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Using supervised learning for the binary classification of Type 2 Diabetes

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CMP6202 - Artificial Intelligence & Machine Learning

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Abstract

Probably would benefit from an abstract. You can't really write this until the very end though, so return to it then. **The example work is from a previous year wherein this assessment was a group task. You can see that each group member developed one ML model, but you seem to be developing all of them yourself, so don't be misled by the report titles only mentioning one model.**

Introduction

Diabetes mellitus, or type 2 diabetes, accounts for 90% of the 4.4 million cases of diabetes in the UK, and it is estimated that there are 1.2 million undiagnosed cases of type 2 diabetes across the country (Diabetes UK, 2024a). The rate of type 2 diabetes per 100,000 individuals is rapidly increasing, with M. A. B. Khan et al. (2020)'s analysis projecting that by 2030, the rate will reach 7,079 per 100,000. Many people with diabetes suffer immensely reduced quality of life, with approximately 50% of patients suffering from peripheral neuropathy (Dhanapalaratnam et al., 2024), an irreversible disability which causes immense pain due to nerve damage from high blood sugar (NHS, 2022), which can occur when the patient was unaware they even had diabetes.

Therefore, it is imperative that systems are put in place to enable the swift diagnosis of diabetes, especially type 2 diabetes given its major prevalence. This can be accomplished by training machine learning models on existing clinical datasets to identify common trends in those with and without type 2 diabetes. This report will document the planning, development and evaluation of multiple machine learning models in their classification of whether individuals have type 2 diabetes based on multiple clinical factors, specifically through the stages of:

- Dataset Identification
- Data Integration
- Data Preprocessing
- Exploratory Data Analysis (EDA)
- Model Development
- Model Evaluation
- Research Conclusions

1.1 Dataset Identification

Machine learning models require large amounts of data to train upon, meaning a dataset must be identified consisting of many rows and features. This project identified two datasets which could be integrated into one larger dataset, the first of which being the well-reputed Pima Indian Diabetes Database (UCI Machine Learning, 2024), downloaded from [Kaggle](#), a platform for students and researchers alike to download and upload datasets and code for research purposes. The data originates from the National Institute of Diabetes and Digestive and Kidney Diseases, who collected this data from Pima Indian¹ women aged 21 and over in hospitals in Phoenix, Arizona, USA, and it has previously seen wide use across academic literature relating to machine learning (AlZu'bi et al. (2023), Zou et al. (2024), Joshi and Dhakal (2021), Hayashi and Yukita (2016)), where other researchers have also aimed to solve the problem of diabetes classification via supervised learning. This dataset contains 768 rows with 9 features.

This project also includes a second dataset, also from [Kaggle](#), that has been previously used in literature by Zou et al. (2024). This dataset (John DaSilva, 2024) is based on data from female patients in Frankfurt, Germany, and includes the same 9 features as the Pima Indian dataset, but includes 2000 rows. By integrating these two datasets into one larger dataset of 2768 rows, it will be possible to give the machine learning models more data to train upon.

Table 1.1 details the 9 features seen in both datasets and their descriptions.

| Feature | Description |
|--------------------------|---|
| Pregnancies | The number of pregnancies the patient has had. |
| Glucose | Plasma glucose concentration over 2 hours in an oral glucose tolerance test. |
| BloodPressure | Diastolic blood pressure in mm/Hg. |
| SkinThickness | Triceps skin fold thickness (mm) |
| Insulin | 2-hour serum insulin. |
| BMI | Body Mass Index, calculated from the patient's weight and height. |
| DiabetesPedigreeFunction | The product of a function to ascertain the probability of diabetes based on family genetics. (Akmeşe, 2022) |
| Age | The patient's age. |
| Outcome | Whether the patient is likely to develop diabetes. |

Table 1.1: The features seen in both datasets.

¹"Pima Indian" refers to a specific Native American ethnic group rather than people from India.

1.2 Supervised learning task identification

As previously mentioned, it is possible for patients to have diabetes without knowing. Therefore, it is paramount that swift and simple diagnosis methods are put in place, which can be achieved through the use of supervised learning classification models. This requires the existence of the "ground truth", which refers to the label given to data that indicates its class (c3.ai, 2024). Within these datasets, the ground truth is present as the 'Outcome' feature, which will be used as the target variable for the produced classification models.

Exploratory Data Analysis

This chapter details the EDA processes undertaken with the datasets, including key questions that will be answered by the process, as well as the splitting of the data into training and testing sets.

2.1 Data Integration

The two datasets must first be merged into one to allow for an overall analysis to be performed. This is a simple process because they both contain the same 9 features, and is detailed in Figure 2.1.



```
pima_df = pd.read_csv("Data/pima.csv")
pima_df.shape
✓ 0.0s
(768, 9)

frankfurt_df = pd.read_csv("Data/frankfurt.csv")
frankfurt_df.shape
✓ 0.0s
(2000, 9)

df = pd.concat([pima_df, frankfurt_df], axis = 0, ignore_index = True)
df.shape
✓ 0.0s
(2768, 9)
```

Figure 2.1: Integrating the two separate datasets into one larger dataset.

2.2 Question identification and assumptions

The key factors involved in the diagnosis of diabetes are critical to understand, which can be solved through EDA on these datasets. It is possible to make various assumptions based on topical background research of each of the features in the dataset, detailed in Table 2.1

| Feature | Research-based assumptions |
|---------------|---|
| Pregnancies | Approximately 13.4% of pregnant women develop a temporary condition known as Gestational Diabetes Mellitus (GDM), which typically subsides after birth (Adam et al., 2023). However, research by (Dennison et al., 2021) indicates that 33% of women who develop GDM will go on to develop permanent diabetes mellitus within 15 years. Therefore, it is assumed that pregnancies will positively correlate with the diabetes outcome. It is also expected that pregnancies should naturally positively correlate with age. |
| Glucose | Glucose concentrations are an enormous factor in the diagnosis of diabetes mellitus, being one of the main metrics used to certify the condition, where results over 200mg/dL mean an absolute diagnosis ¹ (Aftab et al., 2021). It is therefore assumed that the glucose concentrations will be one of the strongest influences of the outcome, and that it will also correlate heavily with insulin levels. |
| BloodPressure | Diastolic blood pressure (DBP) does influence the diagnosis of diabetes mellitus, as 56.2% of recently diagnosed patients presented with elevated DBP in Nelaj et al. (2023)'s limited study of 126 patients, but it is not a decisive factor by itself. Therefore, it is assumed that there will be some correlation between DBP and the outcome, but not as major as other factors like plasma glucose levels. |
| SkinThickness | It is a frequent assumption even non-academically that people who weigh more, and by consequence have higher skin thickness in certain areas such as the triceps, have a higher risk of developing conditions like type 2 diabetes. This is backed by a study by Ruiz-Alejos et al. (2020), which found strong associations between skin thickness and diabetes mellitus, as well as high blood pressure. Therefore, it is assumed that there will be a strong correlation between tricep skin thickness and the outcome, as well as an expectation of strong correlations between thickness, BMI and blood pressure. |
| Insulin | Diabetes mellitus is directly associated with insulin deficiency, and as such, it is assumed that this factor will be the strongest influence in the outcome. This is because 2-hour serum insulin tests, as used in this dataset, are frequently part of HOMA-IR ² assessments. |

¹The other main metric is insulin deficiency, meaning that the patient could have glucose levels lower than 200mg/dL and still be diagnosed if they are instead insulin deficient. (Aftab et al., 2021).

²Homeostasis Model Assessment of Insulin Resistance, used to measure insulin resistance (Tahapary et al., 2022), which can be used in both type 1 and type 2 diabetes diagnosis (Khalili et al., 2023).

| | |
|---------------------------|---|
| BMI | BMI is likely to be a significant factor in the outcome, which is backed by previous academic studies indicating that 71% of studied individuals showed increases in BMI prior to diagnosis (Donnelly et al., 2024). Additionally, BMI is used in insulin resistance measurement assessments, which are key assessments in diabetes diagnosis, meaning that it is a safe assumption that BMI will be a large factor in the outcome. |
| DiabetesPedigree-Function | People are more likely to develop diabetes mellitus if there is a family genetic history of the condition, though it is not directly caused by any one particular gene (Diabetes UK, 2024b). With the pedigree function aiming to quantify the inheritance probability, it can be assumed that it will likely correlate heavily with the outcome. |
| Age | Suastika et al. (2012) studied the effects of age as a risk factor for diabetes mellitus, finding that many natural associated factors of ageing including increases in body fat and decreases in lipid metabolism had considerable influence on the development of insulin resistance and diabetes mellitus by consequence. Therefore, it is likely that there will be a noticeable correlation between a patient's age and the outcome. |

Table 2.1: Research-based assumptions prior to any EDA.

Based on these assumptions, the questions that this EDA process aims to answer are:

| ID | Research-based assumptions |
|----|---|
| 1 | Are there any missing values or values that are not physically possible? |
| 2 | Are there any significant outliers? |
| 3 | Is the dataset evenly balanced in terms of the outcome? If not, what should be done? |
| 4 | Does the rate of diabetes positively correlate with the amount of pregnancies a woman has had? |
| 5 | Does the amount of pregnancies influence any of the other features? |
| 6 | What is the distribution of blood glucose levels in patients with and without diabetes? |
| 7 | Does BMI influence glucose levels? |
| 8 | Is diastolic blood pressure a worthwhile diagnosis method in this dataset? |
| 9 | Is the average skin thickness of those with diabetes actually higher than those without? |
| 10 | How does the relationship between insulin and glucose change between those with and without diabetes? |

Table 2.2: The questions that this EDA process aims to answer.

2.3 Splitting the dataset

It is good practice to first split the data into training and testing sets before performing exploratory data analysis to avoid conceptual overfitting, also known as data leakage.

Conceptual overfitting occurs when insights gained from the entire dataset influence model development decisions, which may eventually lead to actual overfitting. By excluding the training data from the analysis, it effectively simulates a real-world environment where the data being given to the model is not known, even to its developers.

Splitting the data is a mandatory process when developing supervised learning models, primarily for the prevention of overfitting. Overfitting is a significant challenge in machine learning, where models can perform exceptionally well on their original training data but are unable to generalize to unseen data, making them unsuitable for deployed use. The training set must consist of a large portion of the data so that the model has enough information to analyse and discover trends within, whereas the testing set is a smaller, unseen remainder of the data that the model's predictions can be evaluated against using various metrics. A key point of determination is the proportions of the dataset that should go in each set - there is no 'one-size-fits-all' percentage that can provide the best results for every possible dataset (Sivakumar et al., 2024), and factors such as the size of the dataset play a large part in this. Most commonly, splits are either 70:30 or 80:20 for training and testing sets respectively.

The integrated dataset for this project is 2,768 rows. This is considered to be a small dataset, and as such, it will be best to maximize the size of the training split, so a split of 80% training and 20% testing was used, visualized in Figure 2.2.

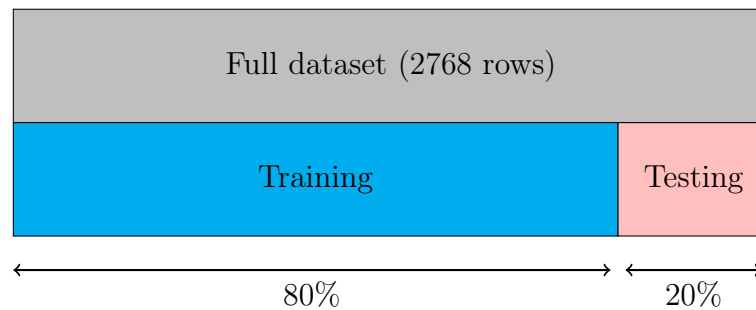


Figure 2.2: A visual representation of the train/test split.

To accomplish this, the data must first be split into X and y tables, where X consists of the eight features, and y is the target variable. After the data is split to X and y , it can be split into training and testing sets through Scikit-Learn's "train_test_split" method, as depicted in Figure 2.3

```
X = df.drop(columns = "Outcome", axis = 1)
y = df["Outcome"]
✓ 0.0s

print(X.shape)
print(y.shape) # No columns because y is now a Series consisting only of the Outcome column.
✓ 0.0s

(2768, 8)
(2768,)

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 0.2, random_state = 42)
✓ 0.0s

print(f"X_train: {X_train.shape}")
print(f"y_train: {y_train.shape}")
print(f"X_test: {X_test.shape}")
print(f"y_test: {y_test.shape}")
✓ 0.0s

X_train: (2214, 8)
y_train: (2214,)
X_test: (554, 8)
y_test: (554,)
```

Figure 2.3: Splitting the data at an 80:20 ratio.

By default, this method will first shuffle all rows in the dataset before splitting it, which introduces an element of randomness which can damage reproducibility. To combat this, the "random_state" parameter can be set to ensure that the same shuffle will occur every time.

When performing EDA, the Outcome column will be necessary to the analysis, so a deep copy³ of X_train was made with y_train (the Outcome column) being added to it, merging the two back into a full training set, shown in Figure 2.4.

```
# It's important to make a deep copy, so that none of the data is tampered with.
fullTrainSet = X_train.copy(deep = True)
fullTrainSet["Outcome"] = y_train.values
✓ 0.0s
```

Figure 2.4: Duplicating X_train and adding the Outcome column for EDA.

³A complete copy rather than a pointer to the original data

2.4 EDA process and results

In the interest of report conciseness, the full EDA process and results accompany this report as Appendix A. They were performed using the Seaborn Python library, which uses Matplotlib to produce convenient visualisations to answer each question posed in Table 2.2. The topics and issues identified during the process are solved in Section 3.3.

2.5 EDA conclusions

The extensive EDA conducted in Appendix A provided clear answers to each question posed in Table 2.2, which are detailed below in Table 2.3.

| ID | EDA-based answer |
|----|---|
| 1 | There are missing values in the dataset that were not originally presented as such; they were instead 0s in columns where this would be physically impossible. After converting the impossible 0s to missing values with NumPy, it was established that there were 18 missing Glucose values, 125 missing BloodPressure values, 800 missing SkinThickness values, 1330 missing Insulin values, and 39 missing BMI values. |
| 2 | The analysis identified significant outliers across various features using box plots. Particularly extremely outliers were noted in the SkinThickness, BMI, and Insulin columns. These outliers could affect data scaling and model performance, and will need to be transformed in data cleaning. |
| 3 | The dataset is imbalanced, with 65.5% of rows in the training set having an outcome of 0, while the remaining 35.5% had an outcome of 1. |
| 4 | The EDA did show a somewhat positive correlation between the number of pregnancies and diabetes outcomes, although pregnancies alone are not decisive in predicting diabetes. |
| 5 | Pregnancies are found to correlate with age, as expected, but do not significantly influence other features. |
| 6 | There is a clear and significant distinction in glucose levels between diabetic and non-diabetic individuals, with higher levels being mostly present in those with diabetes, making it a strong indicator. |
| 7 | A slight positive correlation is observed between BMI and glucose levels, indicating that higher BMI could be associated with higher glucose levels. |
| 8 | Blood pressure shows some correlation with diabetes outcomes but is not a strong standalone diagnostic factor. However, like pregnancies, previously mentioned academic research specifies that it is still a useful feature to keep. |
| 9 | Individuals with diabetes tend to have higher skin thickness on average, although this feature contains significant high outliers in both individuals with and without diabetes. |
| 10 | The relationship between insulin and glucose varies between diabetic and non-diabetic individuals, with diabetic individuals showing higher glucose levels as a result of lower insulin levels, which is expected of type 2 diabetes. |

Table 2.3: Answers to the questions after the completion of the EDA process.

Overall, the EDA process conducted in Appendix A has been highly beneficial for many reasons. Firstly, it identified critical data issues, such as the abundance of missing values and outliers, which are essential to address to improve model accuracy and reliability. By recognizing these issues early, the EDA ensures that data preprocessing steps can be effectively planned to mitigate their impact. Secondly, the EDA highlighted significant correlations between features and the diabetes outcome, such as the strong influence of glucose levels and BMI on diabetes diagnosis. Understanding these relationships helps in feature selection and engineering, which are crucial for building effective predictive models. Additionally, the EDA revealed class imbalances in the dataset, guiding the development of strategies to handle this imbalance during model training to prevent biased predictions.

The insights gained from the EDA therefore provide a solid foundation for informed decision-making in the experimental design and model development, ensuring that the models are trained on clean, balanced, and relevant data, ultimately enhancing their predictive performance. This is especially crucial given that the models would be used in the medical field, where incorrect predictions could have life-changing ramifications.

Experimental Design

This chapter details the planned algorithms to be leveraged against this dataset, as well as the metrics to evaluate them. Furthermore, the data cleaning and preprocessing stages will be deeply explored, as well as some potential limitations relating to their use.

3.1 Identification of chosen algorithms

Five classification algorithms will be leveraged on this dataset, these being Random Forests, Support Vector Machines, Logistic Regression, Naïve Bayes, and K-Nearest Neighbours. These were selected due to their previous use in literature based on these datasets, and also due to their high prevalence across many fields. Detailed descriptions of each algorithm, including their mathematical formulae, can be found in Appendix B - Classification Algorithms.

3.2 Identification of appropriate evaluation techniques

When evaluating classification models, it is crucial to select appropriate metrics that provide a comprehensive understanding of the model's performance. For this project, three key evaluation metrics will be used: accuracy, recall, and F1 score. By using these three metrics in combination, we can gain a comprehensive understanding of our classification models' performance. Accuracy provides an overall measure of correctness, recall ensures positive cases are not missed, and the F1 score offers a balanced view that accounts for both precision and recall. This multi-metric approach will allow for a detailed evaluation of the five models.

3.2.1 Accuracy

Accuracy is the most straightforward metric, measuring the overall correctness of the model's predictions. It is calculated as the ratio of correct predictions (both true positives [TP] and true negatives [TN]) to the total number of predictions, including false positives [FP] and negatives [FN] (Google, 2024), shown in Equation 3.1.

$$\text{Accuracy} = \frac{\text{TP} + \text{TN}}{\text{TP} + \text{TN} + \text{FP} + \text{FN}} \quad (3.1)$$

While accuracy is intuitive and easy to interpret, it can be misleading in cases of imbalanced datasets, which is a concern in this dataset that will need to be addressed in preprocessing.

3.2.2 Recall

Recall, also known as sensitivity or true positive rate, is particularly important in medical diagnosis scenarios like diabetes detection. It measures the model's ability to correctly identify all positive cases. In our context, high recall ensures that we minimize the number of diabetic patients who are incorrectly classified as non-diabetic (false negatives). This is crucial because missing a diabetes diagnosis could have serious health implications for the patient such as neuropathy, vision problems and other health complications such as heart disease or strokes (NHS, 2024).

$$\text{Recall} = \frac{\text{TP}}{\text{TP} + \text{FN}} \quad (3.2)$$

3.2.3 F1 Score

The F1 score provides a balanced measure of the model's performance by combining precision¹ and recall into a single metric, and is particularly useful with imbalanced datasets such as the one used in this project. The F1 score is calculated as the harmonic mean² of precision and recall, giving equal weight to both metrics, which is useful because in a medical context, false positives and negatives are extremely important and can bear significant consequences.

$$\text{Precision} = \frac{\text{TP}}{\text{TP} + \text{FP}} \quad (3.3)$$

¹The rate of correctly classified positives. Often has an inverse relationship with Recall (Google, 2024).

²The reciprocal of the mean of the reciprocals of the features. A reciprocal is 1 divided by the number, such as 4's reciprocal being 1/4.

$$\text{F1-Score} = 2 \times \frac{\text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}} \quad (3.4)$$

3.3 Data Cleaning and Pre-processing Transformations

3.3.1 Data encoding

Data encoding was not necessary in this dataset as all features were already numeric. However, a detailed description of typical encoding processes can be found in Appendix C.

3.3.2 Data cleaning

The EDA revealed the necessity for data cleaning in this dataset through the transformation of outliers and imputation of missing values.

Outlier handling

It was observed that all columns had outliers, with some having particularly extreme outliers that caused massive skew in the data and the visualisations produced from it. To address these, data was constrained to be within the 1st and 99th percentiles, and any data outside of these would be increased or decreased to one of these boundaries.

```
# Transforming rows under the 1st percentile or over the 99th percentile.
for column in X_train.columns:
    lowerBound = X_train[column].quantile(0.01)
    upperBound = X_train[column].quantile(0.99)
    # Where data in the column is less than the 1st percentile or more than the 99th,
    # transform it to the percentile.
    X_train[column] = np.clip(X_train[column], lowerBound, upperBound)
    # np.clip will make values lower than the lower bound into the lower bound,
    # and values over the upper bound into the upper bound.
✓ 0.0s
```

Figure 3.1: Using np.clip to transform values less than or greater than the 1st and 99th percentiles.

Missing data imputation

After handling the outliers in the data, missing data can be imputed. The selected method for this was KNN imputation, which uses the KNN algorithm to aggregate data from the k nearest data points and imputes the average of these points in place of the missing value (TrainInData, 2024). This method can be very useful as it will not impute many rows of the same number as mean or median imputation would do, and instead imputes reasonable values based on similar rows, which is especially beneficial given the high correlations between some of the missing data (such as Insulin) and data that is mostly present (such as Glucose).

```
# Creates a KNN Imputer that aggregates data from the 6 nearest neighbours to fill missing
# data across the previously identified columns.
imputer = KNNImputer(n_neighbors = 6)

# Fit the imputer on the training data and transform missing values.
X_train = imputer.fit_transform(X_train)
# This converts X_train to a NumPy array, thereby removing the column names.
# This is solved by converting it back to a DataFrame with the column names
# of the original X.
X_train = pd.DataFrame(X_train, columns = X.columns)

# The imputer is not fitted to the testing set, and instead only transforms
# missing rows within it.
X_test = imputer.transform(X_test)
# As with X_train, the column names are passed back by converting the
# NumPy array to a DataFrame with the column names of the original X.
X_test = pd.DataFrame(X_test, columns = X.columns)

print(X_train.isna().sum())
print(X_test.isna().sum())
```

✓ 0.0s

| | |
|--------------------------|---|
| Pregnancies | 0 |
| Glucose | 0 |
| BloodPressure | 0 |
| SkinThickness | 0 |
| Insulin | 0 |
| BMI | 0 |
| DiabetesPedigreeFunction | 0 |
| Age | 0 |
| dtype: int64 | |
| Pregnancies | 0 |
| Glucose | 0 |
| BloodPressure | 0 |
| SkinThickness | 0 |
| Insulin | 0 |
| BMI | 0 |
| DiabetesPedigreeFunction | 0 |
| Age | 0 |

Figure 3.2: Using KNN imputation to resolve missing data.

K was set to 6 in the imputer to increase the amount of data each imputed point is based on, but also to not average too many data points, as the data still varies despite containing many less outliers.

3.3.3 Data scaling

After imputing missing data, scaling can occur. Algorithms such as KNN and SVMs rely heavily on the distance between data points, meaning they can be heavily skewed by large distances between real numbers. Due to the high variance in the dataset as many features use different scales (Age, Insulin, SkinThickness, and BMI for example), it was decided that standardisation will be the scaling procedure. Standardisation uses the formula in Equation 3.5 to scale data so that it has a mean of 0 and a standard deviation of 1.

$$Z = \frac{X - \mu}{\sigma} \quad (3.5)$$

Z is the standardized value (also known as "z-score")

X is the original value of the feature

μ is the mean of the feature

σ is the standard deviation of the feature

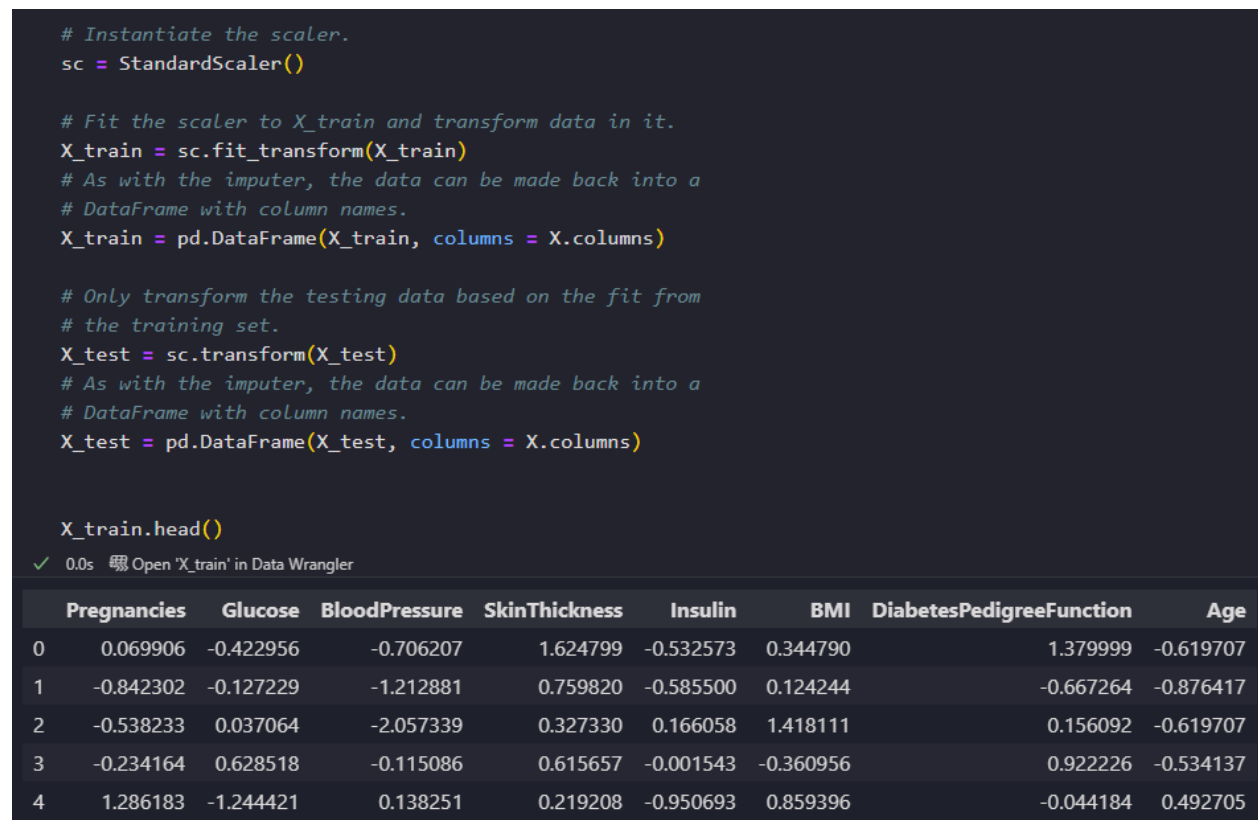


Figure 3.3: Using a StandardScaler to standardise the data.

3.3.4 Data balancing

It was also established during EDA that the dataset is imbalanced, mostly containing rows without diabetes. Therefore, the Synthetic Minority Oversampling Technique (SMOTE) was used to generate synthetic data to balance the classes. SMOTE also uses the KNN algorithm to generate data, but randomly selects nearest neighbours and generates data in-between the selected sample and the neighbour (TrainInData, 2023). This is repeated until the classes are balanced.

```
# Instantiate SMOTE, to be applied on the training set.
smote = SMOTE()

# View the original class imbalance.
print(y_train.value_counts())

# Fit SMOTE to the training set, and also generate data to balance it.
X_train, y_train = smote.fit_resample(X_train, y_train)

# We can now see that the classes are balanced.
y_train.value_counts()
✓ 0.0s
```

Outcome

| | | |
|---|------|---------------------|
| 0 | 1449 | |
| 1 | 765 | Pre-SMOTE imbalance |

Name: count, dtype: int64

Outcome

| | | |
|---|------|------------|
| 1 | 1449 | |
| 0 | 1449 | Post-SMOTE |

Name: count, dtype: int64

Figure 3.4: Using SMOTE to balance the training set.

SMOTE is not used to balance the testing set, as the testing set should be exclusively real data so that an accurate representation of the model's ability to predict real data can be gathered (Ozbun, 2021).

3.4 Limitations and Options

A key limitation in this design comes from the datasets themselves; they contain colossal amounts of missing data, with almost half of the Insulin values missing. With Insulin being such an integral part of type 2 diabetes diagnosis, the issue of having so much missing data cannot be overlooked. While it was addressed using KNN imputation, the synthetic data generated by this approach could possibly be of poor quality.

Furthermore, SMOTE was used to balance the classes. While SMOTE is a useful tool, it can introduce noise to a dataset. Additionally, SMOTE was performed after the KNN imputation, meaning that a substantial amount of the dataset was then synthetic data.

In future projects, it would be best to use more organised and clean datasets, where such substantial preprocessing measures would not be necessary. Furthermore, the features in the dataset are all numerical. While this is good for the development of machine learning models, it did not allow for the demonstration of encoding techniques, which were instead described in Appendix C.

Model Development

This chapter details the training and evaluation processes of the original produced models before any iterative improvements such as hyperparameter tuning.

4.1 Predictive modelling process

4.2 Results on seen data

Evaluation and further improvements

This chapter details the extensive evaluation of each model, as well as iterative improvements that were made to enhance their performance.

Conclusion

6.1 Summary of results

6.2 Reflection on Individual Learning

Over the course of this module and others, I have enhanced my skills with a wide variety of tech stacks to a degree I previously thought impossible. I have thoroughly enjoyed expanding my Python skills for data science and machine learning with the use of industry standard packages like Pandas and NumPy. This project in particular has heavily challenged me, requiring extensive research into many academic papers and web resources to further my knowledge of the medical field and machine learning trends.

I have always enjoyed writing code from as young as 11 years old. I originally began by creating games on the Roblox platform using their specialised fork of the Lua language, and expanded beyond that into Python as I furthered my knowledge of computing and IT. Also, I have a [personal GitHub account](#), which I use for version control and iterative saving of my University work, including for this module in the [CMP6202 repository](#), where every step taken in the production of this report is documented across many commits.

Irrespective of my personal appreciation and enjoyment in writing code, the particular topic of this project was one that is close to my heart - members of my family suffer from type 2 diabetes and other health complications that arose from it, including neuropathy (intense pain and/or weakness), retinopathy (loss of vision) and even heart attacks and strokes. Therefore, I am intensely interested in the applications of my passions in AI and Machine Learning to make a positive difference for others, and I believe that the knowledge I have gained through this project will be a strong asset in doing so.

Appendix A - EDA Process and Results

Problems identified through the EDA conducted in this Appendix were resolved in Section 3.3.

A.1 Identification of missing or impossible values

An initial glance at the dataset would make it appear as though as there are not any missing values in the dataset, as shown in Figure A.1.

```
fullTrainSet.isna().sum()
✓ 0.0s
Pregnancies      0
Glucose           0
BloodPressure     0
SkinThickness     0
Insulin           0
BMI               0
DiabetesPedigreeFunction  0
Age              0
Outcome          0
```

Figure A.1: An initial count of missing values before any further analysis.

This would be very good - if it were true. Instead of missing values, this dataset contains impossible values in five columns, highlighted in red in Figure A.2.¹

```
fullTrainSet.describe()
```

| | Pregnancies | Glucose | BloodPressure | SkinThickness | Insulin | BMI | DiabetesPedigreeFunction | Age | Outcome |
|-------|-------------|-------------|---------------|---------------|-------------|-------------|--------------------------|-------------|-------------|
| count | 2214.000000 | 2214.000000 | 2214.000000 | 2214.000000 | 2214.000000 | 2214.000000 | 2214.000000 | 2214.000000 | 2214.000000 |
| mean | 3.780036 | 121.210479 | 69.093496 | 20.599819 | 79.662150 | 32.058988 | 0.473864 | 33.284101 | 0.345528 |
| std | 3.321450 | 31.967589 | 19.319345 | 16.041849 | 111.192963 | 8.091686 | 0.328880 | 11.826703 | 0.475648 |
| min | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.078000 | 21.000000 | 0.000000 |
| 25% | 1.000000 | 99.000000 | 64.000000 | 0.000000 | 0.000000 | 27.300000 | 0.244000 | 24.000000 | 0.000000 |
| 50% | 3.000000 | 117.000000 | 72.000000 | 23.000000 | 40.000000 | 32.050000 | 0.375500 | 29.000000 | 0.000000 |
| 75% | 6.000000 | 141.000000 | 80.000000 | 32.000000 | 129.750000 | 36.600000 | 0.629000 | 41.000000 | 1.000000 |
| max | 17.000000 | 199.000000 | 122.000000 | 110.000000 | 846.000000 | 80.600000 | 2.420000 | 81.000000 | 1.000000 |

Figure A.2: The overall dataset description. Physically impossible values are in red.

¹The mean of the outcome is highlighted in blue, as the fact that it is under 0.5 indicates that there are more cases of outcome 0 (no diabetes) than 1 (diabetes). This will be further analysed in Section A.2.

It is not possible for a living person to have a 0 in any of the five highlighted columns, and these datasets do not contain information of the deceased. Therefore, it can be deduced that these values are erroneous, and should be treated as though they are missing. It is theorised by some in Kaggle discussions of these datasets that the zeroes in the Insulin column actually meant "imperceptible levels", which would have been useful data. However, a further review of literature around the datasets, especially Hayashi and Yukita (2016)'s paper, led to the discovery that these zeroes truly are missing values that were missing due to experimental invalidity at the time of their collection.

```
X_train[["Glucose","Insulin","BloodPressure","SkinThickness","BMI"]] = X_train[["Glucose","Insulin","BloodPressure","SkinThickness","BMI"]].replace(0, np.nan)
# These changes also need to be made to the full training set.
fullTrainSet[["Glucose","Insulin","BloodPressure","SkinThickness","BMI"]] = fullTrainSet[["Glucose","Insulin","BloodPressure","SkinThickness","BMI"]].replace(0, np.nan)
✓ 0.0s
```

Figure A.3: Converting the impossible values to NaNs which are recognised by Pandas.

This conversion is applied to the actual `X_train` set for model training, as well as to the `fullTrainSet` copy made in Figure 2.4. Now that there are officially recognised missing values, they can be visualised using the Missingno package, which can produce a matrix of missing values by column, seen in Figure A.4.

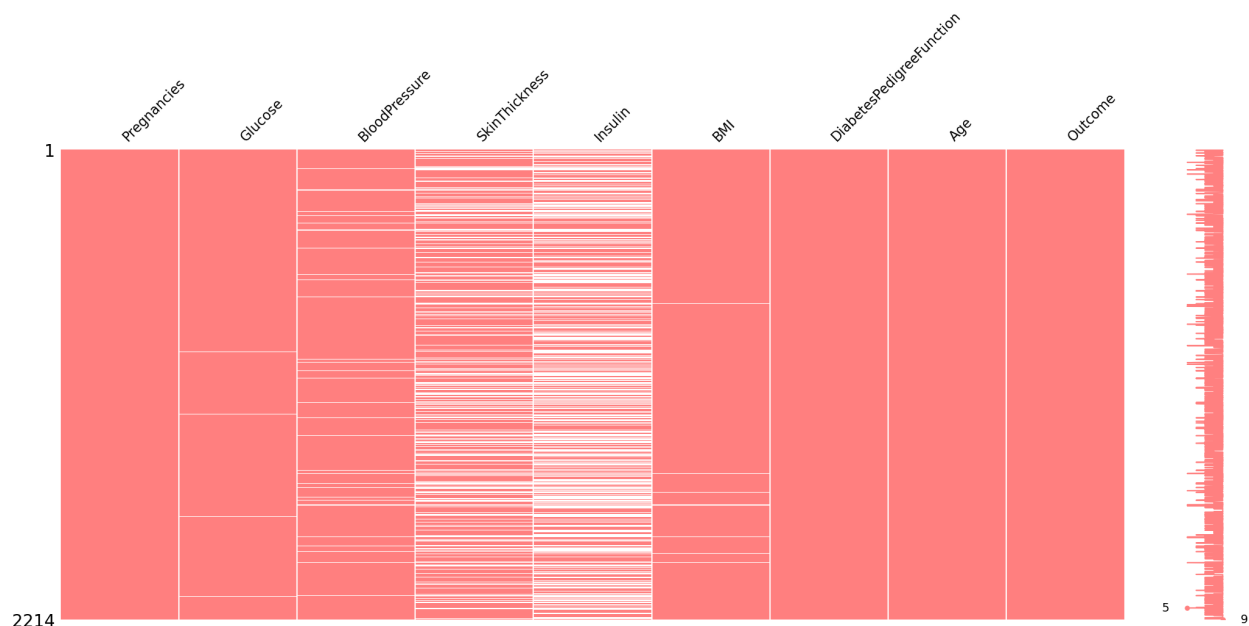


Figure A.4: A Missingno matrix of the missing data per column.

This matrix shows that the Insulin and SkinThickness columns contain considerable amounts of missing data alongside many missing rows of BloodPressure, and some missing rows of BMI and Glucose, which will need to be fixed before any model can be trained. This is accomplished through imputation in Section 3.3.

A.2 Target univariate analysis

Binary classification models can develop bias if they do not have enough data of both classes to accurately predict what combinations of values should determine each class. Therefore, it is essential to view the balance between classes as in Figure A.6.

```
# We're only performing EDA on the training set. Y_train consists of the training set's Outcome column.
print(y_train.value_counts())
sns.countplot(X_train, x = y_train, color = "cyan")
```

| Outcome | count |
|---------|-------|
| 0 | 1449 |
| 1 | 765 |

Figure A.5: The code to produce Figure A.6.

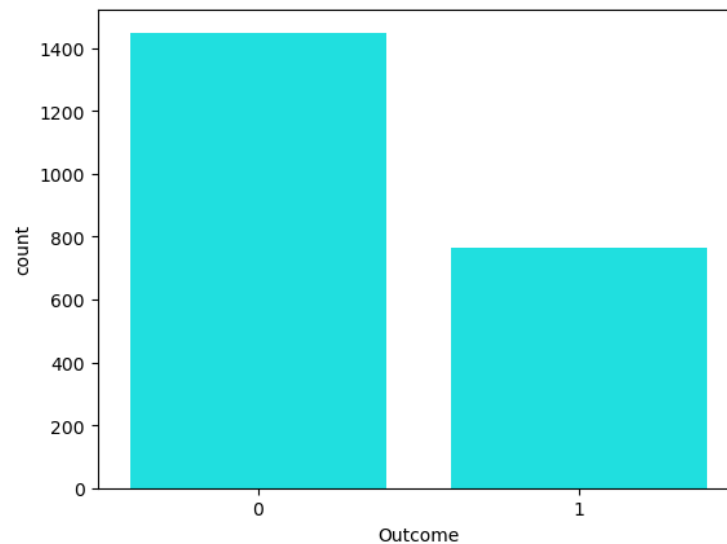


Figure A.6: The class distribution of the training set (0: 1449, 1: 765).

The dataset is imbalanced, favouring an outcome of 0. The exact percentages of each class can be calculated as seen below.

$$\text{Outcome 0} = \frac{1449}{2214} = 0.655 \times 100\% = 65.5\% \quad (\text{A.1})$$

$$\text{Outcome 1} = \frac{765}{2214} = 0.345 \times 100\% = 34.5\% \quad (\text{A.2})$$

The training set is 80% of the data, hence why it is 2214 rows rather than 2768. From these calculations, it can be determined that there is an imbalance present in the training set, and we can also assume there will be a similar imbalance in the unseen testing set, as the `train_test_split` method aims to maintain the original class balances where possible. The class imbalance will be resolved in Section 3.3.

A.3 Multivariate analysis

To compare each variable to each other and the outcome, the full training set previously created in Figure 2.4 was used.

A.3.1 Data distributions by Outcome

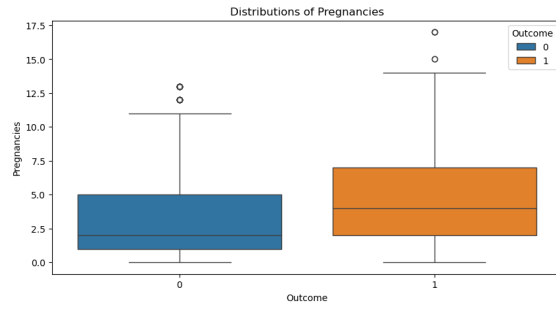
It is important to identify significant outliers in the dataset so that models do not become skewed by the inflated variance, standard deviation and mean that they cause. Outliers that are very high in comparison to the primary distribution of the data will cause the standard deviation and mean to increase, whereas low outliers will make them decrease. Their identification is important not only for data analysis, but also for model development, as outliers can cause some algorithms to perform poorly or overfit, most notably distance-based algorithms such as K-Nearest Neighbours (KNN) and Support Vector Machines (SVM), which is further discussed in Section 3.1.

The simplest way to visualise outliers in the dataset is through box plots, which present the spread and skewness of numerical data in a simple visual format by showing the inter-quartile range (IQR), with rows outside of these being outliers. The boxplots of each column in the training set are shown below in Figure A.8. Each of the plots contains two boxplots, where one is for individuals without diabetes, and one is for those with diabetes.

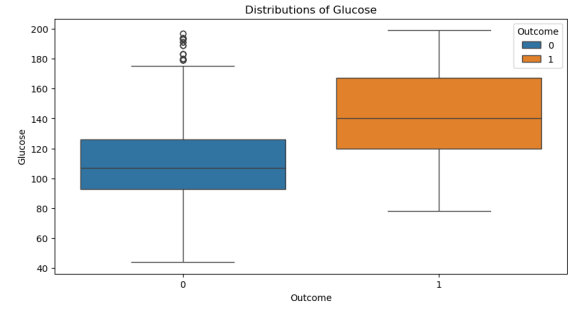
In the figure, it can be seen that all columns contain some outliers. However, most of these outliers are still relevant statistical data that would be possible, such as the outliers in Age being elderly people. Some of these outliers are less feasible, however; most notably the extreme high outliers in SkinThickness, BMI, and Insulin. Leaving these outliers in would affect the scaling of the data, and because it is generally ill-advised to remove rows of data especially with smaller datasets, they could instead be transformed to the upper bound to give a more even distribution. This will be accomplished in Section 3.3.

```
# Iterates through each column, producing a boxplot titled "Distributions of [column name]"
# Only iterates through X_train so that it doesn't produce one for the Outcome column itself.
for col in X_train:
    plt.figure(figsize = (10, 5))
    sns.boxplot(data = fullTrainSet, y = col, x = "Outcome", hue = "Outcome")
    plt.title(f'Distributions of {col}')
    plt.show()
✓ 0.7s
```

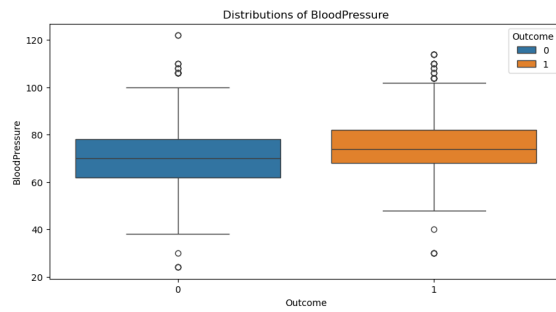
Figure A.7: The code used to produce Figure A.8.



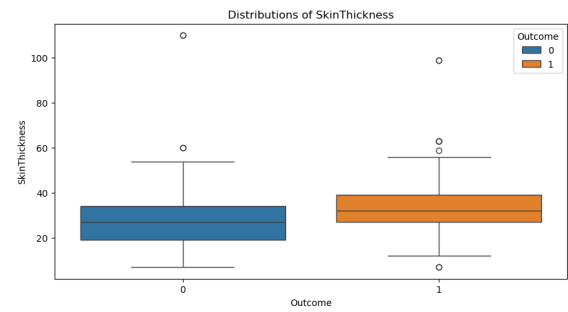
(a) Pregnancies



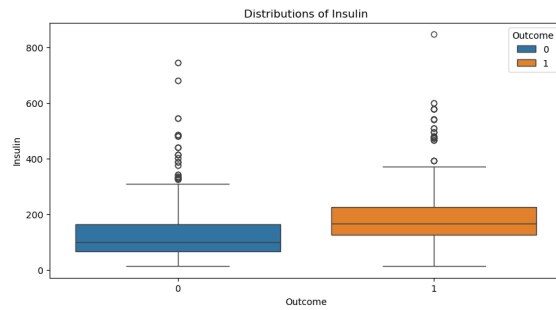
(b) Glucose



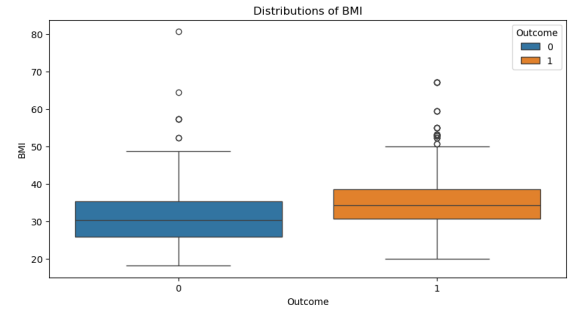
(c) BloodPressure



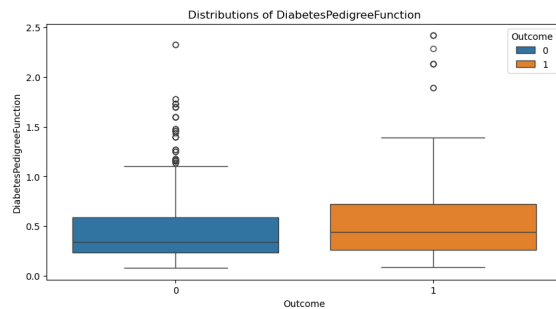
(d) SkinThickness



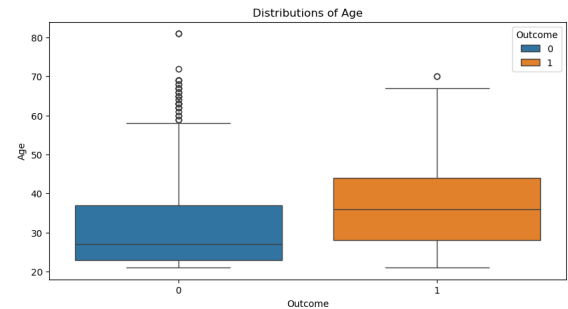
(e) Insulin



(f) BMI



(g) DiabetesPedigreeFunction



(h) Age

Figure A.8: Boxplots of all features by the outcome (Blue: No diabetes, Orange: Diabetes).

Pregnancies

It was assumed in Table 2.1 that the amount of pregnancies a woman has had may bear a strong correlation on whether they develop type 2 diabetes. This box plot does support the original assumption that the amount of pregnancies can positively correlate with the diabetes outcome, as the median and upper quartiles of the distributions of those with diabetes are higher than those without, though it also confirms that pregnancies are not a decisive factor on their own, as some patients had many pregnancies without having diabetes.

Glucose

This feature clearly shows a direct and strong correlation with the outcome; individuals with diabetes have much higher glucose values, with a clear upward shift in both the median and interquartile range (IQR). The lower whisker of the boxplots begins much higher with patients with diabetes, which implies that low glucose is a strong indicator that a patient does not have diabetes.

BloodPressure

Blood pressure values are fairly similar between the two groups, though individuals with diabetes show a slightly higher median. Both groups have similar variability and range, indicating that blood pressure is not as strong a distinguishing factor. However, this slight correlation is still useful information, so this column should be kept.

SkinThickness

This column contains significant outliers that will cause issues with data scaling. Aside from these outliers, it does appear that skin thickness positively correlates with the outcome.

Insulin

This column contains many outliers, with some of these being extremely high. Aside from these, the main IQRs of the plots appear to indicate that higher insulin values are indicative of diabetes, showing a positive correlation.

BMI

Individuals with diabetes tend to have higher BMI values on average. The median BMI for the diabetic group is higher, with a slightly larger IQR, showing that BMI is an important factor in distinguishing diabetes outcomes.

DiabetesPedigreeFunction

The diabetes pedigree function has a slightly higher median for individuals with diabetes, but the difference is not substantial. Both groups share significant overlap, suggesting that this feature alone may not strongly differentiate between outcomes, which differs from the original assumption.

Age

Individuals with diabetes tend to be older on average, as indicated by a higher median age for the diabetic group, and the fact that the IQR for the diabetic group is shifted upwards. However, many outliers without diabetes exist.

A.3.2 Pair plot

To view every column in the dataset plotted against each other, a pair plot can be created using Seaborn, pictured in Figure A.10.

```
# Produces a pair plot of all columns, colouring each point by the outcome.
sns.pairplot(fullTrainSet, hue = "Outcome")
```

✓ 12.7s

Figure A.9: The code to produce Figure A.10.

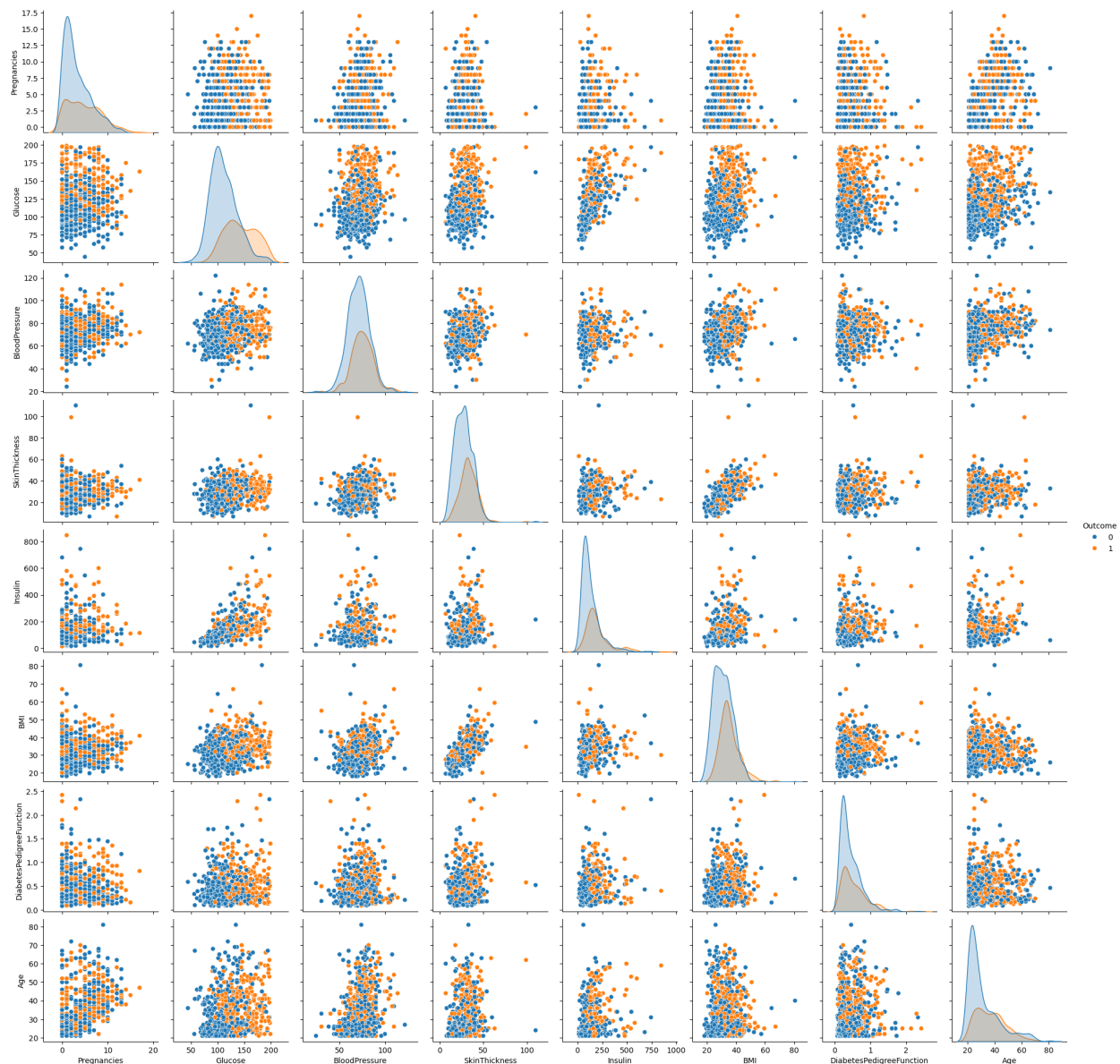


Figure A.10: The pair plot of the full training set (Blue: No diabetes, Orange: Diabetes).

There are multiple observations on the relationships between features to be made from this pair plot, such as:

- Glucose, BMI and Outcome
 - Glucose and BMI appear to be the two strongest predictors, with there being more cases of diabetes as each of these features increase, shown by the higher clustering of points.
 - Glucose also appears to slightly increase as BMI increases, suggesting a slight positive correlation between the two features.
- Pregnancies and Age
 - As expected, pregnancies do typically increase with age.
- Pregnancies and Outcome
 - There is no clear separation in the outcome based on pregnancies alone, suggesting it may not be a decisive factor.
- Age
 - While a person's age appears to not be directly relevant to them having diabetes, it instead appears that older individuals instead typically have higher glucose levels and BMI, which are decisive factors.
- Insulin
 - Appears to be a good predictor, but not quite as much as glucose. Most rows where Insulin is between 400 and 600 are diabetic.
- SkinThickness and BMI
 - As expected, these two features are closely interlinked as seen by the mostly tight clustering between them in their associated plot.

Relation between Insulin and Glucose by Outcome

A particular relation of note given the subject matter is the relation between insulin and glucose dependent on whether the individual has diabetes or not. Type 2 diabetes is characterised by insulin resistance and underproduction, meaning that lower insulin values are expected as glucose rises. Figure A.12 details this relation in patients with and without diabetes.

```
# Scatter plot using Linear Regression to produce a line of best fit.  
# "scatter_kws" refers to keywords for the scatter points. "s: 5" makes the points smaller.  
sns.lmplot(x = "Glucose", y = "Insulin", data = fullTrainSet, hue = "Outcome", scatter_kws={"s": 8})  
✓ 0.2s
```

Figure A.11: The code to produce Figure A.12.

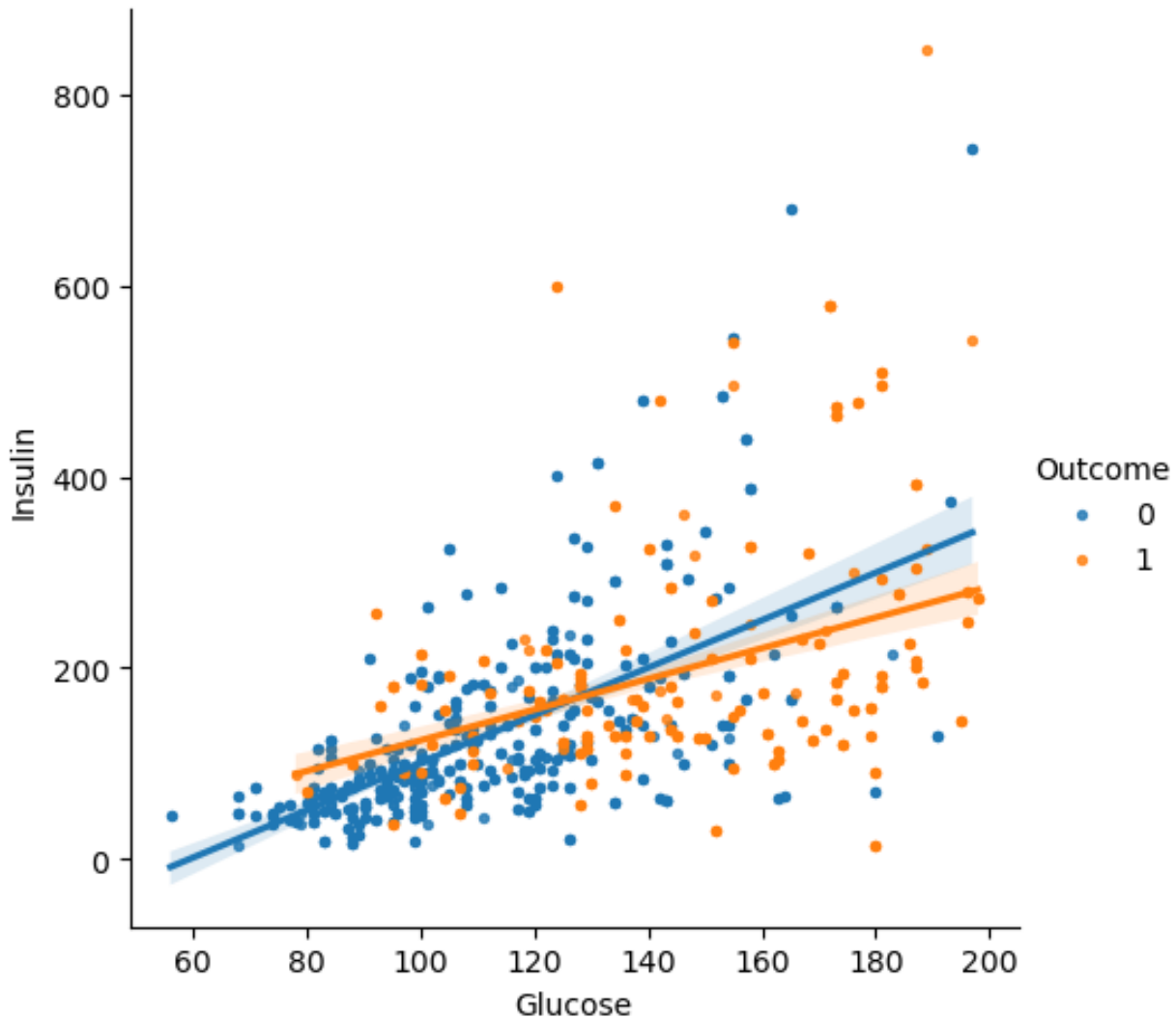


Figure A.12: A scatter plot with lines of best fit to show the trends in Insulin and Glucose.

The expectation is matched, as glucose rises more than insulin in patients with diabetes, and slower than insulin in patients without diabetes.

A.3.3 Correlation Matrix

An alternative and simpler way to visualise the correlations between features in a dataset is through a correlation matrix as pictured in Figure A.14. The matrix uses the full training set created earlier to show the correlations between the dataset's features in an annotated heatmap format, quantifying each correlation as a number. Correlation matrices only work with numerical features, though all features are numeric in this dataset which enables the matrix to show all features.

```
sns.heatmap(fullTrainSet.corr(), annot = True)
```

✓ 0.2s

Figure A.13: The code to produce Figure A.14.

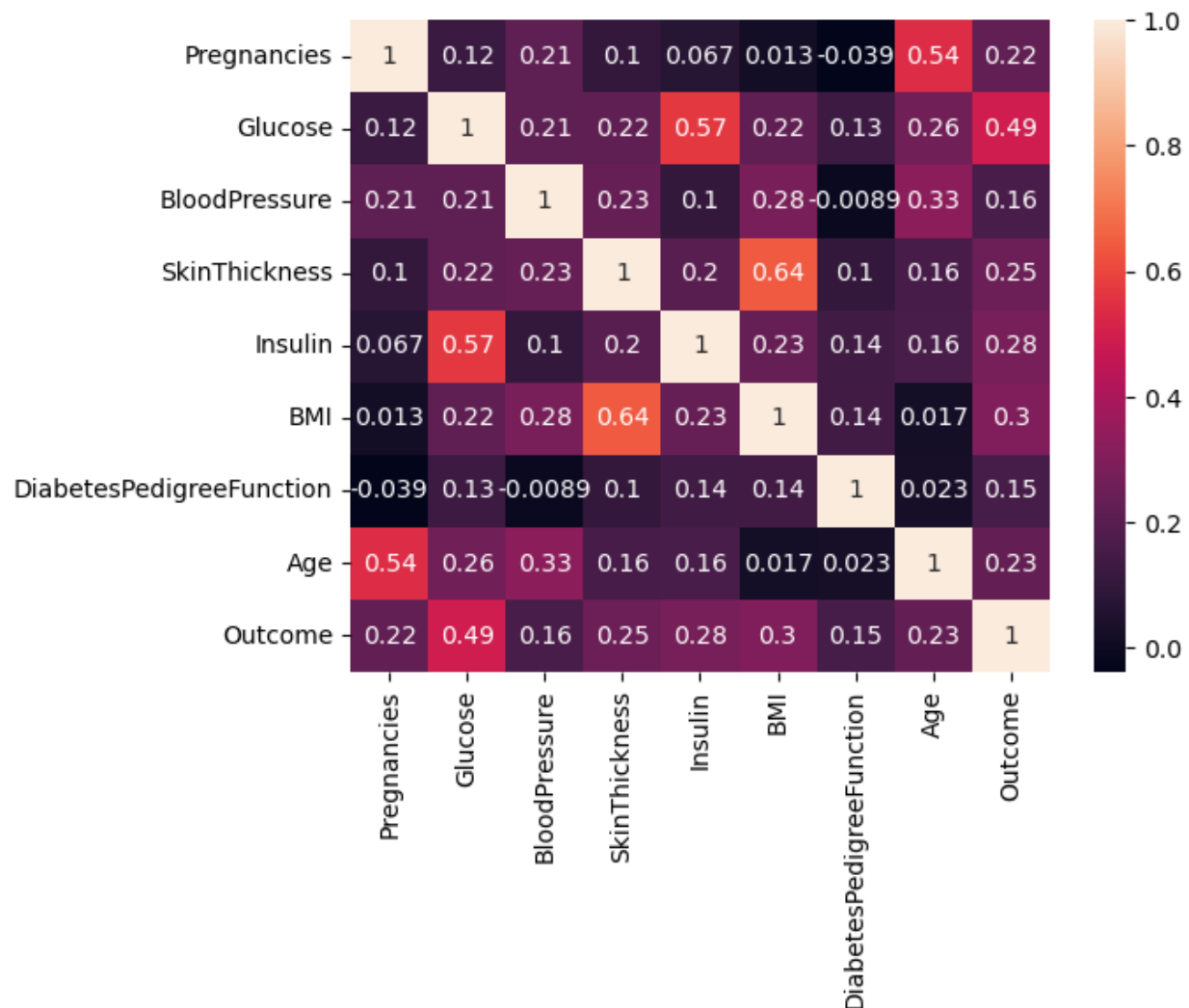


Figure A.14: The correlation matrix of the full training set.

The correlation matrix reflects many of the observations noted in the pair plot and data distributions. It shows the relationships between all features, including many expected relations like those of Glucose and Outcome, Pregnancies and Age, and BMI and SkinThickness. However, the matrix also reveals insights that subvert the previous assumptions about the dataset, such as the pedigree function actually having the weakest correlation with the outcome. This can be explained through other insights in the data as well as academic research.

Mambiya et al. (2019) argue that diabetes mellitus can be caused by genetic predisposition, which is represented by the pedigree function in this dataset, though lifestyle factors such as weight gain and poor dietary variance can be a more significant factor in the cause of the disease in both those with and without genetic predispositions. Their findings are also echoed within this dataset, with high BMIs representing overweightness/obesity and high Glucose values representing high sugar intake, which are the two most significant factors in the outcome according to the correlation matrix.

Appendix B - Classification Algorithms

B.1 Random Forest

Random forests are ensemble models, meaning that they leverage multiple other models and average their findings to give a single result. The other models used by a random forest are decision trees, which are flowchart-like structures where data is split at each node of the tree based on feature values to arrive at a classification. Random forests create many decision trees based on randomly sampling the dataset, and these trees then classify rows based on what they learn. Then, the predictions for each row by all decision trees are aggregated, and the prediction reached by the most trees is used. The amount of decision trees used is a parameter that can be set, and the computational requirements of the algorithm also increase alongside this amount.

Random forests are reputed as one of the best classification algorithms, and are used frequently in many fields including diabetes diagnosis as seen in works from Chang et al. (2023) and AlZu'bi et al. (2023), demonstrating their suitability for this classification task.

B.2 Support Vector Machine

Support vector machines aim to find the optimal hyperplane² which separates classes with the highest possible margin, and are commonly used in classification problems (IBM, 2023). Data points on either side of the margin are known as support vectors. Figure B.15 shows how a perfect SVM would look in a two-dimensional dataset for demonstrative purposes.

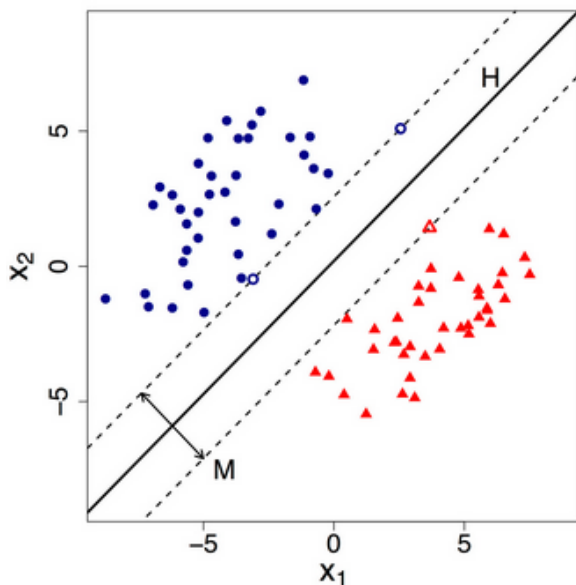


Figure B.15: An optimal SVM that demonstrates the algorithm's key features. Rows on the dotted line are the support vectors, the solid line is the hyperplane, and the space between the hyperplane and support vectors is the margin. (Kirchner and Signorino, 2018)

²A decision boundary that separates the classes. In a two-dimensional graph, this would be a line of best fit, but in a multidimensional dataset, it would be a hyperplane.

Kirchner and Signorino (2018) state that SVMs are computationally intensive, requiring lots of memory and processing power to run optimally. Additionally, Atla et al. (2011) mention that SVMs are particularly sensitive to noise in datasets, meaning their quality can be poor when there are many outliers. Despite these drawbacks, however, they can still be useful in diabetes classification as observed in the work of Zou et al. (2024).

B.3 Logistic Regression

Logistic regression computes a weighted sum of all input features, where the appropriate weights are learned by the algorithm as it trains. A sigmoid function, shown in Equation B.3, is then used to transform the sum to a value between 0 and 1, which is then used to classify the row as 0 if it is below 0.5, or classify it as 1 if it is above 0.5.

$$f(x) = \frac{1}{1 + e^{-x}} \quad (\text{B.3})$$

Logistic regression is a very common algorithm in binary classification tasks, as it is simple to implement and interpret, and can perform well even with limited amounts of training data (Kavya et al., 2024). It has also been widely used in previous analyses of the Pima Indian dataset. (AlZu'bi et al. (2023), Joshi and Dhakal (2021), Zou et al. (2024))

B.4 Naïve Bayes

Naïve Bayes is an example of a probabilistic classification algorithm (IBM, 2021), as it is based on Bayes' theorem, which calculates the probability of an event given that another event has occurred, shown in Equation B.4. In binary classification, it is the probability of the target given the other features. Naïve Bayes gets its name from its naïve assumption that features are all independent of each other.

$$P(A|B) = \frac{P(B|A) \cdot P(A)}{P(B)} \quad (\text{B.4})$$

This theorem calculates that the probability of an event occurring is equal to the probability of the event given prior knowledge multiplied by the prior probability of the event. This can be contextualised to this specific dataset, shown in Equation B.5.

$$P(\text{Diabetes}|\text{Other features}) = \frac{P(\text{Other features}|\text{Diabetes}) \cdot P(\text{Diabetes})}{P(\text{Other features})} \quad (\text{B.5})$$

Gaussian Naïve Bayes is used in this project, as it is best suited to continuous data as seen in this dataset's features. Interestingly, Naïve Bayes typically has lower accuracy than other models such as Random Forests (A. Khan et al., 2023), though it has been used in previous diabetes classification tasks (Aftab et al., 2021; Chang et al., 2023; Zou et al., 2024).

B.5 K-Nearest Neighbours (KNN)

The k-Nearest Neighbours (kNN) algorithm is a fundamental machine learning classification method that operates by identifying the k closest training examples to a data point across all features and assigns the most common class among these neighbours as the prediction. K is a parameter that can be set within the algorithm, and has a heavy influence over its accuracy. KNN doesn't make any assumptions about the distribution of the data, making it useful for complex, real-world scenarios such as healthcare (Thomas and Rajabi, 2021), and has also been used on the Pima Indian and Frankfurt datasets to high success (AlZu'bi et al., 2023; Zou et al., 2024).

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