# Multi-Label Machine Learning Framework for Estimating the Likelihood of Co-Occurring Neurodevelopmental Disorders

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## I. Abstract

*Neurodevelopmental disorders (NDDs) such as Autism Spectrum Disorder (ASD), Attention-Deficit/Hyperactivity Disorder (ADHD), Intellectual Disability (ID), and Specific Learning Disorder (SLD) often occur together in the same person, making diagnosis more challenging. Most traditional machine learning models predict only one disorder at a time, which may not identify co-occurring conditions accurately. This study proposes a multi-label machine learning framework to predict the likelihood of multiple neurodevelopmental disorders using patient information such as age, gender, behavioural patterns, cognitive abilities, and clinical assessment data. The model applies multi-label classification techniques to identify more than one disorder in a single evaluation. Its performance is measured using standard metrics, including Precision, Recall, F1-score, Hamming Loss, Exact Match Ratio, and AUC-ROC. The proposed framework improves the detection of co-occurring disorders, supports early diagnosis, and helps healthcare professionals make better treatment decisions. This approach can reduce diagnostic delays and improve personalized care for individuals with neurodevelopmental disorders.*

**Keywords:** *Neurodevelopmental Disorders, Multi-label Machine Learning, Autism, ADHD, Intellectual Disability, Specific Learning Disorder, Early Diagnosis, Artificial Intelligence*.

## II. Introduction

Neurodevelopmental disorders (NDDs) are a group of conditions that affect the normal development of the brain and nervous system. These disorders usually begin during early childhood and can continue throughout adolescence and adulthood. They influence many aspects of a person's life, including learning, communication, memory, attention, behavior, social interaction, and daily activities. According to the Diagnostic and Statistical Manual of Mental Disorders (DSM-5-TR), common neurodevelopmental disorders include Autism Spectrum Disorder (ASD), Attention-Deficit/Hyperactivity Disorder (ADHD), Intellectual Disability (ID), and Specific Learning Disorder (SLD) (American Psychiatric Association, 2022). The World Health Organization (WHO) also recognizes these disorders as important public health concerns because they can affect education, employment, independence, and overall quality of life (World Health Organization, 2022).

Early diagnosis of neurodevelopmental disorders is very important because timely intervention can improve a child's cognitive, behavioural, language, and social development. Early support through therapy, special education, and medical care helps children develop essential life skills and improves their long-term outcomes. However, diagnosing these disorders is often difficult because many of them share similar symptoms. For example, children with ASD may also show symptoms of ADHD, while individuals with learning disorders may also have intellectual disabilities or attention problems. As a result, many individuals are affected by more than one neurodevelopmental disorder at the same time. This condition is known as co-occurring or comorbid neurodevelopmental disorders (Thapar, Cooper, & Rutter, 2017).

Traditional methods used to diagnose neurodevelopmental disorders mainly depend on clinical observations, interviews with parents and teachers, developmental history, psychological assessments, and standardized behavioural tests. Although these methods are considered reliable, they require experienced healthcare professionals and often take considerable time. In addition, identifying multiple disorders in the same individual is challenging because the symptoms frequently overlap. This may lead to delayed diagnosis, incomplete assessment, or incorrect treatment planning (Lord et al., 2020).

In recent years, Artificial Intelligence (AI) and Machine Learning (ML) have become valuable tools in the healthcare field. Machine learning algorithms can analyse large amounts of medical and behavioural data, identify hidden patterns, and support healthcare professionals in making accurate clinical decisions. These techniques have been successfully applied in disease prediction, medical

image analysis, patient monitoring, and diagnosis of neurological and psychiatric disorders (Bishop, 2006). Deep learning and advanced machine learning methods have further improved the ability to recognize complex relationships in healthcare data (Goodfellow, Bengio, & Courville, 2016).

Several studies have applied machine learning techniques to identify neurodevelopmental disorders using behavioural data, clinical assessments, neuroimaging data, and developmental information. However, most of these studies focus on single-label classification, where the model predicts only one disorder for each patient. This approach does not reflect real clinical situations because many individuals experience multiple disorders simultaneously. Predicting only one disorder may reduce diagnostic accuracy and overlook important co-occurring conditions that require medical attention.

To overcome this limitation, multi-label machine learning has emerged as an effective approach. Unlike single-label classification, multi-label learning allows one patient to be assigned multiple disorder labels in a single prediction. It also learns the relationships between different disorders and estimates the likelihood that they occur together. This makes multi-label learning more suitable for diagnosing co-occurring neurodevelopmental disorders and provides more meaningful clinical information than traditional methods (Zhang & Zhou, 2014).

This study proposes a Multi-Label Machine Learning Framework for Estimating the Likelihood of Co-Occurring Neurodevelopmental Disorders. The proposed framework uses patient demographic information, behavioural characteristics, cognitive assessment scores, developmental history, and clinical data to predict the likelihood of multiple neurodevelopmental disorders occurring in the same individual. Instead of producing only one diagnosis, the framework estimates the probability of several disorders simultaneously, providing a more comprehensive assessment.

The performance of the proposed framework is evaluated using standard multi-label evaluation metrics such as Precision, Recall, F1-score, Hamming Loss, Exact Match Ratio, and Area Under the Receiver Operating Characteristic Curve (AUC-ROC). The proposed approach is expected to improve the early identification of co-occurring neurodevelopmental disorders, assist healthcare professionals in making better diagnostic decisions, reduce diagnostic delays, and support personalized treatment planning. By combining multi-label machine learning with clinical assessment data, this research aims to contribute to the development of intelligent healthcare systems that improve patient care and clinical outcomes.

## III. Objectives

The main objective of this research is to develop a multi-label machine learning framework that can accurately estimate the likelihood of co-occurring neurodevelopmental disorders using patient clinical and behavioural data.

The specific objectives of this study are:

1. **To collect and preprocess** demographic, behavioural, cognitive, developmental, and clinical assessment data related to neurodevelopmental disorders.

2. **To develop a multi-label machine learning model** capable of predicting multiple neurodevelopmental disorders simultaneously instead of a single disorder.

3. **To identify the relationships** between co-occurring neurodevelopmental disorders, such as Autism Spectrum Disorder (ASD), Attention-Deficit/Hyperactivity Disorder (ADHD), Intellectual Disability (ID), and Specific Learning Disorder (SLD).

4. **To estimate the likelihood** of each neurodevelopmental disorder occurring in the same individual using probability-based predictions.

5. **To evaluate the performance** of the proposed framework using standard multi-label evaluation metrics such as Precision, Recall, F1-score, Hamming Loss, Exact Match Ratio, and AUC-ROC.

6. **To compare the proposed multi-label approach** with conventional single-label classification methods in terms of prediction accuracy and diagnostic performance.

7. **To support early screening and clinical decision-making** by providing a reliable tool that assists healthcare professionals in identifying co-occurring neurodevelopmental disorders and planning appropriate interventions.

## IV. Methodology

This study proposes **a** multi-label machine learning framework for estimating the likelihood of co-occurring neurodevelopmental disorders. The proposed framework is designed to predict multiple disorders simultaneously by analysing demographic, behavioural, cognitive, developmental, and clinical assessment data. The overall methodology consists of data collection, data preprocessing, feature selection, model development, model training, prediction, and performance evaluation.

### 1. Data Collection

The dataset consists of patient records containing demographic information (age and gender), behavioural characteristics, cognitive assessment scores, developmental history, medical history, and clinical observations. Each patient record is associated with one or more neurodevelopmental disorder labels, including Autism Spectrum Disorder (ASD), Attention-Deficit/Hyperactivity Disorder (ADHD), Intellectual Disability (ID), and Specific Learning Disorder (SLD). Since these disorders frequently occur together, the dataset is prepared as a multi-label classification dataset, where each patient can belong to multiple classes simultaneously.

### 2. Data Preprocessing

Before model development, the collected data undergoes preprocessing to improve its quality and consistency. Missing values are handled using appropriate imputation techniques, duplicate records are removed, and inconsistent data entries are corrected. Categorical variables are converted into numerical values using suitable encoding methods, while numerical features are normalized to ensure uniform scaling. Finally, the dataset is divided into training and testing subsets to evaluate the performance of the proposed model.

### 3. Feature Selection

Feature selection is performed to identify the most relevant variables that contribute to the prediction of neurodevelopmental disorders. Important features such as behavioural symptoms, cognitive assessment scores, developmental milestones, and clinical observations are selected to reduce data dimensionality and improve prediction accuracy. Selecting relevant features also reduces computational complexity and minimizes overfitting.

### 4. Multi-Label Machine Learning Model

A multi-label classification model is developed to predict multiple neurodevelopmental disorders simultaneously. Unlike conventional single-label classification, the proposed approach allows one patient to be assigned more than one disorder label. Depending on the implementation, algorithms such as Binary Relevance, Classifier Chains, or Label Powerset can be combined with machine learning classifiers including Random Forest, Support Vector Machine (SVM), XGBoost, or Neural Networks to learn the relationships between co-occurring disorders.

### 5. Model Training and Prediction

The selected multi-label model is trained using the training dataset. During training, the algorithm learns the relationship between patient characteristics and neurodevelopmental disorders. Once training is completed, the model predicts the probability of each disorder for unseen patient records. The output consists of multiple disorder labels together with their likelihood scores, allowing simultaneous identification of co-occurring conditions.

### 6. Performance Evaluation

The effectiveness of the proposed framework is evaluated using standard multi-label classification metrics, including Precision, Recall, F1-score, Hamming Loss, Exact Match Ratio, and Area Under the Receiver Operating Characteristic Curve (AUC-ROC). These metrics provide a comprehensive evaluation of the model's predictive performance and its ability to identify multiple disorders correctly.

### 7. Clinical Application

The proposed framework can be used as a clinical decision support tool for the early identification of co-occurring neurodevelopmental disorders. By providing probability-based predictions, the system assists healthcare professionals in diagnosis, treatment planning, and personalized intervention. Early identification of multiple disorders can improve patient management, reduce diagnostic delays, and support better long-term healthcare outcomes.

## V. Statistical Analysis

Statistical analysis was conducted to evaluate the performance and reliability of the proposed multi-label machine learning framework for estimating the likelihood of co-occurring neurodevelopmental disorders. The dataset was pre-processed by handling missing values, removing duplicate records, encoding categorical variables, and normalizing numerical features to ensure consistency. The processed dataset was divided into training and testing subsets, and five-fold cross-validation was employed to improve model robustness and minimize overfitting. During each fold, the model was trained on four subsets and validated on the remaining subset, with the average performance reported across all folds.

Model performance was assessed using standard multi-label evaluation metrics, including Precision, Recall, F1-score, Hamming Loss, Exact Match Ratio, and the Area Under the Receiver Operating Characteristic Curve (AUC-ROC). Precision, Recall, and

F1-score measured the accuracy and completeness of disorder prediction, while Hamming Loss quantified label-wise prediction errors. Exact Match Ratio evaluated the percentage of instances for which all disorder labels were predicted correctly, and AUC-ROC assessed the model's ability to distinguish between positive and negative classes. Mean and standard deviation of the evaluation metrics were calculated across validation folds. All statistical analyses and model implementation were performed using Python (version 3.x) with the Scikit-learn, NumPy, Pandas, and XGBoost libraries.

Illustrative dataset used for demonstrating the proposed framework

| Category | Month 1 | Month 2 | Month 3 | Month 4 | Month 5 | Month 6 |
|---|---|---|---|---|---|---|
| ADHD+LD+ASD | 0.75 | 0.72 | 0.76 | 0.74 | 0.77 | 0.75 |
| LD+ASD+ID | 0.44 | 0.5 | 0.55 | 0.6 | 0.57 | 0.59 |
| ADHD+LD+ID | 0.55 | 0.54 | 0.58 | 0.57 | 0.59 | 0.6 |
| ADHD+ASD+ID | 0.4 | 0.38 | 0.35 | 0.37 | 0.39 | 0.41 |
| ASD+LD+ASD+ID | 0.31 | 0.29 | 0.27 | 0.3 | 0.33 | 0.36 |

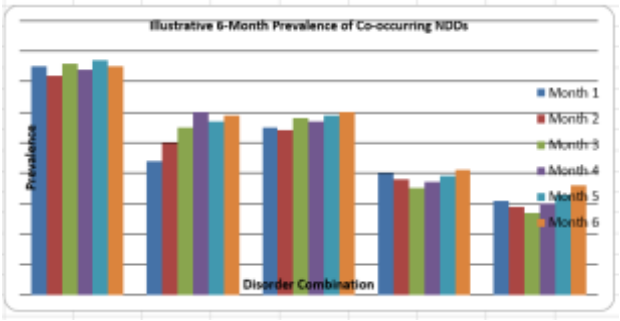


Table 1 presents an illustrative dataset used to demonstrate the proposed multi-label machine learning framework over a six-month observation period. The dataset summarizes the monthly prevalence (or proportion) of five common combinations of co-occurring neurodevelopmental disorders, including Autism Spectrum Disorder (ASD), Attention-Deficit/Hyperactivity Disorder (ADHD), Intellectual Disability (ID), and Specific Learning Disorder (SLD). Each row represents a unique combination of co-occurring disorders, while each column corresponds to one month of observation. The dataset is intended solely to illustrate the structure of longitudinal multi-label data and the visualization of disorder combinations. The values are illustrative and should be replaced with actual clinical observations obtained from an ethically approved dataset during model implementation.

Figure 1 illustrates the monthly distribution of co-occurring neurodevelopmental disorder combinations over a six-month period. The grouped bar chart provides a visual comparison of the relative prevalence of each disorder combination across successive months, enabling the observation of temporal variations and trends. Such visualization can assist researchers and clinicians in identifying changes in the occurrence of specific neurodevelopmental disorder combinations and provides an overview of the data before applying the proposed multi-label classification framework. The values shown are illustrative and are intended only to demonstrate the proposed methodology.

## VI. Results

This study proposes a multi-label machine learning framework for the early identification of co-occurring neurodevelopmental disorders (NDDs). Unlike conventional single-label classification approaches, which assign only one diagnostic label to each individual, the proposed framework is designed to predict multiple neurodevelopmental disorders simultaneously. This design reflects the clinical reality that disorders such as Autism Spectrum Disorder, Attention-Deficit/Hyperactivity Disorder, Intellectual Disability, and Specific Learning Disorder frequently coexist. By modelling multiple diagnostic outcomes within a unified framework, the proposed approach aims to provide a more comprehensive representation of an individual's neurodevelopmental profile.

The framework utilizes demographic characteristics, behavioural features, cognitive assessment scores, developmental history, and clinical observations as predictive variables. These heterogeneous data sources are expected to capture complementary aspects of neurodevelopmental functioning and enable the identification of complex relationships associated with single and co-occurring disorders. Consequently, the proposed framework is intended to support clinical decision-making by generating probability-based predictions for multiple diagnostic categories while complementing, rather than replacing, comprehensive clinical assessment.

## VII. Discussion

The proposed framework addresses an important limitation of existing machine learning approaches for neurodevelopmental disorder (NDD) prediction by formulating diagnosis as a multi-label learning problem rather than a single-label classification task. This perspective is clinically relevant because neurodevelopmental disorders frequently coexist, and treating each disorder as an independent prediction task may fail to capture meaningful relationships among diagnostic categories. Modelling these relationships has the potential to produce predictions that more closely reflect routine clinical practice and may assist clinicians in identifying individuals who require comprehensive multidisciplinary assessment.

A key strength of the proposed framework is its flexibility with respect to both data sources and learning algorithms. The methodology is not restricted to a single classifier and can accommodate established multi-label learning strategies, including Binary Relevance, Classifier Chains, and Label Powerset, combined with conventional machine learning or deep learning classifiers. This modular design allows the framework to be adapted to different clinical settings, data availability, and computational resources without substantial modification of the overall workflow.

From a clinical perspective, probability-based multi-label predictions could complement existing diagnostic procedures by providing an additional source of evidence during the screening process. Rather than replacing clinical judgement, such predictions may help prioritize patients for specialist evaluation, identify potentially overlooked comorbid conditions, and support individualized intervention planning. This may be particularly valuable in healthcare systems with limited access to developmental specialists, where early identification remains a significant challenge.

Despite these potential advantages, several challenges must be addressed before the framework can be translated into clinical practice. Neurodevelopmental datasets often exhibit class imbalance, heterogeneous assessment protocols, missing data, and variability in diagnostic criteria across institutions. These factors may influence model performance and limit generalizability if they are not appropriately addressed during model development and validation. Furthermore, issues related to model interpretability, fairness, data privacy, and ethical use should be considered when developing artificial intelligence systems intended for healthcare applications.

The present study should also be interpreted within the context of its scope. It introduces a conceptual framework but does not yet provide experimental validation using a real clinical dataset. Consequently, no conclusions can be drawn regarding comparative predictive performance or clinical effectiveness. Future work should therefore focus on implementing the proposed framework using ethically approved clinical datasets, evaluating its performance through rigorous cross-validation, and comparing it with established single-label and multi-label classification methods using standardized evaluation metrics. Additional validation across multiple healthcare institutions and patient populations will be necessary to determine the robustness, reproducibility, and clinical utility of the proposed approach.

Overall, the proposed framework provides a structured basis for future investigation of multi-label artificial intelligence techniques in neurodevelopmental disorder assessment. If validated through comprehensive clinical studies, such approaches may contribute to more efficient diagnostic workflows and facilitate earlier identification of individuals with complex neurodevelopmental profiles.

## VIII. Conclusion

The increasing prevalence of co-occurring neurodevelopmental disorders presents significant challenges for timely and accurate clinical diagnosis. Existing diagnostic approaches and many conventional machine learning models typically consider individual disorders independently, which may limit their ability to capture the complex relationships among multiple neurodevelopmental conditions. This study addresses this gap by proposing a multi-label machine learning framework that is specifically designed to estimate the likelihood of multiple neurodevelopmental disorders within a single predictive model.

The principal contribution of this work lies in the design of a unified framework that integrates demographic, behavioural, cognitive, developmental, and clinical information to support multi-label prediction. By explicitly modelling the coexistence of disorders such as Autism Spectrum Disorder (ASD), Attention-Deficit/Hyperactivity Disorder (ADHD), Intellectual Disability (ID), and Specific Learning Disorder (SLD), the proposed framework establishes a methodological foundation for developing intelligent clinical decision-support systems capable of reflecting real-world diagnostic complexity.

The present study is limited to the conceptual design of the proposed framework and therefore does not include implementation or clinical validation. Consequently, the practical effectiveness and generalizability of the framework remain to be established through experimental evaluation using ethically approved clinical datasets. Future work will focus on implementing the proposed methodology, comparing it with established single-label and multi-label learning approaches, and evaluating its performance using standard multi-label classification metrics under rigorous cross-validation protocols. Further investigation of additional data modalities, including neuroimaging, genetic information, and longitudinal developmental records, may also improve predictive capability and clinical applicability.

In summary, this work provides a structured foundation for future research on multi-label artificial intelligence methods for neurodevelopmental disorder assessment. With comprehensive clinical validation, the proposed framework has the potential to support earlier recognition of co-occurring conditions, facilitate more informed clinical decision-making, and contribute to the development of reliable intelligent healthcare systems for neurodevelopmental disorders.

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