**1. Introduction**

* 1. **Background on Autism Spectrum Disorder (ASD)**

Autism Spectrum Disorder (ASD) is a neurological condition that affects how a person thinks, communicates, interacts socially, and processes sensory information. The term "spectrum" reflects the wide range of characteristics and abilities individuals with autism may have. While some may face significant challenges in their day-to-day existence, others may have exceptional skills and live independently.

ASD usually starts to show up in early childhood, and by the time a child is two or three years old, there are often clear signs. Some common signs are trouble communicating verbally and nonverbally, doing the same things over and over, having few interests, and having trouble getting along with others. It's important to understand and help people with ASD because they are all different.

Early diagnosis is very important. If kids with ASD get the right kind of help and support, like occupational therapy, behavioural therapy, speech therapy, or educational support, they are more likely to learn important skills and become independent over time. Support is still very important in adolescence and adulthood; it helps people with their mental health, careers, and social lives.

Although the exact cause of ASD is still unknown, researchers think that a combination of environmental and genetic factors contributes to the disorder. Parenting styles or individual decisions are not to blame. As ASD has become more widely recognised and diagnosed in the past few decades, there are now more resources and support networks available.

Early assistance in the development of vital life skills is very beneficial for children with ASD. Personalised treatment plans and educational support can make a significant difference. Importantly, the increasing acceptance of the abilities and contributions of people on the spectrum is promoting an open culture that values neurodiversity. Acceptance and inclusion are becoming increasingly important in today's society. Numerous communities and advocacy organisations are trying to change the conversation away from "curing" autism and towards embracing neurodiversity. Individuals with ASD can contribute unique perspectives, innovative concepts, and useful abilities, and they can lead fulfilling lives in the correct setting.

In conclusion, autism spectrum disorder is a collection of differences that impact how individuals view and engage with the world instead of a single illness. People with ASD can succeed in every aspect of life if they are understood, accepted, and given the proper support. Making the world more inclusive and supportive begins with understanding ASD. We can all help people on the autism spectrum live better lives if we have patience, empathy, and knowledge.

**1.2 Importance of Early Detection**

Early detection of Autism Spectrum Disorder (ASD) is one of the most critical factors in ensuring a better quality of life for individuals on the spectrum. Identifying signs of autism at an early age, typically between 18 months and 3 years, allows for timely intervention, which is essential during the critical period of brain development. Children can get the help they require during the most critical phases of brain development if the early symptoms of autism, such as delayed speech, limited eye contact, or repetitive behaviours, are identified.

During early childhood, the brain is especially adaptable. A child's brain is most capable to learn new behaviours and skills during this time, which is frequently referred to as the "critical window." If ASD is identified early, targeted therapies can begin when they are most effective. According to research, learning, social interactions, and communication skills can all significantly improve with early intervention.

Additionally, early detection gives carers and parents more power. It allows them to learn how to support their child's special requirements, access the right services, and understand their child's condition. Children with ASD may not receive the necessary support if they are not diagnosed early, and parents may feel overwhelmed or confused if they are unaware of the causes of their child's behaviour.

Schools, medical professionals, and therapists all gain from early identification. Early diagnosis allows professionals to create specialised education and support plans for the child. The child benefits from these specialised methods in both educational and social environments.

It's also critical to remember that early detection decreases long-term difficulties. Early support increases a child's likelihood of becoming self-sufficient, confident, and emotionally resilient. As they age, they might also need less intensive support.

In conclusion, early identification of ASD is transformative rather than just helpful. It creates the basis for a happy life, boosts the likelihood of positive development, and provides access to early support.

Early identification of ASD can alter a child's entire developmental trajectory in addition to providing a head start. It makes it possible for professionals and families to interact right away, setting the foundation for development, education, and deep connections with society.

* 1. **Motivation for using Machine Learning**

Machine learning (ML) has emerged as an increasingly essential asset in the healthcare sector, enabling the analysis of extensive and intricate datasets, uncovering concealed patterns, and making highly accurate predictions. In relation to Autism Spectrum Disorder (ASD), ML offers a distinctive opportunity to revolutionize the conventional diagnostic approach, which is frequently subjective, labour-intensive, and time-consuming.

One significant reason for implementing ML in ASD detection is its capacity to facilitate early screening through automation and standardization. Traditional techniques heavily depend on expert interpretation of behavioural symptoms, which can differ significantly among clinicians. In contrast, machine learning can analyze objective data - such as responses to questionnaires, developmental history, and even video or audio signals - to produce predictions based on learned patterns from previously classified cases.

ML models, including decision trees, support vector machines (SVM), random forests, and deep learning networks, can be trained on labelled ASD datasets to differentiate between individuals with ASD and those without. These models can also pinpoint which characteristics (e.g., lack of eye contact, delayed speech) are most indicative of an ASD diagnosis, thereby enhancing the refinement of current screening tools.

The scalability of ML represents another significant benefit. Once trained and validated, these models can be integrated into mobile applications, online platforms, or diagnostic software, thereby making screening more accessible in under-resourced or rural regions. Additionally, ML models function efficiently, providing predictions within seconds and alleviating the workload of healthcare professionals.

Moreover, ML paves the way for personalized diagnostics by continuously learning from new data and adjusting to specific population traits. As more data becomes available, models can be updated to reflect evolving diagnostic trends and enhance generalizability across diverse populations.

In conclusion, the rationale for employing machine learning in ASD detection is rooted in its ability to support early and accurate diagnosis.

**1.4 Project Objectives**

The main aim of this initiative is to utilize machine learning algorithms for the early identification of Autism Spectrum Disorder through the analysis of real-world datasets. This encompasses the design, implementation, and assessment of predictive models capable of categorizing individuals as either likely or unlikely to have ASD based on behavioural, demographic, or developmental characteristics.

The project is directed by the following specific goals:

* To gather and pre-process dependable ASD datasets that encompasses pertinent features such as age, gender, responses to screening questionnaires, and developmental history.
* To conduct exploratory data analysis (EDA) to comprehend the structure, distribution, and correlations within the data, which will guide feature selection and model development.
* To train and evaluate various machine learning algorithms, including logistic regression, decision trees, random forests, and support vector machines, and to compare their effectiveness using metrics such as accuracy, precision, recall, F1-score, and ROC-AUC.
* To pinpoint the most critical predictive features that influence ASD classification, which may assist in enhancing current screening tools or inform the creation of new ones.
* To assess the practical implications and constraints of employing machine learning in a real-world clinical environment, taking into account ethical considerations, data privacy, and interpretability.

By fulfilling these goals, the project aims to advance the integration of artificial intelligence into healthcare, particularly in domains that can benefit from early intervention and improved accessibility, such as autism diagnosis.

* 1. **Organization of the Report**

2. DATASETS USED

**2.1 Dataset Overview**

Two distinct but complementary datasets were used in our project on Autism Detection using Machine Learning: the *ABIDE phenotypic dataset* and a publicly available *autism screening dataset*. These datasets, though differing in structure and content, together provided a robust foundation for exploring autism spectrum disorder (ASD) classification from both clinical and behavioural perspectives. While the ABIDE dataset offered rich phenotypic data linked to MRI imaging, the screening dataset supplied accessible, structured questionnaire data commonly used in early autism detection. The combination allowed for a dual approach—leveraging both medically-validated information and real-world screening tools—to train, validate, and compare machine learning models aimed at distinguishing individuals with ASD from typically developing individuals.

**2.2 Autism Screening Dataset**

The second dataset (autism\_data.csv) is a tabular dataset that resembles standardized autism screening forms. It includes individual-level responses to a series of binary or multiple-choice questions, typically administered in self-report or caregiver-report formats. These questions are designed to identify behavioural patterns commonly associated with autism, such as social withdrawal, difficulty with communication, and repetitive behaviours.

Alongside these questionnaire responses, the dataset also includes demographic fields such as age, gender, country of residence, and education level, as well as a binary target label indicating whether a subject was classified as autistic or not. Compared to the ABIDE dataset, this data is more simplified but allows for rapid prototyping and evaluation of machine learning models using structured, easy-to-obtain data. It is particularly relevant for real-world applications where clinical or imaging data may not be readily available.

In the project, this dataset was instrumental in testing several baseline classifiers and tuning algorithms based on common metrics like accuracy, precision, recall and f1-score. Its clean structure also made it suitable for exploratory data analysis and feature selection.

The dataset contains information related to autism screening, with the following 21 columns:

1. **A1\_Score to A10\_Score**: These are binary (0 or 1) responses to ten screening questions from the Autism Spectrum Quotient (AQ-10) test. A response of 1 typically indicates behavior associated with autism.
2. **age**: The age of the individual (in years).
3. **gender**: The gender of the individual, typically 'm' for male and 'f' for female.
4. **ethnicity**: The individual's ethnic background (e.g., 'White-European', 'Latino', 'Asian', etc.).
5. **jundice**: Whether the individual had neonatal jaundice ('yes' or 'no').
6. **austim**: Whether the individual has a family history of autism ('yes' or 'no').
7. **contry\_of\_res**: Country of residence of the individual (note the typo: "contry" instead of "country").
8. **used\_app\_before**: Whether the individual has used a screening app before ('yes' or 'no').
9. **result**: The screening result score from the AQ-10 test (a numerical value).
10. **age\_desc**: Description of the age group (e.g., '18 and more').
11. **relation**: The relationship of the person filling out the form to the individual being screened (e.g., 'Self', 'Parent', etc.).
12. **Class/ASD**: The final classification based on the test — 'YES' if the person is likely to have autism, 'NO' otherwise.

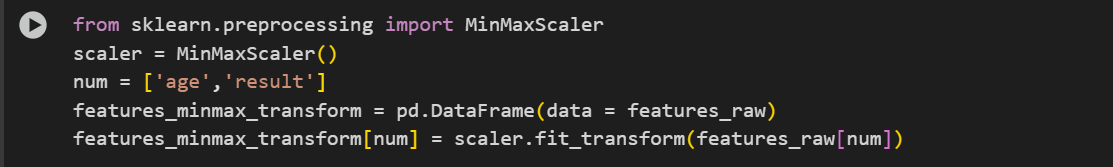
**2.2.1 Preprocessing techniques used:**

1. **Handling Missing Values:**

* **Technique:** The code uses data.dropna(inplace=True) to remove rows with missing values.
* **Reasoning:** Missing values can cause issues with many machine learning algorithms. Removing them is a simple way to handle this problem.

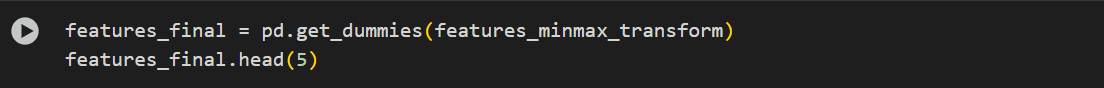
**2. Feature Scaling:**

* **Technique:** MinMaxScaler is used to scale numerical features ('age' and 'result') to a range between 0 and 1.
* **Reasoning:** This ensures that features with different scales (e.g., age and result) have a similar impact on the model. It can improve the performance of algorithms like SVM and KNN.



**3. One-Hot Encoding:**

* **Technique:** pd.get\_dummies() is used to convert categorical features into numerical representations using one-hot encoding.
* **Reasoning:** Machine learning algorithms typically work with numerical data. One-hot encoding creates new binary columns for each category, preventing the model from misinterpreting categorical values as ordinal.



**4. Label Encoding:**

* **Technique:** The target variable ('Class/ASD') is converted from 'YES' and 'NO' to 1 and 0, respectively, using a lambda function.
* **Reasoning:** Similar to one-hot encoding, this converts the target variable into a numerical format suitable for machine learning models.



**2.3 ABIDE Phenotypic Dataset**

The ABIDE phenotypic dataset (Phenotypic\_V1\_0b\_preprocessed1.xlsx) is part of the larger Autism Brain Imaging Data Exchange project. It includes subject-level metadata corresponding to participants whose neuroimaging data was collected from 17 international sites. Although this project focused on the phenotypic (non-imaging) data, the dataset remains closely tied to fMRI-based research in autism.

Each row in the dataset represents an individual participant and contains a wide array of variables. These include demographic information such as age at scan, sex, and handedness; diagnostic classification (Autism or Control); cognitive assessments like Full-Scale IQ (FIQ), Verbal IQ (VIQ), and Performance IQ (PIQ); and various clinical and behavioural scores derived from standardized instruments such as the ADOS (Autism Diagnostic Observation Schedule), SRS (Social Responsiveness Scale), and SCQ (Social Communication Questionnaire). In addition, quality control metrics for scan reliability—such as framewise displacement and root mean square (RMS) motion estimates—are included for filtering participants during data preprocessing.

This dataset enabled a detailed understanding of the characteristics typically associated with autism and was used in the project to construct feature sets for machine learning classifiers. It was particularly useful for examining how demographic and cognitive variables could influence ASD diagnosis and how predictive such features could be when used in isolation or combination.

The dataset contains 106 fields, many of these are clinical, diagnostic, or quality control measures.

1. Subject Identifiers

* i, Unnamed: 0, X: Internal or indexing fields (can usually be ignored).
* SUB\_ID: Subject ID.
* subject: Often duplicate or formatted version of SUB\_ID.
* SITE\_ID: Data acquisition site (e.g., NYU, UCLA).
* FILE\_ID: File name identifier.

1. Diagnosis and Demographics

* DX\_GROUP: Diagnosis group (1 = Control, 2 = Autism).
* DSM\_IV\_TR: DSM-IV-TR classification.
* AGE\_AT\_SCAN: Age in years at time of scanning.
* SEX: 1 = Male, 2 = Female.
* HANDEDNESS\_CATEGORY: Right, Left, Ambidextrous.
* HANDEDNESS\_SCORES: Numeric handedness score.

1. IQ Scores and Test Types

* FIQ, VIQ, PIQ: Full, Verbal, and Performance IQ.
* FIQ\_TEST\_TYPE, VIQ\_TEST\_TYPE, PIQ\_TEST\_TYPE: Corresponding test types used.

1. ADI-R (Autism Diagnostic Interview – Revised) Scores

* ADI\_R\_SOCIAL\_TOTAL\_A
* ADI\_R\_VERBAL\_TOTAL\_BV
* ADI\_RRB\_TOTAL\_C: Restricted/repetitive behavior.
* ADI\_R\_ONSET\_TOTAL\_D: Age of symptom onset.
* ADI\_R\_RSRCH\_RELIABLE: Whether interview was research-reliable.

1. ADOS (Autism Diagnostic Observation Schedule) Scores

* ADOS\_MODULE: Module used (depends on age/verbal ability).
* ADOS\_TOTAL, ADOS\_COMM, ADOS\_SOCIAL, ADOS\_STEREO\_BEHAV: Scores across domains.
* ADOS\_RSRCH\_RELIABLE: Research-reliable status.
* ADOS\_GOTHAM\_SOCAFFECT, ADOS\_GOTHAM\_RRB, ADOS\_GOTHAM\_TOTAL, ADOS\_GOTHAM\_SEVERITY: Gotham algorithm scores.

1. SRS (Social Responsiveness Scale) Scores

* SRS\_VERSION: Version used.
* SRS\_RAW\_TOTAL: Total raw score.
* SRS\_AWARENESS, SRS\_COGNITION, SRS\_COMMUNICATION, SRS\_MOTIVATION, SRS\_MANNERISMS: Subscale scores.

1. Other Behavioral Assessments

* SCQ\_TOTAL: Social Communication Questionnaire total.
* AQ\_TOTAL: Autism Quotient score.

1. Medical and Comorbidity

* COMORBIDITY: Comorbid conditions.
* CURRENT\_MED\_STATUS: Medication usage status.
* MEDICATION\_NAME: Name of medications.
* OFF\_STIMULANTS\_AT\_SCAN: Was off stimulants during scan?

1. Vineland Adaptive Behavior Scales (Used to assess personal and social skills)

* VINELAND\_RECEPTIVE\_V\_SCALED, ..., VINELAND\_COPING\_V\_SCALED: Scaled subdomain scores.
* VINELAND\_COMMUNICATION\_STANDARD, VINELAND\_DAILYLVNG\_STANDARD, VINELAND\_SOCIAL\_STANDARD, VINELAND\_ABC\_STANDARD: Standard scores.
* VINELAND\_SUM\_SCORES: Sum of scaled scores.
* VINELAND\_INFORMANT: Person reporting the scores (e.g., parent).

1. WISC-IV (Wechsler Intelligence Scale for Children - Fourth Edition)

* WISC\_IV\_VCI, WISC\_IV\_PRI, WISC\_IV\_WMI, WISC\_IV\_PSI: Composite scores.
* Subtest scaled scores like:
* WISC\_IV\_SIM\_SCALED, VOCAB\_SCALED, INFO\_SCALED, ...
* WISC\_IV\_BLK\_DSN\_SCALED, MATRIX\_SCALED, DIGIT\_SPAN\_SCALED, ...

1. Scan Status and Motion

* EYE\_STATUS\_AT\_SCAN: Eyes open/closed during scan.
* AGE\_AT\_MPRAGE: Age at T1-weighted scan.
* BMI: Body Mass Index.

1. Quality Metrics (Anatomical and Functional MRI)

* anat\_cnr, anat\_efc, anat\_fber, anat\_fwhm, anat\_qi1, anat\_snr: Structural scan quality.
* func\_efc, func\_fber, func\_fwhm, func\_dvars, func\_outlier, func\_quality: Functional scan quality.
* func\_mean\_fd, func\_num\_fd, func\_perc\_fd: Framewise displacement (motion).
* func\_gsr: Whether global signal regression was applied.

1. Quality Control Ratings

* qc\_rater\_1, qc\_notes\_rater\_1, ... qc\_anat\_rater\_2/3, qc\_func\_rater\_2/3: Manual ratings.
* qc\_anat\_notes\_\*, qc\_func\_notes\_\*: QC notes from different raters.

1. Final Inclusion Status

* SUB\_IN\_SMP: Whether the subject was included in the sample used in publication.

**Combined Use**

By combining the clinical depth of the ABIDE phenotypic data with the practical accessibility of the autism screening data, this project was able to evaluate autism detection from two complementary angles: one rooted in comprehensive, medically-reviewed data, and the other based on everyday behavioural screening tools. This approach not only strengthened the reliability of the classification models but also showcased the potential for scalable autism detection solutions that bridge clinical research and real-world usability.

**3. Methodology**

**3.1 Overview of Project Workflow**

Data collection, pre-processing, feature selection, model training, and evaluation are all part of the project's organized pipeline. Two different datasets—a neuroimaging dataset (ABIDE) and a text-based dataset with questionnaire responses—were employed. Every dataset needed a different approach to modelling and pre-processing. The high-level process consists of:

* **Data Collection**: Gathering data from two primary sources — a structured questionnaire dataset and the ABIDE (Autism Brain Imaging Data Exchange) repository.
* **Pre-processing**: Customized pre-processing for each dataset type, including cleaning, normalization, and skull-stripping for MRI data.
* **Feature Engineering and Dimensionality Reduction**: Extracting meaningful features and reducing dimensionality to avoid overfitting and computational overhead.
* **Model Building**: Training classical machine learning models like Logistic Regression, SVM, and KNN tailored to each dataset.
* **Evaluation and Analysis**: Using performance metrics and visual tools like confusion matrices to assess model effectiveness.

This modular approach ensures flexibility, scalability, and robust handling of heterogeneous data sources.

**3.2 Data Pre-processing Techniques**

**3.2.1 Text Dataset:**

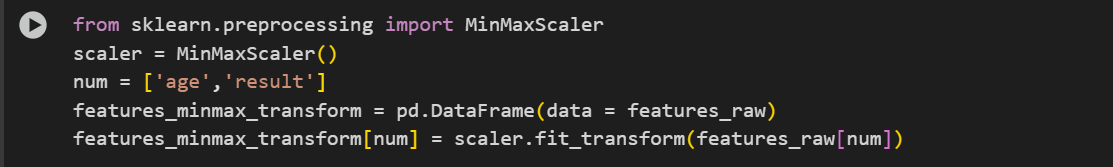
The study's text dataset comes from standardized diagnostic questionnaires that evaluate demographic and behavioural indicators linked to autism spectrum disorder (ASD). Age, gender, ethnicity, country of residence, history of familial ASD, and screening results are among the characteristics included in this dataset. Such data must go through a methodical pre-processing pipeline to be cleaned, consistent, and machine-readable before it can be used for machine learning.

1. **Handling Missing Values:**

* **Technique:** The code uses data.dropna(inplace=True) to remove rows with missing values.
* **Reasoning:** Missing values can cause issues with many machine learning algorithms. Removing them is a simple way to handle this problem.

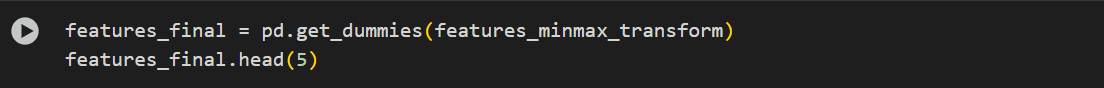
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* **Reasoning:** Similar to one-hot encoding, this converts the target variable into a numerical format suitable for machine learning models.



The pre-processing of the text dataset is a crucial step that changes raw, unstructured data into a well-formed and numerical form suitable for machine learning models. This rigorous preparation improves data quality, reduces bias, and ensures better generalization of the trained models.

**3.2.2 ABIDE Dataset: Pre-processing and Feature Preparation**

The Autism Brain Imaging Data Exchange (ABIDE) dataset used in this study was obtained from the Pre-processed Connectomes Project (PCP), specifically the ‘rois\_aal’ derivative. This version of the dataset provides resting-state fMRI data that has already undergone a standardized pre-processing pipeline, ensuring consistency and reproducibility across studies.

**Pre-processing Performed by PCP**

The following pre-processing steps were completed by the PCP team:

* **Skull-stripping**: This involves removing non-brain tissues such as the skull, scalp, and other surrounding structures from anatomical scans, focusing the analysis solely on the brain.
* **Spatial Normalization**: Individual brain scans are aligned to a common anatomical space, typically the MNI152 template. This step allows data from different subjects to be compared voxel-by-voxel or region-by-region in a standardized framework.
* **Smoothing and De-noising**: Spatial smoothing using a Gaussian kernel improves signal-to-noise ratio and accommodates anatomical variability. De-noising procedures such as regression of confounding signals (e.g., motion, white matter, CSF) help reduce artifacts and enhance data quality.
* **Temporal Filtering**: A band-pass filter is applied to the time-series data to retain frequencies typically associated with neural activity while removing low-frequency drift and high-frequency noise.
* **Parcellation with AAL Atlas**: The brain is divided into 116 distinct anatomical regions using the Automated Anatomical Labeling (AAL) atlas. For each region, the average BOLD signal across all voxels within that region is extracted, resulting in a region-wise time series.

**Feature Engineering and Additional Steps**

On top of the pre-processed time series, the following steps were performed in this study to prepare features suitable for machine learning:

* **Flattening the Correlation Matrix**: Since the Pearson correlation matrix is symmetric, only the upper triangular values (excluding the diagonal) are extracted and flattened into a 1D feature vector. This dramatically reduces the number of features while preserving all unique pairwise relationships.
* **Dimensionality Reduction**: To address the curse of dimensionality and enhance model generalization, feature reduction techniques such as Principal Component Analysis (PCA) or correlation-based selection can be applied. These helped remove redundant or non-informative features.

This carefully structured pre-processing pipeline ensures that the derived features are neuro-biologically grounded, noise-reduced, and optimized for machine learning-based classification between ASD and control subjects.

**3.3 Feature Selection and Dimensionality Reduction**

In the context of ML, high-dimensional datasets can lead to several challenges, including overfitting, increased computational load, and difficulty in model interpretation. This is especially true for the ABIDE dataset, which involves hundreds to thousands of functional connectivity features derived from correlation matrices, as well as the text-based dataset that includes multiple categorical and numerical attributes.

To address these issues, dimensionality reduction and feature selection techniques were employed. These approaches aim to retain the most relevant information while reducing redundancy, noise, and computational complexity.

**Principal Component Analysis (PCA)**

Principal Component Analysis is a widely used linear technique for dimensionality reduction. In this work, PCA was largely used on the ABIDE dataset following feature extraction from the functional connectivity matrices. The key goals of using PCA were:

* **Noise Reduction**: By projecting the data onto directions of maximum variance, PCA helps eliminate features that contribute less to the overall variance (and often represent noise).
* **Redundancy Elimination**: Many brain areas show linked activity, resulting in redundant connectivity patterns. PCA combines linked features into orthogonal principal components.
* **Improved Training Efficiency**: Reducing the amount of features speeds up the training process and allows for the adoption of simpler models that perform better on untested data.
* **Visualization**: PCA also allows for data visualization in lower dimensions (e.g., 2D or 3D), helping assess cluster separation between ASD and control subjects.

The number of components maintained was determined using the cumulative explained variance criteria, which generally retains components that explain 95% or more of the overall variation.

**Rationale for Dimensionality Reduction**

These feature selection and dimensionality reduction methods were crucial, particularly because:

* The **ABIDE dataset** involved 6670 unique pairwise correlations (from 116 AAL regions), which is large relative to the number of subjects.
* The **textual questionnaire data**, while not extremely high-dimensional, included categorical variables with multiple levels and required transformation to numeric space.

**3.4 Tools and Technologies Used**

This project's implementation required the use of a variety of robust open-source tools and libraries, the majority of which were created around the Python programming language. These tools helped at different phases of the workflow, including data preprocessing, model training, and visualization, allowing for effective handling of both structured questionnaire data and high-dimensional neuroimaging data.

**Python**

Python formed the foundation of the entire project. Its rich ecosystem of scientific and machine learning libraries, paired with its ease of use and readability, made it perfect for quick prototyping, data analysis, and experimentation. Python's adaptability enabled the smooth integration of neuroimaging technologies with traditional machine learning frameworks.

**Pandas and NumPy**

* **Pandas** was utilized for structured data processing, namely with questionnaire-based datasets. It was useful for dealing with missing values, encoding categorical characteristics, and converting tabular data into model-friendly representations.
* **NumPy** provided efficient array-based operations and numerical computations, which were essential during normalization, matrix transformations, and implementation of custom algorithms when needed.

**Scikit-learn**

Scikit-learn was the primary machine learning framework used for both classification tasks and preprocessing. It provided built-in functions for:

* Splitting datasets into training and test sets
* Feature scaling and normalization
* Implementing classifiers such as Logistic Regression, SVM, and KNN
* Performing dimensionality reduction using PCA
* Evaluating model performance through accuracy, precision, recall, and F1-score metrics

Its intuitive API and well-documented utilities significantly accelerated development.

**Nilearn**

Nilearn is a specialized Python library built on top of NiBabel and scikit-learn, designed for statistical learning on neuroimaging data. It played a crucial role in:

* Loading and handling 4D fMRI images from the ABIDE dataset
* Applying pre-processing steps such as masking and smoothing
* Extracting regional time series and computing functional connectivity matrices
* Reducing the complexity of raw neuroimaging data into structured features suitable for machine learning

This library was central to bridging the gap between raw brain imaging data and ML model inputs.

**Matplotlib and Seaborn**

These visualization libraries were used for generating insightful plots during analysis. Their key use cases included:

* Plotting correlation heatmaps of features
* Visualizing the distribution of diagnostic labels
* Displaying performance metrics (e.g., confusion matrix, ROC curves)
* Tracking model behavior and feature relationships

Seaborn’s high-level API helped in creating aesthetically appealing and informative statistical graphics.

**Jupyter Notebook and Visual Studio Code**

* **Jupyter Notebook** was used to interactively explore, visualize, and record the data analysis process. The cell-based execution architecture allowed for gradual testing of pre-processing processes and algorithms.
* **Visual Studio Code (VS Code)** was used for organizing and managing larger scripts and modules, particularly when transitioning from prototype code to more structured implementations.

**GitHub**

GitHub was used for version control, project tracking, and collaboration. The entire codebase, including data processing scripts, model implementations, and result visualizations, was maintained in a public repository. This ensured transparency, reproducibility, and ease of access for future research or peer review.

These environments offered a productive development workflow and were instrumental in maintaining reproducibility and version control throughout the project.

1. **Experimental Results and Analysis**

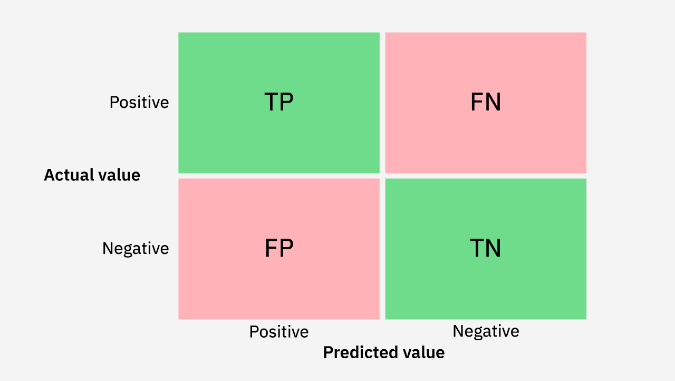
**5.1 Evaluation Metrics**

Evaluation metrics are used to assess the performance of trained models. We employed the following evaluation metrics on our models.

1. **Accuracy**: Accuracy measures the ratio of correct predictions made by the model to the total number of predictions. It gives us a general idea of how often the model is correct, but can be unreliable for unbalanced datasets.
2. **Precision**: Precision measures the accuracy of positive predictions. It is the ratio of true positive predictions to the total number of positive predictions that was made by the model. Models having a high precision have a very low rate false positives.
3. **Recall (or Sensitivity)**: Recall measures the ability of a model to correctly identify all relevant positive cases. It is the ratio of correctly predicted positive instances to the total actual positive instances. A high recall indicates a low false negative rate.
4. **F1-Score**: F1 Score is the harmonic mean of precision and recall. Its value lies in the range of 0 and 1, both included. It balances the trade-off between precision and recall and tells us how precise (correctly classifies how many instances) and robust (doesn’t miss any significant number of instances) our classifier is. It is particularly useful when the class distribution is imbalanced.
5. **Confusion Matrix**: Confusion Matrix is the visual representation of the relation between actual values and predicted values.

It helps us determine the following values-

* **True Positive**: The values which were actually positive and were predicted positive.
* **False Positive**: The values which were actually negative but falsely predicted as positive. Also known as Type I Error.
* **False Negative**: The values which were actually positive but falsely predicted as negative. Also known as Type II Error.
* **True Negative**: The values which were actually negative and were predicted negative.



*Figure 1: Confusion Matrix (*[*https://developer.ibm.com/tutorials/awb-confusion-matrix-r/*](https://developer.ibm.com/tutorials/awb-confusion-matrix-r/)*)*

**5.2 Results on Text-Based Questionnaire Dataset**

The text-based dataset used in our project consists of responses to standard Autism Spectrum Disorder (ASD) screening questionnaire. This data was preprocessed and used to train six different machine learning models: Logistic Regression, Support Vector Machines (SVM), Decision Tree, Random Forest, k-Nearest Neighbor, and Naïve Bayes. The dataset was split in training and testing samples using 80:20 ratio.

**5.2.1 Performance Comparison**

The following table summarizes the performance metrics of the six models:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Model** | **Accuracy** | **Precision** | **Recall** | **F1-Score** |
| Decision Trees | 0.957 | 0.925 | 0.925 | 0.925 |
| Random Forest | 0.900 | 1.000 | 0.650 | 0.787 |
| Support Vector Machines | 0.978 | 1.000 | 0.925 | 0.961 |
| K-Nearest Neighbors | 0.950 | 0.923 | 0.900 | 0.911 |
| Naïve Bayes | 0.950 | 0.923 | 0.900 | 0.911 |
| Logistic Regression | 0.992 | 1.000 | 0.975 | 0.987 |

**5.2.2 Confusion Matrices**

A confusion matrix gives us a detailed analysis of a model's classification performance, displaying the number of correct and incorrect predictions made on each class. It includes four key components:

* **True Positives (TP)**: Correctly predicted ASD cases
* **True Negatives (TN)**: Correctly predicted non-ASD cases
* **False Positives (FP)**: Non-ASD cases incorrectly classified as ASD
* **False Negatives (FN)**: ASD cases incorrectly classified as non-ASD

Below are the confusion matrices for the two best performing models i.e. Logistic Regression and Support Vector Machines (SVM)-

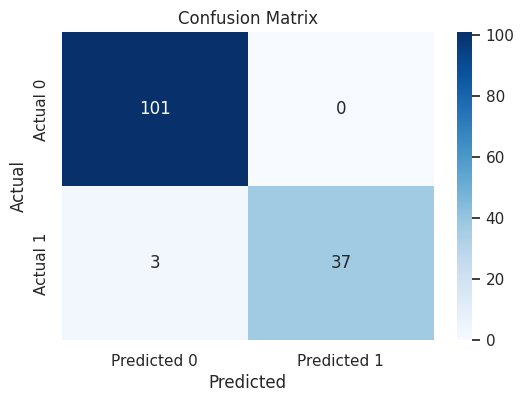
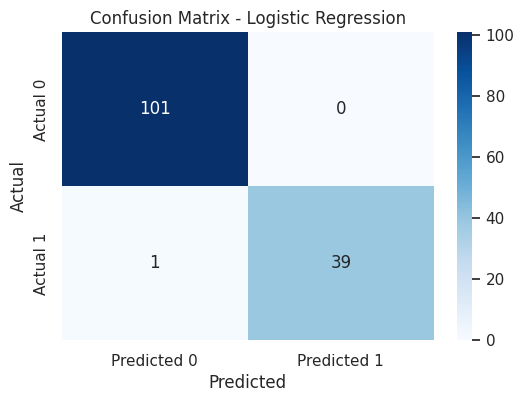


Figure 2: Confusion Matrix for Support Vector Machines

Figure 2: Confusion Matrix for Logistic Regression

**Interpretation**:

* Logistic Regression achieved a nearly perfect classification, with only 1 false positive and 0 false negatives.
* SVM also performed strongly, with three false positives but no false negatives.
* Both of these models, showed high recall and precision which makes them reliable for ASD detection.

**5.2.3 Discussion**

* With the best accuracy and F1-score, Logistic Regression showed outstanding performance and reliability.
* SVM was also quite successful, particularly when it came to high recall and perfect precision.
* Recall was marginally lower for Decision Trees and k-NN than for the best performers, but they still performed admirably.
* Despite having excellent precision, Random Forest missed a lot of good cases because of its much weaker recall.
* Although it performed rather well, Naïve Bayes trailed somewhat behind the other models.

**5.3 Results on ABIDE Dataset**

The Autism Brain Imaging Data Exchange (ABIDE) dataset consists of resting-state functional MRI (fMRI) scans from people with and without ASD. In this project, we’ve only worked with data from the **NYU site** to maintain uniform imaging protocols and reduce inter-site variability.

Data was fetched using the “fetch\_abide\_pcp” function with the **‘rois\_aal’ derivative**, which extracts mean regional time-series features from brain regions defined by the **AAL (Automated Anatomical Labelling)** atlas. This approach reduces the high dimensionality of raw fMRI data by computing average signals from predefined anatomical regions.

**5.3.1 Preprocessing**

Since the data was already pre-processed by the Pre-processed Connectomes Project (PCP), standard pre-processing steps like motion correction, skull stripping, normalization, and nuisance regression had already been applied. The AAL-based ROI features were then directly used for training machine learning models.

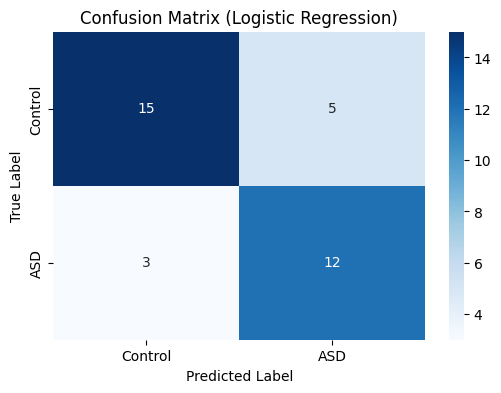
**5.3.2 Performance Comparison**

Three classical machine learning models were evaluated on the extracted ROI-based features:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Model** | **Accuracy** | **Precision** | **Recall** | **F1-Score** |
| Logistic Regression | 0.807 | 0.772 | 0.772 | 0.772 |
| Support Vector Machines (SVM) | 0.677 | 0.666 | 0.736 | 0.700 |
| k-Nearest Neighbors (KNN) | 0.673 | 0.692 | 0.409 | 0.514 |

**5.3.3 Confusion Matrix**

Below is the confusion matrix for the model which performed the best i.e. Logistic Regression.



*Figure 2: Confusion Matrix for Logistic Regression Model on the ABIDE dataset*

**5.3.4 Discussion**

* **Logistic Regression** performed the best among the three models, with an accuracy of 77.1%, a high recall of 0.800, and an F1-score of 0.750. This suggests that Logistic Regression was able to identify a significant proportion of ASD cases, although its precision is slightly lower compared to its recall.
* **SVM** exhibited lower overall performance, with an accuracy of 67.7% and an F1-score of 0.700. While it performed reasonably well, it had lower precision and recall than Logistic Regression, indicating that it may have been more conservative in predicting ASD cases, potentially leading to more false positives and negatives.
* **KNN** performed the worst among the three models, with an accuracy of 67.3%, precision of 0.692, recall of 0.401, and an F1-score of 0.514. The low recall indicates that KNN struggled significantly to identify positive ASD cases, leading to many false negatives.

These results indicate that **Logistic Regression** is the most reliable model for ASD detection on the ABIDE dataset, though the overall performance of the models was lower compared to the text-based dataset. This highlights the challenges associated with working with neuroimaging data, which is complex and high-dimensional. Pre-processing and feature engineering are critical factors that can influence model performance in this domain.

**5.3.5 Challenges**

* **Pre-processing Complexity**: Neuroimaging data require extensive pre-processing including normalization, brain region extraction, and feature selection.
* **Data Heterogeneity**: Differences in scanner types, imaging protocols, and demographics across acquisition sites introduce variability.
* **Sample Size**: Despite the richness of each sample, the number of subjects remains limited, making generalization difficult.

**6. Discussion**

**6.1 Interpretation of Results**

The results demonstrate that traditional machine learning models can accurately distinguish between ASD and non-ASD cases using both questionnaire-based data and neuroimaging-derived features. On the questionnaire dataset, Logistic Regression achieved the highest accuracy (0.992) and F1-score (0.987), indicating strong predictive performance and generalization capability. Support Vector Machines also performed exceptionally well, with an accuracy of 0.978 and an F1-score of 0.961.

On the ABIDE neuroimaging dataset, however, Logistic Regression once again performed best, with an accuracy of 0.807 and an F1-score of 0.772. This stability across both modalities shows that it can handle a variety of data formats, even with limited sample numbers. SVMs performed moderately, however KNN underperformed due to its susceptibility to irrelevant characteristics and high complexity in neuroimaging data.

These results highlight the significance of model selection based on data characteristics. Simpler, interpretable models, such as Logistic Regression, can be extremely useful in domains where data volume is limited but structure is abundant.

**6.2 Key Findings and Insights**

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* **Logistic Regression Demonstrates Strong Generalizability**: Across both datasets, logistic regression consistently outperformed alternative models in terms of accuracy and F1 score. Its superior performance demonstrates that even simple linear models can thrive when the features are well-preprocessed and relevant. Furthermore, its interpretability makes it ideal for medical applications in where comprehending model decisions is crucial.
* **Effectiveness of Pre-processing Pipelines**: The success of the models highlights the importance of data preparation. Label encoding, normalization, and outlier removal in the questionnaire dataset, as well as skull-stripping, smoothing, and standardization in the ABIDE dataset, all helped to improve input quality and learning outcomes.
* **Dimensionality Reduction Was Pivotal for Neuroimaging**: Using PCA on the high-dimensional ABIDE data helped to minimize noise, reduce overfitting, and improve training efficiency. Without this phase, models such as SVM and KNN would most likely have suffered more from the curse of dimensionality. This emphasizes the need of dimensionality reduction in neuroimaging applications.
* **Model Performance Reflects Data Nature**: Models such as Random Forest scored badly on the ABIDE dataset when compared to questionnaire data, demonstrating that algorithms sensitive to high-dimensional or noisy data are unsuitable for neuroimaging until further improved. KNN, too, demonstrated a significant performance loss on ABIDE, emphasizing the need of model-data compatibility.
* **Insights into Real-World Utility**: The fact that a simple model, such as logistic regression, may achieve over 99% accuracy on structured questionnaire data indicates a significant potential for scalable, low-cost screening tools. Meanwhile, even mediocre performance on ABIDE data shows that machine learning can identify clinically significant signals from complex brain imaging, but more work is needed to improve resilience and interpretability.

**6.3 Challenges in Multimodal ASD Detection**

* **Data Imbalance and Size**: The very limited sample size, particularly for neuroimaging data, presents difficulties in training deep learning models and assuring generalization. With inadequate data, models may fail to catch unusual but important patterns, increasing the danger of overfitting.
* **Heterogeneity in Data Sources**: Varying scanning parameters, equipment, and methods amongst ABIDE sites can cause discrepancies and noise in neuroimaging results. This diversity makes generalization difficult and necessitates harmonization measures.
* **Feature Integration Complexity**: To ensure meaningful representation, diverse data from behavioural questionnaires and neuroimaging modalities must be carefully pre-processed and aligned. Differences in feature scale, dimensionality, and type (categorical vs. continuous) complicate the procedure.
* **Computational Load and Resource Demands**: Working with high-resolution fMRI data, particularly during pre-processing and feature extraction with tools like Nilearn, requires a significant amount of resources. This prevents real-time or large-scale adoption in clinical contexts unless computationally efficient processes are built.

**6.4 Ethical Considerations in Medical ML**

* **Patient Privacy**: Using neuroimaging and personal health data requires rigorous adherence to anonymisation standards and data governance.
* **Bias and Fairness**: Models trained on imbalanced datasets may exhibit demographic biases, such as gender or regional skew.
* **Interpretability**: Clinicians demand interpretable models to defend their decisions. As a result, simpler models such as logistic regression are occasionally selected over complicated black-box designs.
* **Informed Consent and Transparency**: Any future use of such technologies must ensure that patients or their guardians are fully aware of how their data will be utilized.

**6.5 Clinical Relevance**

The study shows that integrating clinical questionnaires with neuroimaging biomarkers can aid in the early diagnosis of autism spectrum disorder. Such models, once fully tested, could help clinicians with screening and diagnosis, particularly in places without expert access. The strong performance of logistic regression also offers promise for real-world application, provided that data scalability and generalizability issues are addressed.

Furthermore, the success of questionnaire-based models paves the way for the development of low-cost, non-invasive digital screening instruments that may be quickly deployed. Neuroimaging-based models, albeit more resource-intensive, can aid in confirming diagnosis in clinical settings with access to imaging infrastructure. Overall, the combination of computational techniques and clinical experience shows promise for improving ASD diagnosis and enabling timely intervention.

**Chapter 7: Conclusion and Future Work**

**7.1 Summary of Contributions**

This study explored the application of machine learning techniques to the multimodal detection of Autism Spectrum Disorder (ASD) using two distinct data sources: structured diagnostic questionnaires and the ABIDE neuroimaging dataset. Extensive preprocessing pipelines were designed for each modality to ensure data quality and consistency. The performance of multiple classical machine learning models was evaluated, with logistic regression emerging as the most robust and generalizable model across both datasets.

On the questionnaire dataset, high accuracy (up to 99.2%) was achieved, demonstrating the strength of structured behavioral data in ASD detection. The ABIDE dataset, although more complex and limited in sample size, also yielded promising results, with logistic regression achieving an accuracy of 80.7%. The use of dimensionality reduction, particularly PCA, played a pivotal role in improving model performance on high-dimensional fMRI features. Together, the results underscore the potential of combining behavioral and neuroimaging data for more comprehensive ASD screening tools.

**7.2 Limitations**

Despite encouraging results, the study has several limitations:

* **Sample Size Constraints**: The ABIDE dataset, while rich in information, suffers from limited sample size, especially when filtered to a single site (e.g., NYU). This restricts the generalizability of the findings and hampers the applicability of more data-hungry models like deep learning.
* **Modality Integration**: Although both questionnaire and imaging data were analyzed, a fully integrated model combining both modalities was not implemented in this work. Such integration poses challenges in terms of feature alignment and representation.
* **Computational Resource Requirements**: Neuroimaging data processing is resource-intensive and not yet viable for low-resource or real-time deployment without optimized pipelines.
* **Simplistic Models**: While logistic regression showed strong performance, it may not capture the complex, non-linear relationships present in neurobiological data. More advanced models could uncover deeper patterns.

**7.3 Suggestions for Future Work**

**Deep Learning on ABIDE**

Future studies should explore the use of convolutional neural networks (CNNs) and recurrent neural networks (RNNs) for extracting complex spatiotemporal features from raw or minimally preprocessed fMRI data. Transfer learning and data augmentation techniques could be employed to mitigate the small dataset issue.

**Combining Questionnaire and Imaging**

A key area for future research is the development of integrated models that combine both behavioral and neuroimaging features. Multimodal learning frameworks, including ensemble models and attention-based networks, could help capture the complementary information from both data types and improve diagnostic accuracy.

**Real-Time Diagnostic Tools**

The eventual goal of this research is to contribute to the development of real-time, accessible diagnostic tools that can assist clinicians in early detection of ASD. This will require not only optimized machine learning models but also user-friendly interfaces and validation in clinical settings. Techniques like model compression, edge computing, and explainable AI (XAI) should be considered to bring these models closer to deployment.

In summary, while this study demonstrates the promise of machine learning in ASD detection using multimodal data, substantial opportunities remain for extending and enhancing this work to improve clinical outcomes and accessibility.