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Role of Artificial Intelligence in Increasing Agricultural Productivity and Ensuring Global Food Security through Study of Plant Protein-Protein Interaction Networks and Interactomes

Review Article

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Abstract

To better understand cells, diseases, and how to treat them, researchers focus on protein-protein interactions (PPIs). Since there are many difficulties in food production due to the environment, studying interactomes can ease these problems and help reveal new facts about how crops interact with pathogens. To study PPIs in plants, researchers rely on yeast two-hybrid (Y2H) systems, affinity purification with mass spectrometry (AP-MS), bimolecular fluorescence complementation (BiFC), and computational prediction programmes. Yet, they have some problems, including a high error rate and the difficulty in obtaining similar results on repeating the same experiments. The areas of machine learning and deep learning within AI have helped in PPIs by boosting the accuracy, speed, and ability to work on large datasets. AI is being applied more often to plant protein-protein interaction networks and interactomes, helping people to better understand the details of biological systems that will determine the future prospects of agriculture and global food security.

Keywords: Plant Proteomics; Artificial Intelligence; Protein-Protein Interaction Networks; Host-Pathogen Interactions; Agricultural Biotechnology.

Abbreviations

PPI-Protein-protein Interaction; Y2H-Yeast two-hybrid; AP-MS-Affinity Purification with Mass Spectrometry; BiFC-Bimolecular Fluorescence Complementation; 2D-LC Two-dimensional Liquid Chromatography; 2D-DIGE Two-dimensional Difference Gel Electrophoresis; AI-Artificial Intelligence; ML-Machine Learning; DL-Deep Learning; PAMP Pathogen-associated Molecular Pattern; PTI-PAMP-triggered Immunity; KGF-GNN-Knowledge Graph Fused Graph Neural Network; PAN-Protein-associated Network; CNN-Convolutional Neural Network; RNN-Recurrent Neural Network; GSN-Generative Stochastic Network; LSTM-Long Short-term Memory; GO-Gene Ontology; LC-MS Liquid Chromatography Mass Spectrometry; DIA-Data-independent Acquisition; DDA-Data-dependent Acquisition; GAN- Generative Adversarial Network; IoT-Internet of Things.

Materials and Methods

PubMed (https://pubmed.ncbi.nlm.nih.gov/) was used as the primary resource for searching the relevant articles using keywords/ search terms like “artificial intelligence in plant proteomics”/ “artificial intelligence for prediction of protein-protein interactions”/ “artificial intelligence for prediction of host-pathogen interactions in plants”/ “protein-protein interactions in plant immunity” etc.

Introduction

Understanding how living things work, how diseases start, and ways to treat them all come down to how proteins interact with each other [1]. Hence, addressing issues in food production brought on by environmental stressors can be aided by comprehensive interactome research to understand protein interactions in plants, which are essential for many biological processes like development, stress responses, and signalling pathways [2, 3]. Furthermore, analysis of host-pathogen interactions can provide novel insights into how pathogens manipulate host defences for their own benefit [4]. These findings might help us better understand how plants defend themselves by showing us how plant proteins and pathogen molecules interact and respond to each other.

To understand PPIs in plants, scientists are depending mainly on proteomics techniques since it provides a better insight into various biological processes. Researchers depend on high-throughput tools to look into and understand how cells interact [2, 5]. Using the yeast two-hybrid (Y2H) system, scientists are able to study PPIs that take place naturally in cells, which made it easier to study the binary interactions between individual proteins, and thereby helped with plant biology studies [6].Another way to figure this out is to use a purification method called affinity purification together with mass spectrometry (AP-MS) in plant tissues. It can be made more effective by testing proteins with fluorescent tags and without labels to get rid of any nonspecifically precipitated proteins [7]. Other methods include bimolecular fluorescence complementation (BiFC) for visualizing protein interactions in living cells, and in silico prediction tools for computational analysis of potential interactions [3]. Two-dimensional liquid chromatography (2D-LC) and fluorescence two-dimensional difference gel electrophoresis (2D-DIGE) have also made it easier for researchers to identify proteins regulated by specific stimuli in plants [8].

Recent progress in proteomic technology has led to the development of new methods that can detect very small amounts of proteins more accurately, and allow us to look at a high volume of samples at the same time. These include multidimensional protein identification technology, OFFGEL electrophoresis, and filter-aided sample preparation methods, which allow for the identification of thousands of proteins and the detection of transient or weak affinity interactions [9]. Nevertheless, the integration of multiple techniques, such as Y2H, AP-MS, and computational predictions, is crucial for constructing comprehensive and reliable plant protein interactome networks [2].

In conclusion, the combination of various proteomic methods, including Y2H, AP-MS, BiFC, and advanced mass spectrometry techniques, allows scientists to understand the inter-relationships between proteins in plant systems. With the help of these methods, researchers can study plant development, functions, and diseases, guiding new discoveries and using them in agricultural practice forcrop improvement [2, 3]. Yet, each of them is subject to flaws such as having too many false positives and making results hard to repeat [10]. On the other hand, recent advancements in artificial intelligence (AI), particularly machine learning (ML) and deep learning (DL), have revolutionized the study of PPIs. These computational approaches have improved the reliability, efficiency, and scale of predicting PPIs, helping researchers to explore and discover new connections between proteinsand their biological significance. While there is less comprehensive experimental data available on plant interactomes than for some other organisms, this still creates an opportunity for exploring how plant protein interactions may improve crop yields and help plants resist various factors causingbiotic and abiotic stress. For example, PPIs play a crucial role in regulating plant defense responses against pathogens and pests by detecting pathogen-associated molecular patterns (PAMPs) and initiating PAMP-triggered immunity (PTI), a first line of defense against pathogens [11]. Hence, AI is increasingly being applied to study plant protein-protein interaction (PPI) networks and interactomes, offering new mechanistic insights into plant physiology and host-pathogen interactions.

Methodologies in AI-assisted PPI studies

1. Structure-Based Approaches

Structure-based methods look at the three-dimensional shape of a protein to predict how it might interact, giving better results than methods that rely solely on protein sequences. Taking into account the location and the parts of a protein involved in binding and catalysis boosts the accuracy of these approaches. Even so, issues like lacking structural data and efficient ways of using negative samples continue to exist, so there is a need for bringing together experimental and computational tools [12].

2. Graph Neural Networks (GNNs)

Graph neural networks have emerged as powerful tools for modeling PPIs. The Knowledge Graph Fused Graph Neural Network (KGF-GNN) constructs protein-associated networks (PANs) and extracts topological and semantic features. This end-to-end learning framework fuses features from PANs and PPI networks, significantly outperforming state-of-the-art models [13].

3. Deep Learning Techniques

Deep learning methods, such as convolutional neural networks (CNNs), recurrent neural networks (RNNs), and generative stochastic networks (GSNs), have been widely adopted for PPI prediction. CNNs excel at extracting hierarchical features from biological sequences, while GSNs handle uncertainty effectively. Long short-term memory (LSTM) networks capture temporal dependencies, though scalability remains a challenge [14].

4. Multi-Modal Approaches

The integration of multi-modal data, such as protein sequences, 3D structures, and gene ontology (GO), has enhanced PPI prediction. Vision transformers and pre-trained language models are used to extract features from structural and sequence data, respectively. These multi-modal frameworks have demonstrated superior performance compared to uni-modal approaches [15, 16].

5. Language Models

Large language models, such as ProtBERT, have been fine-tuned for PPI prediction. These models achieve state-of-the-art performance by learning from synthetic and real datasets, demonstrating their utility in high-throughput protein interaction prediction.

Role of AI in in MS-based proteomics

Artificial intelligence (AI) plays a transformative role in mass

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spectrometry (MS)-based proteomics data analysis by enhancing data processing, quality control, and interpretation. AI technologies are integrated across the proteomics workflow to extract meaningful insights from complex datasets as summarized in (Table 1), thereby addressing challenges such as data complexity and the need for standardized analytical frameworks, ultimately refining the quality and practicality of proteomics data, in the following aspects:

- **Quality Control and Data Acquisition:** AI models, such as the one developed in the iDIA-QC software, improve quality control in MS-based proteomics by detecting subtle changes in liquid chromatography-mass spectrometry (LC-MS) status. This model, trained on data-independent acquisition (DIA) files, outperforms traditional data-dependent acquisition (DDA) methods, achieving high accuracy in validation datasets [17].
- **Data Analysis and Interpretation:** AI improves the understanding of MS data by filtering out false signals and increasing its accuracy [18]. This is particularly crucial in the context of infectious diseases, where AI aids in the identification of biomarkers and elucidation of disease mechanisms. Machine learning (ML) strategies are also employed to tackle data challenges in proteomics, with a focus on developing robust models through high-quality datasets and standardization efforts [19]. Techniques like self-supervised pre-training and multitask learning are explored to address data scarcity and improve model performance.

AI applications in studying plant PPI networks

Deep Learning Models: AI models like DWPPI use deep neural networks to predict plant PPIs by integrating multi-source information, achieving high accuracy in datasets from plants like *Arabidopsis thaliana*, maize, and rice [28].

Integration of Data Types: AI methods are advancing by integrating various data types, such as molecular structure and interactome data, to enhance prediction accuracy. This approach has shown significant improvements over traditional methods in predicting protein-compound interactions [29].

Network Biology: AI-driven network biology helps identify critical nodes in plant interactomes, which are often targets for pathogens. This understanding can aid in developing disease-resistant plant varieties [30, 31].

Benefits of using AI in plant proteomics research

Improved Prediction Accuracy: AI models have demonstrated superior performance in predicting PPIs compared to traditional methods, with high accuracy values indicating robust predictive capabilities [32].

Data Integration: Combining different data sources, such as sequence and structural information, enhances the predictive power of AI models, providing a more comprehensive understanding of protein interactions [29].

Pathogen Interaction Studies: AI tools are instrumental in studying host-pathogen interactions, revealing how pathogens target specific nodes in plant interactomes, which can inform strategies for enhancing plant immunity [30, 31].

Potential applications of artificial intelligence in improving agricultural output

Artificial intelligence (AI) could really help find new ways to treat plant diseases and make crops grow better. The integration of AI technologies like generative AI, machine learning, and deep learning can help farmers find and control diseases more effectively by making it easier for them to recognise problems and predict what might happen if something goes wrong. These advancements make it possible to help farmers find easy, accurate, and helpful ways to control plant diseases, which really helps make growing crops better and more reliable so there is enough food for everyone. AI applications in agriculture cover a lot of ground, from checking for diseases in real time to helping predict when outbreaks might occur, and more farmers are using them to make their farming more sustainable.

AI in Disease Detection and Management

Generative AI can enhance disease identification and prediction, offering tools for better management strategies, and optimization of food production processes[32].

Machine learning and deep learning techniques, such as convolutional neural networks (CNNs), are used for accurate disease detection, achieving high accuracy and efficiency in identifying plant diseases [33, 34].

Multi-model deep learning approaches, including VGG16 and MobileNetV2, provide scalable, non-invasive solutions for early disease detection, achieving up to 99% efficiency [35].

Table 1: Summary of AI methods used for AP-MS based proteomics analysis.

Method	Description	Reference
SAINT	A probabilistic scoring tool for assigning confidence scores to protein interactions.	[20]
MaxQuant	Protein identification and quantification workflow for PPI data derived from the AP-MS experiments.	[21]
ProHits	Open source software for MS-based interaction proteomics that manages the entire pipeline from raw MS data files to fully annotated protein-protein interaction datasets, including scoring and filtering interactions.	[22]
Nested Clustering	A model-based biclustering method for analyzing label-free quantitative AP-MS data.	[23]
Biased Random Walk (RWRB)	A random walk-based algorithm for detecting protein complexes by incorporating co-complex relations.	[24]
Reinforce	An ensemble method for inferring PPI networks from AP-MS data using rank aggregation and FDR control.	[25]
Alpha-XIC	A deep neural network method for scoring co-elution of peak groups in DIA-MS data.	[26]
CHIMERYS	An AI-based search engine for improving proteomic comprehensiveness in AP-MS data.	[27]

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Improving Crop Yields

AI-driven systems can optimize crop protection and yield by providing timely and informed decision-making tools for farmers. The judicious use of generative models like Generative Adversarial Networks (GANs) and deep reinforcement learning to simulate scenarios, generate realistic data, and evaluate agricultural strategies, can help in creating predictive analytics for crop yields, and the development of personalized nutrition plans, thereby enabling sustainable and efficient agricultural practices [32, 33].

The integration of AI with IoT-enabled devices and satellite imagery allows for real-time monitoring and prediction of disease outbreaks, which can help in implementing preventive measures to protect crops [36].

AI models trained on comprehensive datasets, such as Leafsnap, can identify patterns and symptoms of leaf diseases, aiding in efficient disease management and minimizing crop losses [34].

Challenges and Future Directions:

Despite significant progress, several challenges remain in AI-driven PPI studies. These include:

Data Limitations: The scarcity of high-resolution structural data and the need for reliable negative samples hinder model training and validation [12].

Scalability: Deep learning models often struggle with scalability, particularly when handling large proteomic datasets [14].

Interpretability: The complexity of deep learning models can make it difficult to interpret predictions, limiting their practical utility [14].

While AI offers transformative potential in agriculture, challenges such as data scarcity, computational constraints, and socioeconomic barriers to AI adoption remain. Addressing these issues is crucial for maximizing the benefits of AI technologies in agriculture. Additionally, fostering user trust and acceptance of AI-driven systems among farmers is essential for widespread adoption and success in improving crop yields and disease prevention [35, 36]. Future work could focus on making sure the data used is more reliable, and that it is easier to understand how the machine learning models work, and also on bringing in different kinds of data to help these methods work better with diverse datasets.

Conclusion

There has been a paradigm shift in the domain of plant biology and agricultural biotechnology by the use of AI in the discovery of plant protein-protein interaction networks. Both AI and machine learning use unique data to predict information about plant interactomes accurately, with remarkable benefits for agriculture and biotechnology. Relying on AI while studying plant PPIs and interactomes provides better understanding of the processes involved in plant growth and development. Leveraging machine learning and deep learning with AI increases the accuracy, speed, and capacity of predicting PPIs. Such progress is necessary to increase food production and protect crops from various challenges brought by climate change.

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