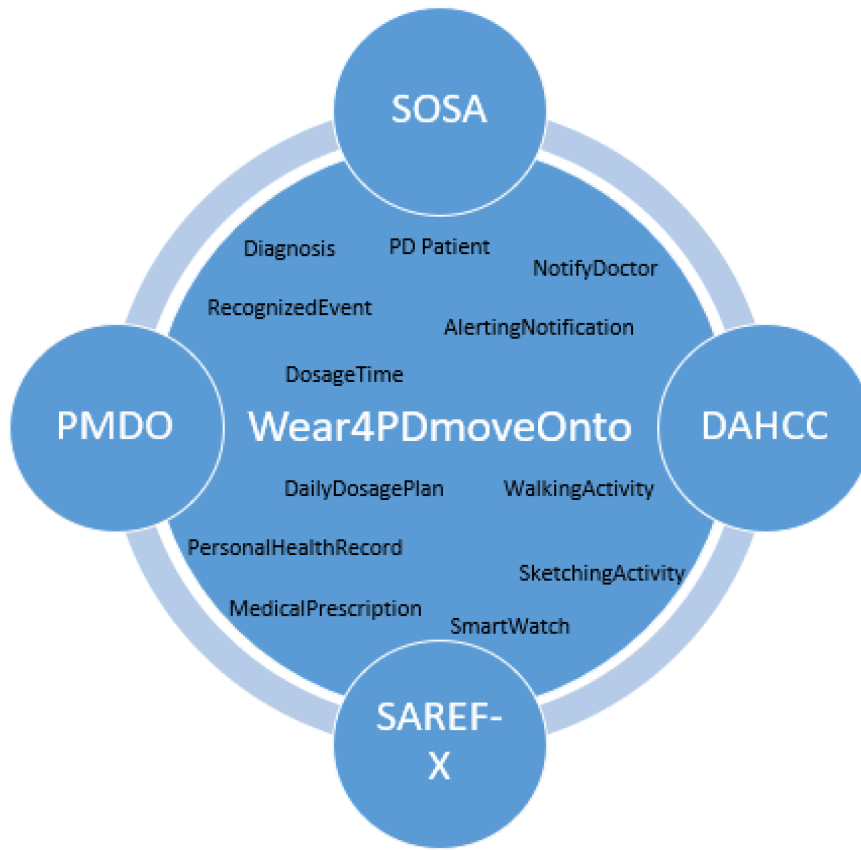


Figure 1. Wear4PDmove ontology key concepts and the reused vocabularies.

DAHCC ontology provides concepts and relationships to model the data analytics process in healthcare applications. SOSA ontology provides a formal model for representing sensors, observations, samples, and actuators and their relationships. SAREF ontology is used to model smart appliances and their features, enabling interoperability among them. PMDO is an ontology for modeling patient medical devices. Importing these ontologies into the core Wear4PDmove ontology allows us to model complex scenarios involving smart devices, sensors, and medical devices in the healthcare domain. Researchers' ontology can be used to support tasks such as monitoring patients, detecting low-level events (e.g., tremors), and providing recommendations for healthcare professionals.

The Wear4PDmove ontology proposed for the PD domain is engineered using an iterative, human-centered, and collaborative approach known as the HCOME ^[18]. This approach incorporates agile practices to encourage continuous development and testing activities in a collaborative manner. A permanent URL for its access is set at W3id: <https://w3id.org/Wear4PDmove/onto> (accessed on 1 January 2024).

5. Evaluating the Ontology in PHKGs and PHGNNs

This part is focused on the evaluation of the Wear4PDmove ontology within the framework of PHKGs and GNNs.

5.1. Experiments Setup and Data

To ensure diverse and comprehensive datasets for researchers' experiments, researchers employed two distinct methods for creating patient data. The first method involves utilizing a Python-based data generator service specifically designed for patient information. This service ensures the generation of realistic and representative observations, simulating various scenarios that might occur in a clinical setting. In the second method, researchers leveraged the Mockaroo tool as a supplementary approach. Mockaroo provides a versatile platform for generating synthetic data, allowing for the customization of attributes and characteristics to mimic real-world scenarios. Simulated observations were collected from three virtual patients for a specific time of the day, with each patient assigned 60 observations per hour (i.e., one for every minute). These two methods enrich and diversify the dataset, enhancing the robustness of researchers' experimental evaluations.

5.1.1. Wear4PDmove in Protégé OE Environment

To exploit and evaluate the engineered ontology, the competency questions were transformed to SPARQL queries and executed on the inferred knowledge represented using as input (a) a PHR database (patient information) and (b) a CSV

file of sensor data gathered from a smartwatch during experimentation with PD patients. Using the Pellet reasoner and the Snap SPARQL plugin, the inferred knowledge was queried to obtain observations related to the 'missing dose' high-level event. The source files of the ontology, the example SPARQL queries, and the SWRL rules can be accessed at <https://github.com/Kotisk/Wear4PDmove/v1.0.0/> (accessed on 1 January 2024).

5.1.2. Wear4PDmove and RDFlib/Python Implementation

In the ontology construction phase, researchers meticulously detailed the connections with recommended classes and features that form the Wear4PDmove ontology. To achieve this, researchers utilized the Protégé 5.5 tool, a widely recognized ontology engineering tool, as already mentioned in the previous section. Protégé 5.5, with its intuitive and user-friendly interface, facilitated the modeling and editing of ontologies using the OWL. The entities, classes, and relationships within researchers' ontology were meticulously defined and structured during this phase, ensuring a comprehensive representation of PD domain knowledge. It is noteworthy that researchers' project can be seamlessly run in a Google Colab environment using Python. This provides an additional layer of accessibility and convenience for users, allowing them to engage with the ontology and its interconnected components.

5.2. Neurosymbolic AI Approach

Researchers aim to explore how a GAT network processes graph-structured data effectively. The GAT network is powerful because of its attention mechanisms, which enable it to capture intricate relationships hidden in the data, providing us with a nuanced perspective on the underlying patterns. GCN complements GAT's capabilities by processing graph-structured data through its convolutional layers. Like GAT, GCN excels in handling nodes and edges representing various entities and relationships within the KG, such as symptoms, treatments, and PHR data. Together, GAT's attention mechanisms and GCN's convolutional approach enable a comprehensive analysis of the intricate relationships in the data.

To embed KG into GNNs, nodes and edges from the KG should be represented in the graph structure used by the PHGNN models. Nodes represent various entities (like symptoms, treatments, and PHR data), while edges represent relationships. To accomplish that task, researchers create a graph-based library called DGL (Deep Graph Library) to load researchers' data and use them for training a GNN model to perform binary classification regarding two different alert labels, namely, 'medium' and 'high'. These alerts are triggered by employing specific features (*hasTremor* and *hasBradykinesia*) related to tremor and bradykinesia, respectively. The "medium" alert is activated when one of these features indicates a positive result. The "high" alert is activated when both features signal a positive outcome. Researchers also evaluate the model accuracy for each level. This algorithm represents the practical implementation of researchers' approach, showcasing how GNN is embedded in researchers' system to handle and classify data effectively.

6. Discussion: Limitations and Open Issues

A noteworthy limitation lies in sustaining the relevance of the Wear4PDmove ontology amid the rapid evolution of technologies and healthcare practices. Continuous efforts are essential to ensure alignment with the latest advancements. While leveraging third-party ontologies enhances comprehensiveness, potential challenges regarding compatibility and alignment with evolving standards necessitate careful attention.

Certainly, when considering GNNs and specific algorithms like GAT and GCN, it is important to acknowledge certain limitations. One limitation is the challenge of scalability. PHGNNs, including GAT and GCN, may face difficulties in efficiently handling large-scale graphs or datasets due to the computational demands associated with the propagation of information across nodes and edges. As the size of the graph increases, the complexity of the computations can become a bottleneck, impacting both training time and resource requirements.

In conclusion, the challenges of overfitting in the context of GNNs, specifically when using GAT and GCN with varying numbers of hidden layers, are:

- **Overfitting in Deeper Architectures**
- **GAT with 8 Hidden Layers vs. 16 and 32 Layers**
- **Comparison of GAT with 8 Layers to GCN with 32 Layers**

Expanding on the discussion of limitations in the use of PHGNNs, it is essential to address the potential risk of overfitting, especially when dealing with models incorporating a higher number of hidden layers. While deeper architectures may offer improved performance on the training data, there is a risk that the model becomes too specialized and fails to generalize

well to new, unseen data. This phenomenon, known as overfitting, can hinder the model's overall effectiveness. Therefore, striking a balance and considering the trade-offs between the number of hidden layers and the risk of overfitting becomes crucial in optimizing the performance of GNNs like GAT and GCN. In summary, balancing model complexity and generalizability in PHGNNs is crucial. It suggests that a GAT with eight hidden layers may offer a more optimal balance compared to higher-layered GAT and GCN models, potentially leading to better performance on unseen data due to reduced overfitting.

7. Conclusions

The research outcomes conducted in the domain of knowledge-based PD monitoring and alerting have been presented, leveraging wearable sensor technology, advanced semantic data analysis techniques, and GNNs—particularly employing GAT and GCN algorithms. The primary objective was to enhance the landscape of PD patient care through a multifaceted approach to knowledge representation and reasoning, culminating in the creation and evaluation of a robust PHKG. Researchers' methodological advancements include the extension of the Wear4PDmove ontology to address the specificity demanded by PD monitoring and the strategic implementation of PHGNNs for nuanced analysis of complex medical data.

By exploring the intricacies of PHGNNs, researchers also demonstrated an approach towards improved analysis of complex medical data, contributing valuable insights to the PD research landscape. The culmination of researchers' efforts is a step forward in advancing the monitoring and alerting of PD.

Abbreviations

Acronym	Description
AI	Artificial Intelligence
KG	Knowledge Graph
AD	Alzheimer's Disease
ADL	Activities of Daily Living
ADO	Alzheimer's Disease Ontology
AHA	American Heart Association
AI	Artificial Intelligence
API	Application Programming Interface
BFGS	Broyden–Fletcher–Goldfarb–Shanno (optimization algorithm)
CQ	Continuous Query
CSADT	Computed Tomography Single-photon Emission Computed Tomography
CT	Computed Tomography
DAHCC	Data Analytics for Health and Connected Care
DD	Daily Dosage
DMFM	Multi-Modal Fusion Model
DQN	Deep Q-Network
GAT	Graph Attention Network
GCN	Graph Convolutional Network
GNN	Graph Neural Network
GO	Gene Ontology
HCOME	Human-Centered Ontology Engineering Methodology
ICD	International Classification of Diseases
KG	Knowledge Graph

LD	Linked Data
LOINC	Logical Observation Identifiers Names and Codes
ML	Machine Learning
MRI	Magnetic Resonance Imaging
NN	Neural Network
OE	Ontology Engineering
OOPS	Ontology Pitfall Scanner
OS	Operating System
OWL	Web Ontology Language
PD	Parkinson's Disease
PDON	Parkinson's Disease Ontology
PHGNN	Personal Health Graph Neural Network
PHKG	Personalized Healthcare Knowledge Graph
PHR	Personal Healthcare Record
PMDO	Parkinson Movement Disorder Ontology
PPMI	Parkinson's Progression Markers Initiative
RDF	Resource Description Framework
RML	RDF Mapping Language
SAREF	Smart Appliances REference ontology
SOSA	Sensor, Observation, Sample, and Actuator
SSN	Semantic Sensor Network
SW	Semantic Web
SWRL	Semantic Web Rule Language
TAM	Triple Access Memory
UMLS	Unified Medical Language System

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