ICS5510 Assignment

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***Abstract*—TODO: abstract here**
***Index Terms*—TODO: keywords**

I. Introduction

This exercise explores the well-known COMPAS dataset using several machine learning techniques, where we will also examine the ethical implications of predictive risk assessment models. In this study, we will apply techniques discussed in ICS5110, such as imputation and encoding, to assist in data preparation. Additionally, we trained a neural network, logistic regressor, and k-nearest neighbours model on the dataset to predict whether a person is likely to recidivate within two years.

The selected dataset is particularly interesting because, in addition to the `two_year_recid` label—which indicates whether an individual has reoffended within two years of an initial charge, it also includes the COMPAS `decile_score`, a risk rating predicting the likelihood of recidivism. This allows us to compare our findings with the COMPAS system and analyze the nuances of applying different techniques.

A. History of the COMPAS tool

The COMPAS (Correctional Offender Management Profiling for Alternative Sanctions) dataset and tool have a controversial history rooted in its use for assessing the likelihood of recidivism among criminal defendants. Developed by Northpointe, COMPAS gained widespread adoption in the U.S. judicial system for pretrial risk assessments and sentencing decisions. This tool is helpful in various stages of the criminal justice process, including bail, sentencing, and parole decisions.

However, in 2016, an investigative report by ProPublica revealed significant racial biases in the tool's predictions. The report found that COMPAS disproportionately labelled Black defendants as high risk for reoffending while underestimating the risk for white defendants, even when both groups had similar criminal histories. This revelation sparked a broader debate about using algorithmic tools in criminal justice and their transparency and fairness.

The COMPAS tool has not been directly the subject of lawsuits, but its use in judicial decisions has led to legal challenges. For instance, in State v. Loomis (2016), the Wisconsin Supreme Court upheld using COMPAS in sentencing. However, judges must be informed about its limitations, particularly its proprietary nature and potential biases. The case highlighted the broader tension between the utility of predictive algorithms and their application's need for accountability and fairness.

B. The COMPAS dataset

The dataset that originates from the COMPAS tool is widely used in criminology and machine learning studies.

The dataset contains attributes such as demographic information, prior charges, juvenile records, and risk scores, including the widely analysed decile score, which categorises individuals into ten different risk groups.

The decile score is a critical feature, assigning a numerical value to an individual's likelihood of reoffending. Other important features include the number of prior offences `priors_count` and the type of offence `c_charge_degree`, provide context for these predictions. At the same time, the label `two_year_recid` indicates whether an individual reoffended within two years of their COMPAS assessment.

While the dataset has been instrumental in research aimed at understanding and improving risk prediction models, it has also been the subject of extensive scrutiny due to its implications for fairness and equity in the justice system. A couple of thoughts resulting from this scrutiny include:

- Multiple studies, including the influential ProPublica investigation in 2016, have highlighted racial disparities in the COMPAS predictions. African-American defendants were found to be nearly twice as likely as Caucasian defendants to be labelled as high-risk for recidivism but not reoffend. Conversely, Caucasian defendants were more likely to be classified as low-risk but later reoffend, raising concerns about systemic bias embedded in the algorithm, which could exacerbate existing inequalities in the justice system.
- The COMPAS tool operates as a proprietary black-box model, meaning its internal workings and feature weights are not disclosed to the public or even to the defendants it evaluates. This lack of transparency prevents meaningful scrutiny and accountability, leaving users unable to fully understand or challenge the tool's predictions.
- The COMPAS algorithm relies on historical criminal justice data, which may reflect social and systemic biases. For example, law enforcement practices that can result in sentencing disparities can all influence the patterns observed in the data. Using such data as input, the COMPAS tool risks perpetuating these biases into an electronic tool.
- Some features in the COMPAS dataset, such as age and criminal history, are static and cannot change over time, as this data is based on the date of the COMPAS assessment. We can argue that these features in risk predictions

without considering the period after the COMPAS assessment undermines the potential for individuals to reform and leads to insensible punitive outcomes.
- The ethical implications of using predictive algorithms in high-stakes decisions, such as sentencing and parole, constitute a significant area of concern. The potential for false positives can lead to unjustly harsher treatment, while false negatives can impact public safety.
- The dataset available for research purposes is a reduced version of the original COMPAS data, with several features anonymised or removed. Missing important data introduces limitations for academic studies aiming to replicate or validate the findings from real-world COMPAS applications.

The criticism of the COMPAS tool emphasises the challenges of deploying machine learning systems in sensitive domains like justice. These challenges are not unique to COMPAS but highlight broader issues in applying algorithmic decision-making tools in socially important contexts. They highlight the need for transparency, fairness-aware modelling techniques, and careful ethical evaluations when designing and implementing such tools.

C. Objectives of this work

The objective of this project is to assess the accuracy and fairness of predictive models compared to the COMPAS system. We will in this investigation.

- Analyse the COMPAS dataset and its predictions.
- Prepare the dataset for machine learning through cleaning, transformation, and feature engineering.
- Train and evaluate a neural network, a logistic regressor and use a k-nearest neighbour to obtain our recidivism risk.
- Investigate potential biases and ethical implications in predictions.

II. BACKGROUND

In this section, we will review the key techniques employed in this study, providing an explanation of their principles to establish a solid foundation for the work presented.

A. Machine learning technique - Neural network

Neural networks are machine learning models inspired by biological neural networks. They comprise layers of interconnected nodes (neurons) that transform input data into meaningful outputs through weights and activation functions. Neural networks are widely used for classification, regression, and generative modelling tasks. This section will look at the important aspects related to neural networks.

1) The perceptron: A perceptron is a basic architecture that consists of a layer of input nodes that is fully connected with an output node and, therefore, does not have any hidden nodes. Perceptrons can only represent linearly separable functions and are used only for binary classification.

The building blocks of a perceptron are the following:

- The perceptron takes several input features that each represent an aspect of the input data.
- Each input feature differently influences the output through a weight parameter. Weights are optimized during the training process.
- A bias is utilized to make input-independent adjustments to the weighted inputs. Bias values are also optimized during training.
- The weighted inputs are summed together, including the bias; this can be expressed as:

$$z = \sum_{i=1}^{n} w_i x_i + b \tag{1}$$

- The weighted sum is passed through a Heaviside step activation function that maps the weighted sum to a binary output, such that:

$$f(z) = \begin{cases} 0 & \text{if } z < \theta \\ 1 & \text{if } z \geq \theta \end{cases}$$

- The output of the perceptron that results from the activation function can then be used to classify the inputs.

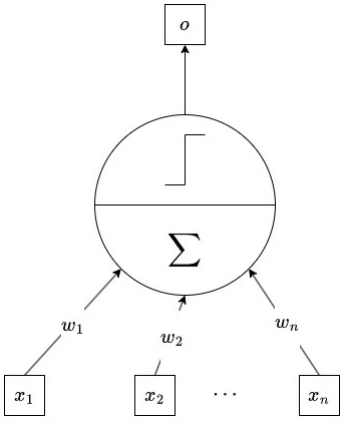


Fig. 1: The perceptron

A simple learning algorithm fits a perceptron to any linearly separable set.

2) Multilayer perceptron: The neural network architecture we use in this work are multilayer perceptrons. A multilayer perceptron is made up of fully connected layers. It contains an input layer, a number of hidden layers, and an output layer. This structure allows us to model more complex relationships when compared to the simpler perceptron.

The building blocks of a perceptron are the following:

- Each input feature is connected directly to an input neuron to forward the features into the network.
- One or more hidden layers, each having a designated number of nodes, follow. These layers transform the feature information at each level.

- Finally, an output layer consisting of one node (if the task is regression or binary classification) or more nodes (if the task is multi-class classification) gives us the result of the network.

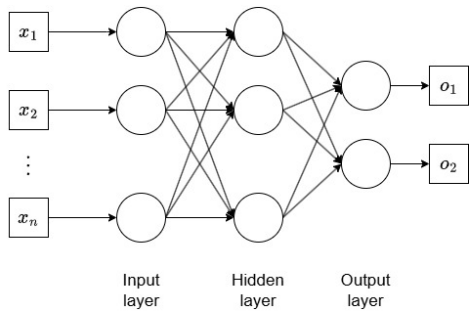


Fig. 2: A multilayer perceptron with a single hidden layer

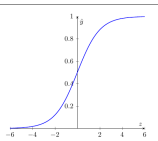
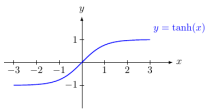
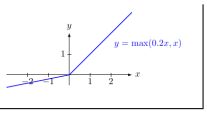
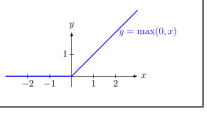
Function	Equation	Diagram
Sigmoid	$\sigma(x) = \frac{1}{1+e^{-x}}$	
Tanh	$tanh(x)$	
Leaky Relu	$max(0.2x, x)$	
Relu	$max(0, x)$	

TABLE I: Activation Functions

I. Forward propagation involves feeding feature information to the input layer, passing it through all hidden layers, and finally to the output layer to generate a predicted output. A linear transformation followed by a non-linear activation generates the output for every node at each layer. Forward propagation is comprised of the following steps:

a) For each neuron in layer j, the weighted sum of its inputs is calculated as:

$$z_j = \sum_{i=1}^{n_j} w_{ij}^{(j)} x_i^{(j-1)} + b_j \tag{2}$$

Where:
$x_i^{(j-1)}$ Input from the i^{th} neuron of the previous layer $j-1$.
$w_{ij}^{(j)}$ Weight connecting the i^{th} neuron of layer $j-1$ to the current neuron in layer j.
b_j Bias term for the neuron in layer j.
z_j Result of the linear transformation at the current neuron in layer j.
n_j Number of inputs (or neurons) in the previous layer $j-1$.

b) The result of the weighted sum, z_j, is passed through a non-linear activation function:

$$a_j = f(z_j)$$

This introduces non-linearity to the model. A list of some common activation functions can be seen in the Table I.

II. The predicted output is compared to the actual output using a loss function to compute the loss. A loss function measures the difference between the actual target values and the model's predicted results. For a single prediction:

$$\mathcal{L}(\hat{y}, y) = f(\hat{y}, y)$$

Where:
$\hat{y}$ Predicted value.
y Actual value.
f Specific loss function formula.

The cost function aggregates the loss over the entire dataset:

$$\frac{1}{m} \sum_{i=1}^{m} \mathcal{L}(\hat{y}, y)$$

Two examples of cost functions are the following:

- Mean Squared Error (MSE):

$$\text{MSE} = \frac{\sum_{i=1}^{n} (\hat{y}^{(i)} - y^{(i)})^2}{n} \tag{3}$$

- Binary Cross-Entropy: Commonly used for binary classification problems:

$$L = -\frac{1}{N} \sum_{i=1}^{N} [y_i \log(\hat{y}_i) + (1 - y_i) \log(1 - \hat{y}_i)] \tag{4}$$

Where:
L The average loss (cost) across all N samples in the dataset.
y_i The true label for the i^{th} sample, where $y_i \in \{0, 1\}$.
$\hat{y}_i$ Predicted probability for $y_i = 1$.

$1 - \hat{y}_i$ Predicted probability for $y_i = 0$.
$\log$ The natural logarithm.

III. Backpropagation is the process by which the network's weights and biases are adjusted to minimize loss. The loss is propagated backwards from the output layer to the input layer. At each step, the gradient of the loss with respect to the parameters determines the adjustment. The following steps make up the backpropagation phase:

a) The gradient of the loss with respect to each weight and bias in every node is calculated, starting from the output layer and moving backwards to the input layer.
b) The gradient for any layer builds on the gradient of the subsequent (later) layers using the chain rule of differentiation.
c) The network's parameters for any node are adjusted in the direction opposite to the respective gradient using optimization algorithms like stochastic gradient descent (SGD) or variants such as the Adam optimizer.

3) Stochastic gradient descent: Stochastic gradient descent is an optimization algorithm that optimizes the parameters Θ of the network, to minimize the loss

$$\Theta = \arg\min_{\Theta} \frac{1}{N} \sum_{i=1}^{n} l(x_i, \Theta)$$

Where:

$x_{1,2,\ldots,N}$ The training set.
$l(x_i, \Theta)$ The loss for a given data point x_i.
N The number of examples in the dataset.

The loss, z is a supervision signal that guides any modifications that should take place on the parameters[3]. The stochastic gradient descent method of such modification is as follows:

$$\theta^i \leftarrow \theta^i - \eta \frac{\partial z}{\partial \theta^i}$$

where i represents the layer index η is the learning rate $\frac{\partial z}{\partial \theta^i}$ is the gradient of the loss z with respect to parameter θ^i

The parameters are updated iteratively, as follows:

$$\theta^i_{t+1} = \theta^i_t - \eta \frac{\partial z}{\partial \theta^i_t}$$

There are a few considerations that are important to note about stochastic gradient descent.

The learning rate affects the step size for each update, that is how much the parameters are adjusted in the direction of the gradient. A large learning rate might result in overshooting and even divergence, whereas a small learning rate leads to more stable convergence, albeit slower

The parameters are updated for every sample or for a small batch of samples, unlike traditional gradient descent that computes that gradients for the entire dataset. This approach leads to faster updates but is also prone to more noise in the optimization process.

4) Momentum: Momentum is a technique used in training neural networks to accelerate optimization. This accelerated optimization is achieved by considering also the values of previous gradients for each parameter. Momentum can, in this way, mitigate oscillations in the optimization path and speed up learning[4].

Momentum acts on the update rule of gradient descent by adding a portion of the update from the previous step to the current step. This approach allows the optimizer to maintain a directional memory, or velocity, effectively smoothing out updates and reducing oscillations.

Momentum is commonly integrated with optimization algorithms like stochastic gradient descent and is a key component of advanced optimizers like Adam optimizer in Section II-A6.

The momentum update rule is given by:

$$v^i_t = \beta v^i_{t-1} + (1 - \beta) \frac{\partial z}{\partial \theta^i_t} \tag{5}$$

$$\theta^i_{t+1} = \theta^i_t - \eta v^i_t \tag{6}$$

Where:

v^i_t The velocity term at step t for the parameters at index i.
β The momentum coefficient (e.g., 0.9), controlling how much of the previous velocity to retain.
$\frac{\partial z}{\partial \theta^i_t}$ The gradient of the loss function z with respect to parameters θ^i at step t.
η The learning rate.
θ^i_t The parameters at layer index i at step t.

A typical value is $\beta = 0.9$, which retains 90% of the previous velocity. Smaller values result in less "memory" of past updates.

5) RMSProp: Root Mean Square Propagation (RMSProp) is an adaptive learning rate optimization algorithm designed to improve the training of neural networks. Its main function is to address challenges such as inconsistent or large gradient magnitudes. RMSProp helps stabilize convergence during optimization due to its effectiveness in dealing with noisy gradients.

RMSProp adjusts the learning rate for each parameter based on the average of recent squared gradients. In this way, the optimizer adapts to the scale of the gradients, preventing large updates that could destabilize training.

The algorithm is similar to momentum, but here it introduces a running average of squared gradients to normalize parameter updates.

The RMSProp update rule is given by:

$$S_t^i = \beta S_{t-1}^i + (1-\beta)\left(\frac{\partial z}{\partial \theta_t^i}\right)^2 \tag{7}$$

Where:

S_t^i Exponentially weighted moving average of squared gradients at step t for the parameters at layer index i.

β Decay rate for the moving average (commonly set to 0.9).

‘$\frac{\partial z}{\partial \theta_t^i}$ Gradient of the loss function z with respect to parameters θ_t^i at step t and layer index i.

The parameters are updated using a learning rate scaled by the square root of S_t^i (with a small value ϵ added for numerical stability):

$$\theta_{t+1}^i = \theta_t^i - \frac{\eta}{\sqrt{S_t + \epsilon}}\left(\frac{\partial z}{\partial \theta_t^i}\right) \tag{8}$$

Where:

η Global learning rate, which is set to 0.001 in most frameworks.

ϵ Small constant (e.g., 10^{-8}) to prevent division by zero.

RMSProp is a widely used optimizer that forms the foundation for more advanced methods such as adam optimizer that is discussed in detail in Section II-A6. It is especially effective in training deep neural networks where gradient magnitudes can vary significantly.

6) Adam optimizer: The Adam Optimizer (Adaptive Moment Estimation) is a widely used optimization algorithm for training deep learning models. It combines the benefits of momentum and rmsprop to provide an efficient, robust, and adaptable optimizer. Adam is particularly effective for problems with sparse gradients and non-stationary objectives.

Adam optimizer had a number of hyper parameters:

- Learning Rate α: `0.001`
- First Moment Decay Rate β_1: `0.9`
- Second Moment Decay Rate β_2: `0.999`
- Numerical Stability Term ϵ: `1e-8`

The Adam-optimizer update rule is given by the following steps:

I. First, calculate the first moment estimate, or the Momentum that we discussed in Section II-A4, which is the exponentially weighted moving average of the gradients. This is done to smooth gradient updates over time by including past gradients and thus maintaining a directional memory:

$$m_t^i = \beta_1 m_{t-1}^i + (1-\beta_1)\frac{\partial z}{\partial \theta_t^i}$$

II. Calculate the second moment estimate, which is the basic idea of RMSProp that we discussed in Section II-A5, to track the exponentially weighted variance of gradients:

$$v_t^i = \beta_2 v_{t-1}^i + (1-\beta_2)\left(\frac{\partial z}{\partial \theta_t^i}\right)^2$$

III. Correct these results for initialization bias:

$$\hat{m}_t^i = \frac{m_t^i}{1-\beta_1^t}$$

$$\hat{v}_t^i = \frac{v_t^i}{1-\beta_2^t}$$

IV. Update the parameters using the corrected estimates:

$$\theta_{t+1}^i = \theta_t^i - \frac{\alpha \hat{m}_t^i}{\sqrt{\hat{v}_t^i} + \epsilon}$$

7) Batch normalization: Batch normalization is used to control the statistics of the activations in the neural networks. It is commonly used in neural network architectures, and it is usually found after layers that have multiplications, like linear or convolutional layers

If we consider a hidden state neural net node

We have basically a pre-activation value, that is the result of

$$z = \left(\sum_{i=1}^{n} x_i w_i\right) + b$$

That is fed into a non-linear element such as RELu or tanh.

- We do not want the pre-activation to be very small as the tanh activation will not effectively activate.
- We also do not want these values to be too large, as the tanh will become saturated.
- Furthermore, we want these values to be roughly Gaussian, that is, with a mean of 0 and a standard deviation of 1.

Sergey Ioffe and Christian Szegedy propose batch-normalization [1] to take the hidden states and normalize them to be Gaussian.

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1\ldots m}\}$;
Parameters to be learned: γ, β
Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m}\sum_{i=1}^{m} x_i \qquad \text{// mini-batch mean}$$

$$\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m}\sum_{i=1}^{m}(x_i - \mu_{\mathcal{B}})^2 \qquad \text{// mini-batch variance}$$

$$\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} \qquad \text{// normalize}$$

$$y_i \leftarrow \gamma \widehat{x}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(x_i) \qquad \text{// scale and shift}$$

Algorithm 1: Batch Normalizing Transform, applied to activation x over a mini-batch.

Fig. 3: Batch normalization algorithm, from [1]

There are two ways whereby batch normalization can be implemented:

- Pre-activation normalization, where batch-normalization is carried out before the activation function is applied.

- Post-activation normalization, where batch-normalization is carried out after the activation function is applied.

The original paper specified pre-activation normalization, however studies have shown that post-activation batch normalization will give superior results.

8) Regularization: Regularization are techniques used to prevent overfitting in machine learning. This is achieved by adding a penalty term to the loss function, that discourage the model from assigning larger weights to features.

L1 regularization or Lasso Regularization adds the sum of the absolute values of the weights to the loss function:

$$\mathcal{L}_{L1} = \mathcal{L} + \lambda \sum_{i=1}^{n} |w_i| \tag{9}$$

Where:

$\mathcal{L}$ The original loss function (e.g., cost-function-mean-square-error, cost-function-cross-entropy).
λ The regularization strength, a hyperparameter.
w_i The weight of the i^{th} node.

L1 regularization drives some weights to zero, thus encouraging sparsity in the network. Since L1 penalizes large weights, it promotes simpler networks with improved generalization.

L2 or Ridge regularization adds the sum of the squared values of the weights to the loss function:

$$\mathcal{L}_{L2} = \mathcal{L} + \lambda \sum_{i=1}^{n} w_i^2 \tag{10}$$

Where:

$\mathcal{L}$ The original loss function (e.g., cost-function-mean-square-error, cost-function-cross-entropy).
λ The regularization strength, a hyperparameter.
w_i The weight of the i^{th} node.

L2 penalizes large weights but does not drive them to zero but shrinks them closer to zero. It hence promotes smoother solutions and avoids sharp changes in parameter values.

B. Machine learning technique - Logistic regression

Logistic regression is a machine learning algorithm commonly used for binary classification tasks.

Given a feature vector $X \in \mathbb{R}^{n_x}$, the goal of logistic regression is to predict the probability $\hat{y}$ that a binary output variable y takes the value 1, given X, that is $\hat{y} = P(y = 1|X)$, $0 \leq y \leq 1$. For example, in the case of image classification, logistic regression can be used to predict the probability that an image contains a cat.

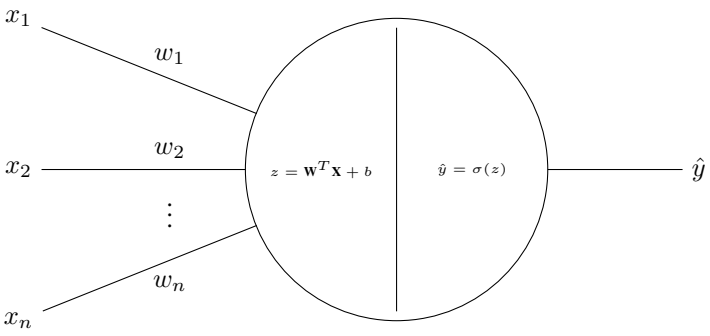


Fig. 4: A logistic regression model

Logistic regression can be visualized as the model shown in Figure 4. It consists of several main components:

- Inputs. The input vector to the model $\mathbf{X} \in \mathbb{R}^{n_x}$.
- Parameters. A weight vector $\mathbf{W} \in \mathbb{R}^{n_x}$ and a bias term $b \in \mathbb{R}$. These will form the coefficients of a linear equation that gives the log odds ratio.
- Pre-activation result: The result is obtained by multiplying the transpose of the weights with the inputs and then adding the bias.

$$z = \mathbf{W}^T\mathbf{X} + b = \begin{bmatrix} w_1 & w_2 & \dots & w_n \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} + b \tag{11}$$

- Sigmoid function. A function as shown in Figure 5, $\sigma(z) = \frac{1}{1+e^{-z}}$, which maps any real number z to the range $(0, 1)$. This function is used to ensure that the predicted probability $\hat{y}$ is always between 0 and 1.

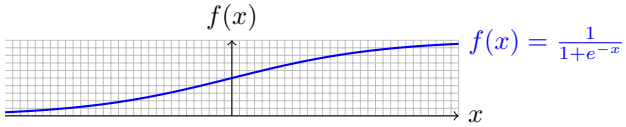


Fig. 5: Sigmoid activation function

- Output. The predicted probability $\hat{y}$ is computed as $\hat{y} = \sigma(z) = \sigma(\mathbf{W}^T\mathbf{X} + b)$.

A term that is often encountered in this scenario is the log-odds ratio or logit. Logistic regression models the probability $P(y = 1 \mid X)$, of the binary dependent variable Y given the predictor variables $\mathbf{X} = \{x_1, x_2, \dots, x_n\}$. The goal is to find a relationship between $P(y = 1)$, and the predictors $\mathbf{X}$.

The probability is modelled using the sigmoid function:

$$P(y = 1 \mid X) = \frac{1}{1 + e^{-\eta}}$$

Where: $\eta = b + w_1x_1 + w_2x_2 + \cdots + w_nx_n$ is the linear regression function

The odds of $y = 1$ are defined as the ratio of the probability of success to the probability of failure:

$$\text{Odds} = \frac{P(y=1)}{1-P(y=1)}$$

Taking the natural logarithm of the odds gives the [log-odds-ratio]] or logit:

$$\text{Log-Odds} = \ln\left(\frac{P(y=1)}{1-P(y=1)}\right)$$

From the sigmoid function, we can derive the relationship between the probability and the log-odds-ratio:

$$P(y=1) = \frac{1}{1+e^{-\eta}}$$

$$1 - P(y=1) = 1 - \frac{1}{1+e^{-\eta}} = \frac{e^{-\eta}}{1+e^{-\eta}}$$

The odds, therefore, are

$$\text{Odds} = \frac{P(y=1)}{1-P(y=1)} = \frac{\frac{1}{1+e^{-\eta}}}{\frac{e^{-\eta}}{1+e^{-\eta}}} = e^{\eta}$$

Taking the natural logarithm of both sides gives the log-odds:

$$ln\left(\frac{P(y=1)}{1-P(y=1)}\right) = \eta$$

Substituting $\eta = b + w_1x_1 + w_2x_2 + \cdots + w_nx_n$

$$\ln\left(\frac{P(y=1)}{1-P(y=1)}\right) = \eta = b + w_1x_1 + w_2x_2 + \cdots + w_nx_n \tag{12}$$

We conclude this overview of logistic regression by looking at how they work and learn. The weight vector **W** and the bias term b are learned from a labelled training set by minimizing a suitable loss function using techniques such as gradient descent or its variants. Once trained, the logistic regression model can be used to predict the probability of the binary output variable for new input examples.

The feedforward process for logistic regression can be described as follows:

1) Compute z as the dot product of the weight vector **W** and the input features, plus the bias term b, transforming the input features info a single scalar z that represents the log-odds of the output being $y = 1$:

$$z = \mathbf{W}^T\mathbf{X} + b \tag{13}$$

2) Pass z through the sigmoid function to map the log-odds z to a probability $\hat{y} = P(y = 1 \mid X)$, ensuring the output is between 0 and 1:

$$\hat{y} = \sigma(z) = \frac{1}{1+e^{-z}} \tag{14}$$

3) During training, we define the loss function $\mathcal{L}$ as the negative log-likelihood of the predicted output given the true label:

$$\mathcal{L} = -\left(y\ln(\hat{y}) + (1-y)\ln(1-\hat{y})\right) \tag{15}$$

For a trained system, we compare $\hat{y}$ to a threshold to convert the probabilistic output into the final binary classification.

We now look at **feedback process** for logistic regression. To optimize the weight vector **W**, we compute the derivatives of the loss function with respect to each weight and the bias term and use these derivatives to update the weights in the opposite direction of the gradient, that is gradient descent.

To compute the derivatives, we use the chain rule:

$$\frac{\partial\mathcal{L}}{\partial w_i} = \frac{\partial\mathcal{L}}{\partial\hat{y}} \cdot \frac{\partial\hat{y}}{\partial z} \cdot \frac{\partial z}{\partial w_i}$$

and

$$\frac{\partial\mathcal{L}}{\partial b} = \frac{\partial\mathcal{L}}{\partial\hat{y}} \cdot \frac{\partial\hat{y}}{\partial z} \cdot \frac{\partial z}{\partial b}$$

We can then use these derivatives to update the weights as follows:

$$w_i \leftarrow w_i - \alpha\frac{\partial\mathcal{L}}{\partial w_i} \tag{16}$$

and

$$b \leftarrow b - \alpha\frac{\partial\mathcal{L}}{\partial b} \tag{17}$$

Where α is the learning rate, which controls the step size of the updates. By iteratively performing these updates on a training set, we can find the optimal weight vector **W** that minimizes the loss function on the training set.

To calculate the derivatives, let us begin by computing the derivative of the loss function with respect to the predicted output $\hat{y}$:

$$\frac{\partial\mathcal{L}}{\partial\hat{y}} = \frac{\partial}{\partial\hat{y}}\left(-\left(y\ln(\hat{y}) + (1-y)\ln(1-\hat{y})\right)\right)$$

since

$$\frac{d(ln(x))}{dx} = \frac{1}{x}$$

we get:

$$\frac{\partial\mathcal{L}}{\partial\hat{y}} = -\left(\frac{y}{\hat{y}} - \frac{1-y}{1-\hat{y}}\right)$$

The derivative of the predicted output $\hat{y}$ with respect to z is solved using the quotient rule, that is

$$\frac{d}{dx}\left(\frac{f(x)}{g(x)}\right) = \frac{f'(x)g(x) - g'(x)f(x)}{g^2(x)}$$

So, if we let

$f(z) = 1$	$f'(z) = 0$
$g(z) = 1 + e^{-z}$	$g'(z) = -e^{-z}$

$$\begin{aligned}\frac{\partial \hat{y}}{\partial z} &= \frac{\partial}{\partial z}\left(\frac{1}{1+e^{-z}}\right) \\ &= \frac{e^{-z}}{(1+e^{-z})^2} \\ &= \frac{1}{(1+e^{-z})}\frac{e^{-z}}{(1+e^{-z})} \\ &= \frac{1}{(1+e^{-z})}\frac{1+e^{-z}-1}{1+e^{-z}} \\ &= \frac{1}{(1+e^{-z})}\left(\frac{1+e^{-z}}{1+e^{-z}} - \frac{1}{1+e^{-z}}\right) \\ &= \hat{y}(1-\hat{y})\end{aligned}$$

The derivative of z with respect to w_i:

$$\begin{aligned}\frac{\partial z}{\partial w_i} &= \frac{\partial}{\partial w_i}\mathbf{W}^T\mathbf{X} + b \\ &= \frac{\partial}{\partial w_i}(w_1x_1 + \cdots + w_ix_i + \cdots + w_nx_n + b) \\ &= x_i\end{aligned} \tag{18}$$

Similarly,

$$\begin{aligned}\frac{\partial z}{\partial b} &= \frac{\partial}{\partial b}\mathbf{W}^T\mathbf{X} + b \\ &= \frac{\partial}{\partial b}(w_1x_1 + \cdots + w_ix_i + \cdots + w_nx_n + b) \\ &= 1\end{aligned} \tag{19}$$

Therefore

$$\begin{aligned}\frac{\partial \mathcal{L}}{\partial w_i} &= \frac{\partial \mathcal{L}}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial z} \cdot \frac{\partial z}{\partial w_i} \\ &= -\left(\frac{y}{\hat{y}} - \frac{1-y}{1-\hat{y}}\right) \cdot \hat{y}(1-\hat{y}) \cdot x_i \\ &= -\left(\frac{-y(1-\hat{y}) + (1-y)\hat{y}}{\hat{y}(1-\hat{y})}\right) \cdot \hat{y}(1-\hat{y}) \cdot x_i \\ &= \left[(1-y)\hat{y} - y(1-\hat{y})\right] x_i \\ &= \left[\hat{y} - y\hat{y} - y + y\hat{y}\right] x_i\end{aligned}$$

$$\frac{\partial \mathcal{L}}{\partial w_i} = (\hat{y} - y)x_i \tag{20}$$

and similarly

$$\frac{\partial \mathcal{L}}{\partial b} = (\hat{y} - y) \tag{21}$$

C. Machine learning technique - K-nearest neighbours algorithm

K-nearest neighbours is simple yet robust for datasets with well-structured local relationships. It is particularly effective for non-linear decision boundaries and finds applications in anomaly detection, pattern recognition, and recommendation systems.

The k-nearest neighbours algorithm is non-parametric, that is, it does not make assumptions about the underlying distribution or functional form of the data; instance-based, that is, it does not explicitly learn a model during a training phase, but it relies on the raw training data to make predictions at query time, unlike parametric models, which "learn" a set of fixed parameters (e.g., coefficients in linear regression) during training, learning method used for classification and regression tasks. It predicts the output of a query point based on the labels or values of its k-nearest neighbours in feature space.

KNN does not assume a specific functional form for the data. Instead, it relies on the local structure of the dataset. For a given query point x, the algorithm uses a distance metric to identify its k-nearest neighbours and infers the prediction by aggregating their outcomes. Typical distance metrics include:

1) Euclidean Distance

$$d(x, x') = \sqrt{\sum_{i=1}^{n}(x_i - x_i')^2}$$

2) Manhattan Distance

$$d(x, x') = \sum_{i=1}^{n}|x_i - x_i'|$$

3) Minkowski Distance. Note that for $p = 2$, this reduces to the Euclidean distance; for $p = 1$, it becomes the Manhattan distance.

$$d(x, x') = \left(\sum_{i=1}^{n}|x_i - x_i'|^p\right)^{1/p}$$

In classification tasks, the predicted class $\hat{y}$ for a query point x is determined by majority voting among its k-nearest neighbours. If we let $N_k(x)$ represent the set of the k-nearest neighbours,he predicted class is given by:

$$\hat{y} = \text{argmax}_c \sum_{x' \in N_k(x)} \mathbb{I}(y(x') = c)$$

Where:

argmax_c	Identifies the class c with the highest count among the neighbours.
$\mathbb{I}(\cdot)$	The indicator function, which equals 1 if $y(x') = c$, and 0 otherwise.

The parameter k determines the number of neighbours considered.

- A small k (e.g., $k = 1$) makes the model sensitive to noise, as predictions rely heavily on individual points.

- A large k smooths the decision boundary but may lead to underfitting.

Finding the optimal value for k is one of the main challenges in the k-nearest neighbour. Cross-validation is typically employed to find a value using the following procedure:

1) Iterate Over Candidate Values of k
   - Choose a range of potential k values, for example, $k = 1, 2, \ldots, 20$.
2) Evaluate Performance for Each k
   - For each k, use K-fold cross-validation:
     - Train the KNN model using $K - 1$ folds.
     - Validate it on the remaining fold.
     - Compute the average performance metric across all K folds.
3) Select k with the Best Performance
   - After evaluating all k values, choose the k that maximizes the performance metric (e.g., accuracy) or minimizes the error.

The k-nearest neighbour algorithm is, therefore, as follows;

1) Input:
- Dataset: $D = \{(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)\}$, where x_i is the feature vector, and y_i is the corresponding label or value.
- Query point: x_{query}, the data point for which the prediction is required.
- Number of neighbours: k, the number of nearest neighbours to consider.
- Distance metric: $d(x, x')$ (e.g., Euclidean distance).

2) Steps::

1) Calculate Distance. For the query point x_{query}, compute the distance to every point x_i in the dataset D using the chosen distance metric. For Euclidean distance:
$$d(x_{query}, x_i) = \sqrt{\sum_{j=1}^{n} (x_{query_j} - x_{i_j})^2},$$
$$\forall i \in \{1, 2, \ldots, N\}.$$
2) Sort Neighbours. Rank all data points x_i in D by their distance to x_{query} in ascending order. Let this sorted set be D_{sorted}.
3) Select k-Nearest Neighbours. Extract the top k data points from D_{sorted}. Denote this set as $N_k(x_{query})$.
4) Aggregate Neighbours' Outputs.
   - For **classification**: Perform majority voting among the labels y_i of the k-nearest neighbours:
   $$\hat{y} = \text{argmax}_c \sum_{x_i \in N_k(x_{query})} \mathbb{I}(y_i = c),$$
   where $\mathbb{I}(y_i = c)$ is an indicator function that equals 1 if $y_i = c$, and 0 otherwise.
5) **Output Prediction:** Return $\hat{y}$ as the predicted label (for classification) or value (for regression) for x_{query}.

3) Output:: The predicted label or value $\hat{y}$ for the query point x_{query}.

D. Feature scaling

Feature scaling is an important data transformation process. It is a very important aspect of many machine learning algorithms including logistic regression, support vector machines and neural networks, as, the performance of such algorithms is adversely impacted when the numerical features have different scales. The two methods to transform features on the same scale are normalization and rescaling.

During normalization or rescaling, values are scaled and shifted so that they are mapped onto the $[0, 1]$ interval. This is achieved by applying the following transformation;

$$x_{normalized} = \frac{x - x_{min}}{x_{max} - x_{min}}$$

Normalization is also sometimes referred to as min-max scaling.

Standardization is particularly suited for algorithms that assume Gaussian distributions, like linear regression and logistic regression. It is achieved by first subtracting values from the mean so that the mean of the normalized values is zero, and then dividing by the standard deviation so that the variance of the normalized distribution is one. Thus;

$$x_{standardized} = \frac{x - \mu}{\sigma}$$

Unlike normalization, the range of standardization is not fixed, and this can sometimes be an issue if a value in the $[0, 1]$ interval is expected. Standardization is however more resilient to the effect of outliers.

Tree based machine learning models, like decision trees and random forests do not normally require feature scaling.

E. Cross-validation

Cross-validation is a technique that can be applied to any ML algorithm that is aimed to reduce overfitting by estimating how well each hypothesis generalizes to unseen data. In practice, a portion of the data is reserved for this purpose.

The K-fold cross validation technique splits the dataset into k folds, training that model on $k - 1$ folds and testing on the remaining one. The test fold is rotated and the process is repeated so that each fold will act as the test set once. Metrics like mean square error are averaged across folds, ensuring a robust estimate.

Therefore, if for example, we split the data into 10 folds, so that each fold will have $n/10$ records, we train the model on 9 folds and test on the remaining one. We then rotate the test fold and repeat this process 10 times. The final performance metric is computed as the mean of the metrics across the 10 folds.

In stratified K-fold cross validation, the folds have the same proportion of the classes as in the original dataset.

Other types of cross validation include Leave one out cross-validation, where each data point is used as a test set once.

F. Principal Component Analysis (PCA)

Principal Component Analysis is a statistical method for dimensionality reduction that transforms high-dimensional data into a lower-dimensional space while maintaining as much variance as possible. It achieves this by identifying directions in the data, called principal components, which maximize the variance. PCA is widely used in data compression, noise reduction, and visualization applications.

PCA relies on variance, which measures data spread, and covariance, which shows how features change together. It transforms the data into a new coordinate system defined by the eigenvectors of the covariance matrix, ordered by their corresponding eigenvalues. These eigenvalues quantify the variance captured by each principal component.

The following steps are carried out in order to determine the principal components of a dataset:

Given a dataset X with n samples and d features, represented as an $n \times d$ matrix:

$$X = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1d} \\ x_{21} & x_{22} & \cdots & x_{2d} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nd} \end{bmatrix}$$

- We start by centring the data. Centering ensures the dataset is zero-centred by subtracting the mean of each feature:

  $$X_{\text{centered}} = X - \mu$$

  where μ is the mean vector:

  $$\mu = \frac{1}{n} \sum_{i=1}^{n} X_i$$

- We then compute the covariance matrix Σ which is calculated as:

  $$\Sigma = \frac{1}{n-1} X_{\text{centered}}^T X_{\text{centered}}$$

- And then solve the eigenvalue equation for the covariance matrix:

  $$\Sigma v = \lambda v$$

  where:

  λ**:** Eigenvalue (variance explained by the principal component).

  v**:** Eigenvector (direction of the principal component).

- We sort the eigenvalues in descending order and select the top k eigenvectors to obtain the principal components:

  $$V_k = [v_1, v_2, \ldots, v_k]$$

- We then transform the data into the new k-dimensional space:

  $$X_{\text{reduced}} = X_{\text{centered}} V_k$$

- The explained variance ratio quantifies the proportion of variance retained by each principal component:

  $$\text{Explained Variance Ratio} = \frac{\lambda_i}{\sum_{j=1}^{d} \lambda_j}$$

  where λ_i is the eigenvalue of the i-th principal component.

G. Feature Selection

Feature selection identifies and retains the most relevant features in a dataset to improve model performance and reduce complexity. It involves reducing the dimensionality of the original problem by selecting a subset of features. For example:

$$\begin{array}{c} \text{Original problem (with} \\ n \text{ dimensions):} \end{array} \longrightarrow \begin{array}{c} \text{Reduced problem (with} \\ k < n \text{ dimensions):} \end{array}$$

In feature selection, k features are selected out of N to minimize the learner error. This process can be mathematically represented as:

$$\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{bmatrix} \xrightarrow{\text{Feature Selection}} \begin{bmatrix} x_{i_1} \\ x_{i_2} \\ \vdots \\ x_{i_k} \end{bmatrix}.$$

Feature selection is essential for several reasons:

- Curse of Dimensionality. High-dimensional datasets often lead to models requiring more data and computation and are prone to poor generalization.
- Overfitting. Excessive features can cause a model to fit noise in the data, leading to overfitting.
- Visualization. Reduced dimensionality makes it possible to visualize data in two or three dimensions.

Filter-based feature selection is a method that selects features based on statistical measures of their relevance to the target variable, independently of any machine learning model.

Filter-based feature selection has two primary aims:

1) Select features that are independent of each other, ensuring that each feature contributes new information.
2) Select features that are highly dependent on the target variable, avoiding features that do not improve model performance.

Types of filter-based feature selection methods include:

- For small numbers of features:
  - Use scatterplots to visually assess relationships between features and the target variable.

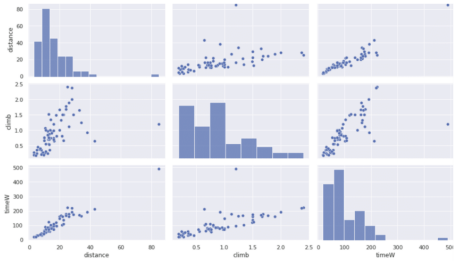


Fig. 6: Scatter plot analysis of a simple dataset with few features. Taken from lecture notes by Dr. Konstantinos Makantasis.

- For analyzing relationships:
  - Use Pearson correlation to measure the linear correlation between features and the target variable.
    The Pearson correlation is a normalized version of covariance[2] and measures the degree of linear correlation between two variables.

$$r = \frac{\sigma_{xy}}{\sigma_x \sigma_y} = \frac{\sum (X_i - \bar{X})(Y_i - \bar{Y})}{\sqrt{\sum (X_i - \bar{X})^2 \sum (Y_i - \bar{Y})^2}}$$

where:

X_i, Y_i: The individual data points.
$\bar{X}$, $\bar{Y}$: The means of the variables X and Y.
r is unitless, meaning it has no associated units of measurement.

H. Measurement

Quantitative measurements numerically represent attributes and are fundamental for evaluating machine learning models by providing an objective means to assess the model's performance. We can analyse the model's effectiveness by comparing model predictions to actual outcomes. Appropriate selection and reporting of measurement methods, including their reliability, validity, and potential biases, are essential to ensure accurate interpretation and meaningful results. This section will look at the measurements used in this study.

The function used in machine learning and statistical modelling to quantify the difference between the predicted outputs of a model and the actual target values is called the loss function. It serves as a measure of the model's performance, guiding the optimisation process to improve predictions.

For a single prediction:

$$\text{Loss}(\hat{y}, y) = f(\hat{y}, y)$$

Where:
$\hat{y}$: Predicted value.
y : Actual value.
f : Specific loss function formula

The aggregation of the loss function across the entire dataset is called the cost function so that;

$$\text{Cost}(\hat{y}, y) = \frac{1}{N} \sum_{i=1}^{N} \mathcal{L}(\widehat{y}_i, y_i)$$

In the problem we are considering, we will try to predict whether a person will recidivate given information about his or her previous criminal history is a binary classifier problem. A binary classifier is a function that can be applied to features X such as $(x_1, x_2, x_3, \ldots, x_n)$ and maps them to an output Y, where $Y \in \{0, 1\}$. It is a supervised learning technique; therefore, a test set is extracted from the available data to validate the model before being deployed in production.

$$f(x_1, x_2, x_3, \ldots, x_n) = Y \in \{0, 1\}$$

The function will return a value between 0 and 1; therefore, a threshold value is operated to classify the result as true or false. The model will subsequently classify predictions as true or false according to the threshold value.

For the classification problem that we have in hand, we will primarily use the log-likelihood cost function defined as:

$$\mathcal{L}_{\text{log-likelihood}} = -\sum_{i=1}^{N} [y_i \ln(\hat{y}_i) + (1 - y_i) \ln(1 - \hat{y}_i)]$$

Negative log-likelihood focuses on the distance between the labels y_i and the predicted probabilities $\hat{y}_i$. If we consider a sample where:

- y_i is one and $\hat{y}_i$ is close to 1: $y_i \ln(\hat{y}_i)$ is close to zero, while $(1 - y_i) \ln(1 - \hat{y}_i)$ is zero, so that the resultant loss is close to zero.
- y_i is 1 and $\hat{y}_i$ is far from 1: $y_i \ln(\hat{y}_i)$ is large, while $(1 - y_i) \ln(1 - \hat{y}_i)$ is zero so that the resultant loss is large.
- y_i is zero and $\hat{y}_i$ is close to 0: $y_i \ln(\hat{y}_i)$ is zero, while $(1 - y_i) \ln(1 - \hat{y}_i)$ is also close to zero so that the resultant loss is close to zero.
- y_i is zero and $\hat{y}_i$ is far from 0: $y_i \ln(\hat{y}_i)$ is zero, while $(1 - y_i) \ln(1 - \hat{y}_i)$ is large so that the resultant loss is large.

In this scenario, we can obtain four kinds of results:

The number of samples that are TP, TN, FP or FN can be organised in what is known as a confusion matrix, that is shown in Figure 7. This tool makes it easy to perform calculations that determine the validity of the model at hand.

Prediction	Classif	Outcome	Description
1	1	True Positive (TP)	The model correctly predicted the positive class.
1	0	False Positive (FP)	The model incorrectly predicted the positive class (a false alarm).
0	1	False Negative (FN)	The model incorrectly predicted the negative class (a miss).
0	0	True Negative (TN)	The model correctly predicted the negative class.

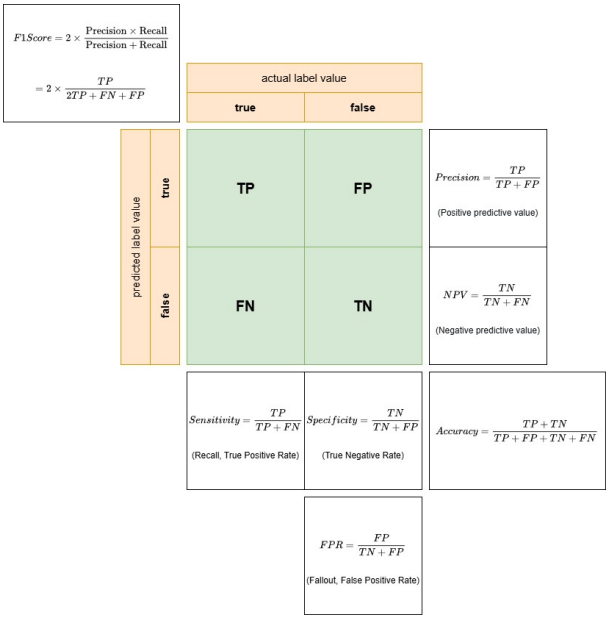


Fig. 7: Confusion matrix and associated equations

There are several key performance metrics derived from the confusion matrix, each offering a different perspective on evaluating the effectiveness of a binary classification model.

The **accuracy** of a model is a straightforward measure that evaluates the proportion of correct predictions (both True Positives and True Negatives) out of the total number of predictions. It can be mathematically defined as:

$$Accuracy = \frac{TP + TN}{TP + FP + TN + FN}$$

for a dataset,

$$Accuracy = \frac{1}{N} \sum_{i=1}^{N} 1(\hat{y}_i = y_i)$$

Precision answers the question: "Out of all the observations predicted to be positive, how many were positive?" In other words, it measures the model's ability to avoid false positives.

$$Precision = \frac{TP}{TP + FP}$$

Recall or **sensitivity** measures the model's ability to correctly identify positive cases. It answers the question: "Out of all the actual positive instances, how many did the model correctly identify as positive?"

$$Recall = \frac{TP}{TP + FN}$$

Specificity measures the model's ability to identify negative cases correctly. It answers the question: "Out of all the actual negative instances, how many did the model correctly identify as negative?"

The formula for specificity is:

$$Specificity = \frac{TN}{TN + FP}$$

The F1-score is the harmonic mean of [precision](model-performance-precision) and [recall](model-performance-recall). It provides a single metric that balances precision and recall, which is useful when there is an uneven class distribution or when false positives and false negatives are important.

The formula for the F1 score is:

$$F1 = 2 \times \frac{\text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}$$
$$= 2 \times \frac{TP}{2TP + FN + FP}$$

As can be seen in Figure 8, the ROC curve is plotted by varying the decision threshold of the classifier and plotting the corresponding values of FPR (on the x-axis) and sensitivity or TPR (on the y-axis). Each point on the ROC curve represents a (FPR, TPR) pair for a particular threshold value.

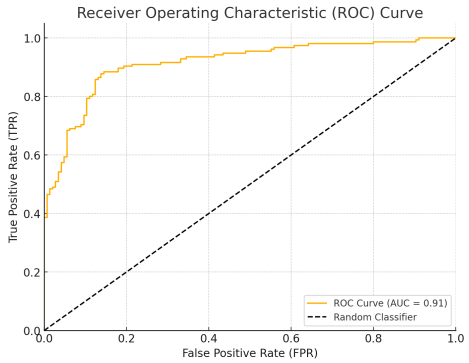


Fig. 8: ROC curve

The Area Under the ROC Curve (AUC) is a key indicator of model performance. The value of the AUC ranges from 0 to 1:

- A perfect classifier has an AUC of 1, indicating it achieves a TPR of 1 while keeping the FPR at 0.
- A model with an AUC of 0.5 performs no better than random guessing.
- Higher AUC values indicate better overall performance.

The goal of a classifier is to maximise the TPR (correctly predicting positive instances) while minimising the FPR (incorrectly classifying negative instances as positive). Ideally, the ROC curve should approach the top-left corner of the plot, indicating a high TPR with a low FPR.

In summary, the ROC curve helps to visualise and compare the trade-offs between true positives and false positives across different thresholds, and the AUC provides a single number summarising the model's ability to discriminate between positive and negative classes.

III. Data preparation

The COMPAS dataset used in this study is publicly available through ProPublica's GitHub repository. This repository contains the dataset and other assets used by ProPublica to investigate the biases present in the COMPAS risk assessment tool.

The file chosen for this analysis is **`compas-scores-two-years.csv`**, as it provides the cleanest and most relevant data for general recidivism prediction. This CSV file contains the key data required for our study, including several attributes related to demographics, criminal history, COMPAS risk scores, and the two-year recidivism outcomes that are important for exploring the predictive capabilities and the ethical implications of machine learning models in the context of recidivism prediction.

The dataset includes important information about individuals. Following an initial analysis, a list of the key fields in the dataset is below.

- Personal Information, includes attributes such as **`age`**, **`race`**, **`age_category`**, etc.
- Case and Event-Related Details are the fields prefixed with **`c_`** that provide a timeline and details of a person's interactions with the criminal justice system.
- Violence Risk Assessment are the fields prefixed with **`v_`** and are associated with the violence risk assessment in COMPAS. This dimension predicts violent recidivism risk.
- Case-Level Details for Violent Recidivism are the fields prefixed with **`vr_`**. These fields provide additional details specific to violent recidivism events.
- Juvenile Criminal Record are the fields prefixed with **`juv_`**. These fields capture information about an individual's juvenile criminal record, which is a key predictor of future adult criminal behaviour.
- Previous Charges and Severity can be deduced from fields such as **`priors_count`** and **`juv_`** fields.
- Additional fields, including **`r_charge_`**, **`r_offense_`**, **`vr_`** fields, **`c_charge_degree`**, and **`c_charge_desc`**, provide a broader perspective on criminal history and severity.
- Two-Year Recidivism, or the **`two_year_recid`** field in the COMPAS dataset, indicates whether an individual reoffended (recidivated) within two years of their initial assessment or release. This field is critical for evaluating the predictive accuracy of the COMPAS risk assessment tool.
- Decile Score is a standardized risk score in the COMPAS dataset. It categorizes an individual's likelihood of recidivism into ten equal groups (deciles) where 1 is the lowest risk, and 10 is the highest risk. Each decile represents approximately 10% of the sample when applied to a norm group.

A. Preparing the data for further analysis and training

Before we can perform any analysis or apply machine learning techniques, it is important to pre-process and prepare the dataset so that we can handle missing values, encode categorical features, and split the data into training, testing, and validation sets. This step will produce a clean dataset for building accurate and unbiased models. The following steps outline the procedures to prepare the dataset for further analysis and training.

B. Initial look at data and missing values handling

The dataset has 7214 instances over 53 columns. The target of the dataset is **`decile_score`**, but the dataset also contains information about whether or not the person recidivised, most notably through the label **`two_year_recid`**.

The first step in data preparation is removing the features irrelevant to this exercise or with over 50% missing records. We removed all the COMPAS-administrative labels and additional recidivism information apart from **`two_year_recid`**, narrowing the dataset to 17 fields.

The difference between **`c_jail_in`** and **`c_jail_out`** was calculated into a new field, **`days_in_jail`** and the difference between **`in_custody`** and **`out_custody`**, in a new field, **`days_in_custody`**. We subsequently removed the features containing date information from the dataset, together with **`days_in_custody`**, as it contained no information. At this stage, the dataset contains thirteen features: eight numerical, four categorical, and one descriptive. It also contains two labels, decile_score, which we will treat as the leading label in this exercise and **`two_year_recid`**, which we are keeping to compare the prediction power of our models to the original one.

C. Imputation of missing data

While examining the resultant dataset, we noticed that **`days_b_screening_arrest`** has 6907 values that are not null. Whilst it is possible to eliminate the rows that contain the null values at this stage, we replaced the missing values using a KNN imputation technique by grouping the numeric values of this dataset so that we can calculate the missing values. We checked this process by plotting the distribution of

days_b_screening_arrest before and after imputation to see if any variations occurred.

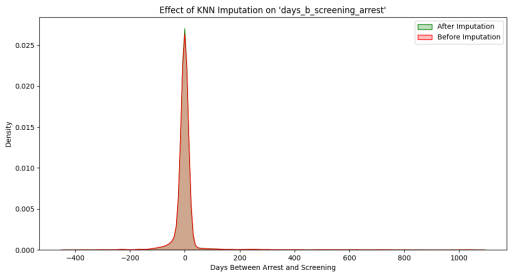


Fig. 9

At this stage, the dataset contains four categorical features that need encoding for machine learning algorithms. This section will focus on converting them into a numerical format using two encoding techniques. The categorical features and their values are listed below:

Feature	Description	Unique Values
sex	Gender of the individual	Male Female
race	Race of the individual	African-American Caucasian Hispanic Asian Native American Other
age_cat	Age category	Less than 25 25 - 45 Greater than 45
c_charge_degree	Degree of the criminal charge	F (Felony) M (Misdemeanor)

The following transformations are applied:

- One-Hot Encoding on **sex**, **race**, and **c_charge_degree**, transforming them into binary columns.
- Ordinal Encoding on **age_cat**. This encoding technique was preferred over one-hot in this case as it preserves order,thus respecting the inherent ranking of the category.

The original categorical columns were retained in the dataset for future use in the analysis steps.

D. Splitting the data into train, test and dev

A stratified shuffle split technique is preferred to create the train, test, and dev datasets whilst ensuring that the splits are proportional by **race**. In the first split, 80% Train and 20% Test are created, whilst in the Second split, The 20% Test is further divided into 10% Test and 10% Dev.

IV. Data Exploration and Visualisation

This section will examine the dataset in more detail to understand the patterns, distributions, and relationships. In this exercise, we will use more of the visual tools available through several Python libraries to identify potential biases, explore correlations between variables, and uncover insights that may influence the outcomes of predictive models.

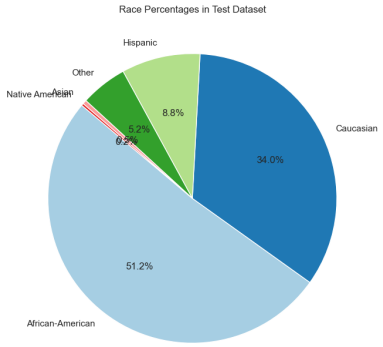


Fig. 10: Caption for the first image

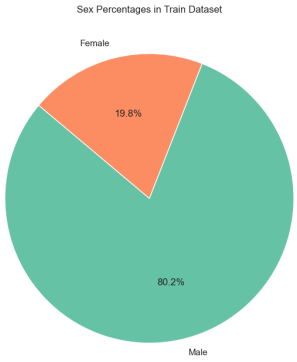


Fig. 11: Caption for the second image

A. Demographic analysis

We begin this analysis by segmenting the dataset based by race and gender.

By examining the racial composition of the dataset, we observe the following:

- Over half of the test dataset is composed of African-American individuals, suggesting that the dataset may be imbalanced, with a disproportionate representation of one racial group.
- Asians and Native Americans each makeup only 0.2% of the dataset; this underrepresentation might raise some concerns as it may lead to challenges in statistical analysis or machine learning models. Such concerns include the lack of reliability or significance for these groups due to insufficient data.

Figure **??** also shows our dataset's male/female split, with females comprising only 19.8%. It is, therefore, evident that the female group is underrepresented, which can lead to biased models as models may overfit male patterns and underperform

on females and misleading conclusions as insights derived might generalise poorly for the female subgroup.

B. Age distribution analysis

We used a boxplot to illustrate the age patterns across racial groups, helping to identify central values, spread, and any anomalies.

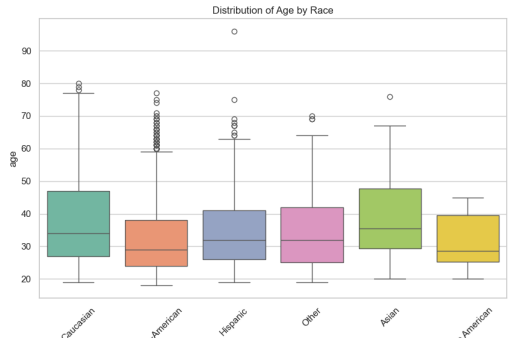


Fig. 12

Race	Median Age	Distribution Description
African-American	≈30 years	Concentrated in the 20–40 range, with a relatively narrow spread. We notice outliers above 60 years, indicating fewer older individuals.
Caucasian	≈40 years	Broader age range, from 20 to 70+ years. We notice more older individuals (upper outliers), making this group appear older on average.
Hispanic	≈30–35 years	Moderately broad spread, with most individuals between 20 and 50 years.
Asian	≈30 years	Narrow distribution, concentrated between 25 and 40 years. No outliers.
Native American	≈33 years	Very tight distribution, with all ages clustered closely around the median (little variability). It is important to note that this group accounts for a tiny portion of the population.
Other	≈35–40 years	Similar to Caucasians but with slightly fewer older individuals. The IQR shows a widespread.

C. Analysing distributions

Next, we plotted the distributions of all the features in our dataset; this is depicted in Figure 13 . From these histograms, we notice

- The age distribution shows a right-skewed pattern, with most individuals falling in the younger age ranges (20–40 years).
- There is a significant over-representation of certain racial groups, particularly African Americans, which could indicate potential biases in the dataset's sampling.
- Most individuals have zero juvenile felony counts, zero juvenile misdemeanour counts, and no recorded "other" juvenile offences, with each distribution rapidly declining for higher counts.
- A large proportion of individuals have a low number of prior offences, but there is a long tail indicating some individuals have a significant number of priors.
- Most individuals have relatively short jail durations, with a few experiencing significantly longer durations.
- The distribution of days between screening and arrest is clustered around zero, with few extreme outliers on both ends.
- The decile scores appear relatively evenly distributed, but slight patterns suggest clustering at specific score levels (e.g., lower decile scores are slightly more frequent).
- Two-year recidivism plot shows a near-equal distribution, indicating a balanced dataset for recidivism outcomes.

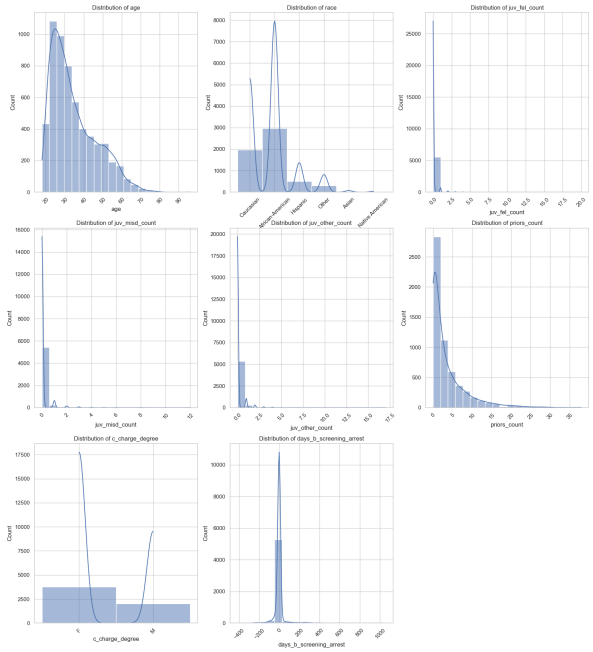


Fig. 13

D. Correlation analysis

The correlation matrix heatmap shown in Figure 14 was created to gather more insights and pinpoint the areas of high correlation. This plot raises a number of interesting observations, namely:

- Individuals with more prior offences tend to have higher risk scores, as prior criminal behaviour is a key factor in risk assessment models. The number of prior offences also correlates positively with recidivism; individuals with more prior offences tend to re-offend more often.
- Older individuals tend to have lower risk scores, suggesting that age may be inversely related to the risk of recidivism, with younger individuals being assessed as higher risk. In addition, older individuals are also less likely to recidivate, supporting this general trend.
- Individuals with higher risk scores are likelier to recidivate within two years, suggesting that the risk score

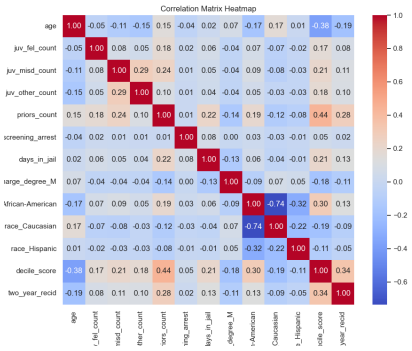


Fig. 14

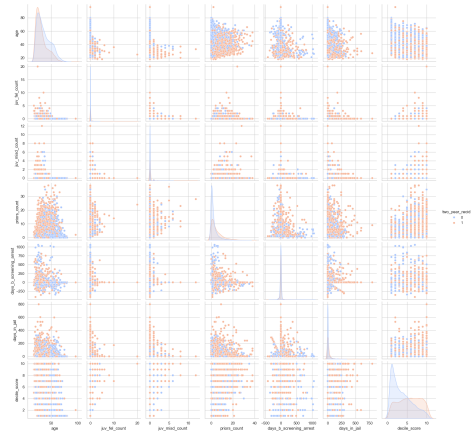


Fig. 15

(**decile_score**) is predictive to a certain extent of recidivism.

- A correlation of 0.30 indicates that being African-American is moderately associated with higher decile scores, raising potential concerns about racial bias in the scoring system. At the same time, Caucasian individuals correlate -0.19 and, therefore, are less likely to receive higher risk scores.
- The time spent in jail has only a small positive relationship with the likelihood of re-offending within two years
- Juvenile felony, misdemeanour, and other counts are positively correlated, indicating that individuals with one type of juvenile record will often have other types.

Figure 15 is a pair plot created to substantiate these observations further to show the relationships among the selected numerical features, with the recidivism outcome (**two_year_recid**) as the hue.

- **age** vs **priors_count**. Younger individuals tend to have fewer prior offences, but the prior count is scattered as age increases, showing that younger offenders tend to continue having problems with the judicial system.
- **age** vs **decile_score**. Older individuals tend to have lower decile scores. Younger individuals are associated with higher scores.

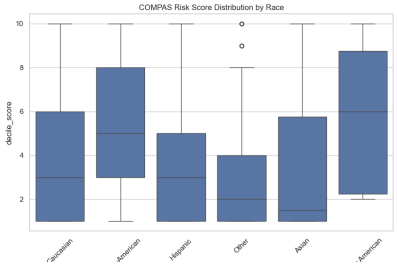


Fig. 16

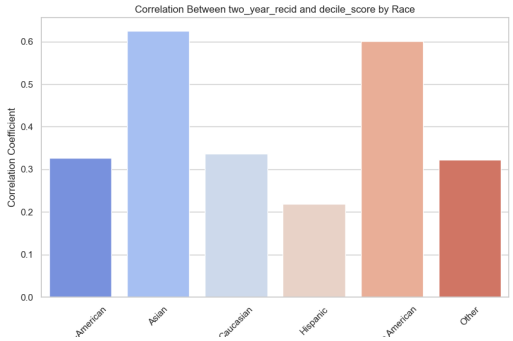


Fig. 17

- **priors_count** vs **decile_score**. Positive trend: Higher priors count leads to higher decile scores, suggesting a strong correlation, indicating the tendency for offenders to be viewed as a risk community
- The distribution of **decile_score**. Two-year recidivists tend to cluster at higher decile scores (6–10 range). Non-recidivists are spread more evenly across scores.

E. Analysis of decile score relationship with race

The COMPAS dataset has been extensively discussed in recent years regarding the fairness of the scores assigned to individuals, especially considering the race component. Although the tool does not use race as one of the features in decile score prediction, there are concerns that race can be associated indirectly with other features. In this section, we will look at the data from the race point of view to see what patterns we can deduce from the dataset.

As a first step, we create a boxplot to compare the distribution of **decile_score** across different racial groups.

From this plot, we notice that African Americans have higher median scores and broader distributions, which suggests a potential bias in the COMPAS scoring system. In addition, Hispanics, Asians, and Other groups scored lower on average, which may indicate differences in the risk assessment process or underlying data inputs.

We then investigated the correlation of **decile_score** with **two_year_recid** by race:

- Asians and Native Americans show the highest correlations, indicating that, for these groups, COMPAS scores align more closely with observed recidivism outcomes.

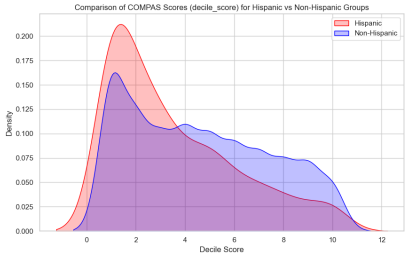


Fig. 18

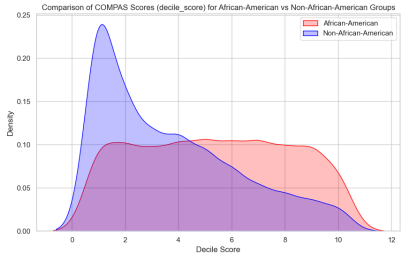


Fig. 19

However, it is important to remember that these groups comprise a tiny percentage of the population.

- African-Americans, Caucasians, and Others have moderate correlations, so COMPAS scores are somewhat predictive for these groups but not as strongly as for Asians or Native Americans.
- The correlation between **`two_year_recid`** and **`decile_score`** for Hispanics is 0.22, the lowest among the groups, suggesting that for Hispanic individuals, the COMPAS scores are less predictive of actual recidivism outcomes than other racial groups. The low correlation for the Hispanic group is an area of concern because if the COMPAS scores do not accurately predict recidivism for this ethnicity, this could mean that the scoring system may overestimate or underestimate their actual risk, which could lead to misclassification of individuals, leading to potential unfair treatment, for example, harsher parole conditions, sentencing).

The distribution of **`decile_score`** for Hispanic individuals was then compared with that of other racial groups using kernel density plots (KDE).

The plots show that the peak density for Hispanic individuals occurs at a lower score of around 2. In contrast, non-Hispanic individuals have a flatter distribution extending to higher scores, albeit peaking in the same region, suggesting that Hispanic individuals are more likely to receive lower COMPAS scores than non-Hispanic individuals.

One has to note that we have previously seen that Hispanic individuals account for 8.8% of the population, which is significantly smaller compared to African-American and Caucasian groups. Although by any means not conclusive, these aspects raise questions about how risk scores are calibrated for underrepresented groups.

1) Analysis of the African-American sector: We created another density plot to compare the distribution of risk scores between African-American individuals and non-African-American individuals.

Here, we notice that African Americans are more likely to receive risk scores in the higher decile range, exceeding a value of six, than non-African Americans, suggesting that the COMPAS tool systematically assigns higher risk scores to African Americans. As noticed previously, non-African-American individuals show a strong peak at around a score of 2, with fewer individuals in this group receiving scores in the higher ranges.

This disparity in score distributions raises concerns about potential bias in the COMPAS scoring system. African Americans appear to be disproportionately classified as higher risk, a factor which could impact downstream decisions such as sentencing or parole.

F. Robustness of ***`decile_score`***

As a final analysis, we compare **`decile_score`** with **`two_year_recid`** to see how many high-risk individuals receded and how many individuals categorised as low-risk did not. This metric is very powerful, as it assesses the validity of the predicted risk metric. Throughout this study, we will also use this test to validate our predicted scores for the machine learning models.

An important decision in this exercise is the selection of the decile score threshold that will dictate that values above it are more likely to recidivate and those below it not. In order to do this, we compared the decile score and two-year record for multiple thresholds. We examined the number of true negatives (the individuals with a decile score lower than the threshold and did not recidivate), true positives (those with a decile score higher or equal than the threshold and did recidivate) and false positives and negatives, and obtained the following results:

Threshold	True Neg	False Pos	True Pos	False Neg
4	2129	1046	964	1632
5	2433	742	1243	1353
6	2661	514	1529	1067
7	2849	326	1805	791
8	2979	196	2087	509

TABLE II: Decile Score Threshold Results

We then used these results to calculate the sensitivity, specificity, precision and accuracy:

Threshold	Sensitivity	Specificity	Precision	Accuracy
4	0.628659	0.670551	0.60941	0.651707
5	0.521186	0.766299	0.645823	0.656039
6	0.411017	0.83811	0.674889	0.645989
7	0.3047	0.897323	0.708147	0.63074
8	0.196071	0.938268	0.721986	0.604401

TABLE III: Performance Metrics for Different Decile Score Thresholds

Following this procedure, a threshold of 5 was decided to provide the best balance of these metrics. With this threshold, the total accuracy and precision are moderate, indicating that while the model performs reasonably well overall, there is room for improvement. We notice a low sensitivity compared to specificity; the model is better at identifying non-recidivists than recidivists.

The metrics for each racial group were then calculated with this threshold.

The Caucasian group has a relatively high specificity but low sensitivity, indicating the COMPAS model more effectively avoids false positives but struggles to identify true positives.

The African-American group shows higher sensitivity but lower specificity compared to Caucasians. This suggests the model identifies more recidivists among African Americans but at the cost of more false positives.

The Hispanic group has low sensitivity, meaning the model struggles significantly to identify true positives in this group. Precision is also the lowest, indicating a high false-positive rate.

The significant disparity in sensitivity and specificity across racial groups highlights potential fairness issues in the model's predictions. For example, the model disproportionately favours Caucasians and Asians in terms of specificity while penalizing African-Americans with higher false-positive rates.

References

[1] Sergey Ioffe. "Batch normalization: Accelerating deep network training by reducing internal covariate shift". In: *arXiv preprint arXiv:1502.03167* (2015).

[2] Will Penny. "Mathematics for Brain Imaging". In: (2008).

[3] Jianxin Wu. "Introduction to convolutional neural networks". In: *National Key Lab for Novel Software Technology. Nanjing University. China* 5.23 (2017), p. 495.

[4] Naimin Zhang. "Momentum algorithms in neural networks and the applications in numerical algebra". In: *2011 2nd International Conference on Artificial Intelligence, Management Science and Electronic Commerce (AIMSEC)*. IEEE. 2011, pp. 2192–2195.

APPENDIX

Field Name	Description	Type	Options (if Categorical)	Used
id	Unique identifier for each individual.	Numeric	N/A	No
name	Full name of the defendant	Text	N/A	No
first	First name of the defendant (anonymized).	Text	N/A	No
last	Last name of the defendant (anonymized).	Text	N/A	No
compas_screening_date	Date of the COMPAS assessment.	Date	N/A	Yes
sex	Gender of the defendant.	Categorical	Male, Female	Yes
dob	Date of birth of the defendant.	Date	N/A	No
age	Age of the defendant at the time of assessment.	Numeric	N/A	Yes
age_cat	Age category of the defendant.	Categorical	Less than 25 25 - 45 Greater than 45	Yes
race	Race of the defendant.	Categorical	African-American Caucasian Hispanic Asian Native American Other	Yes
juv_fel_count	Number of juvenile felony offenses.	Numeric	N/A	Yes
juv_misd_count	Number of juvenile misdemeanor offenses.	Numeric	N/A	Yes
juv_other_count	Number of other juvenile offenses.	Numeric	N/A	Yes
priors_count	Number of prior offenses (adult and juvenile).	Numeric	N/A	Yes
days_b_screening_arrest	Days between arrest and COMPAS screening.	Numeric	N/A	Yes
c_jail_in	Jail booking date for the charge.	Date	N/A	No
c_jail_out	Jail release date for the charge.	Date	N/A	No
c_case_number	Case number associated with the charge.	Text	N/A	No
c_offense_date	Date of the alleged offense.	Date	N/A	No
c_arrest_date	Arrest date for the charge.	Date	N/A	No
c_charge_degree	Degree of the charge.	Categorical	F (Felony) M (Misdemeanor)	Yes
c_charge_desc	Description of the charge.	Text	Free text	No
is_recid	reoffended after COMPAS screening.	Binary	0 (No), 1 (Yes)	No
r_case_number	Case number for the re-offense.	Text	N/A	No
r_charge_degree	Degree of the re-offense charge.	Categorical	F (Felony) M (Misdemeanor)	No
r_charge_desc	Description of the re-offense charge.	Text	Free text	No
r_jail_in	Jail booking date for the re-offense.	Date	N/A	No
r_jail_out	Jail release date for the re-offense.	Date	N/A	No
two_year_recid	Label: offense within two years.	Binary	0 (No), 1 (Yes)	Yes
decile_score	COMPAS risk score (1-10).	Numeric	1–10	Yes
score_text	Risk category for general recidivism.	Categorical	Low, Medium, High	Yes
v_type_of_assessment	Type of COMPAS assessment conducted.	Text	Risk of Recidivism	No
v_decile_score	Violent recidivism COMPAS score (1-10).	Numeric	1–10	No
v_score_text	Risk category for violent recidivism.	Categorical	Low, Medium, High	No
start	Start date of the two-year recidivism period.	Date	N/A	No
end	End date of the two-year recidivism period.	Date	N/A	No
event	offense during the two-year period.	Binary	0 (No), 1 (Yes)	No