Configuration Manual

MSc Research Project
Artificial Intelligence for Business

Khin Sandar Win
Student ID: 24140627

School of Computing
National College of Ireland

Supervisor: Victor del Rosal

National College of Ireland

MSc Project Submission Sheet

School of Computing

Student Name:	Khin Sandar Win ………………………………………………………………………………………………
Student ID:	x24140627 ………………………………………………………………………………………………….……
Programme:	AI for Business ……………………………………………………………… **Year:** 2025 …………………………..
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Lecturer:	Victor del Rosal ……………………………………………………………………………………………….………
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Configuration Manual

Khin Sandar Win
Student ID: x24140627

1 Introduction

The purpose of this Configuration Manual is to provide a detailed, step-by-step guide to reproduce the research project results on the topic: "Beyond Bias with Q-FRE: Benchmarking a Quantum Machine Learning Framework for Fair Recruitment."

This document describes the hardware specifications, software requirements, and the specific implementation architecture required to implement the Quantum-Fairness Recruitment Engine (Q-FRE).

1.1 Intended Audience

This manual assumes that the reader has some familiarity with Python, Conda environments, and Jupyter Notebooks. No prior knowledge of quantum computing is necessary, as all quantum workflows are run using classical simulation offered by Qiskit.

1.2 Technical Constraint & Solution

During the development of Q-FRE a critical library incompatibility was detected between the quantum simulation framework and the explainability framework:

i. Qiskit (required for VQC/QNN) necessitates NumPy >= 2.0 for recent features.
ii. SHAP (required for model interpretability) necessitates NumPy < 2.0.

To address this without compromising functionality, this project adopts a Dual-Environment Architecture. This manual guides the user through process of setting up two different, independent Python environments in order to successfully run the respective workflows.

2 System Requirements

2.1 Hardware Specifications

The experiments were executed on a standard consumer-grade laptop. No dedicated Quantum Processing Unit (QPU) is required, as it is replaced by the Qiskit Statevector Simulator for ideal quantum circuit execution.

Processor (CPU)	Intel Core i5 / AMD Ryzen 5 or higher (Recommended: i7 for faster circuit simulation).
RAM	Minimum 8GB (Recommended: 16GB to handle the 1,470 x 30-dimensional dataset)
Storage	At least 2GB of free space for Anaconda environments and datasets
Operating System	Windows 10/11, macOS, or Linux (Ubuntu 20.04+).

2.2 Software Prerequisites

Anaconda Distribution	Required for managing the conflicting Python environments
Python	Version 3.9 (Standard across both environments).
Jupyter Notebook	For code execution and visualization

3 Environment Architecture Strategy

The technical architecture is divided into two specialized environments in order to ensure library compatibility while maintaining result consistency.

Table 1: Environment Purpose Summary

Environment	Purpose	Key Libraries	Notebook
quantum_ml	Quantum ML experimentation	Qiskit, NumPy $\geq$ 2.0	quantum_ml_notebook.ipynb
classical_xai	Classical ML & Explainability	SHAP, NumPy < 2.0	classical_xai_notebook.ipynb

The following diagram demonstrates the execution flow and how the two environments interact with the shared data and results folder.

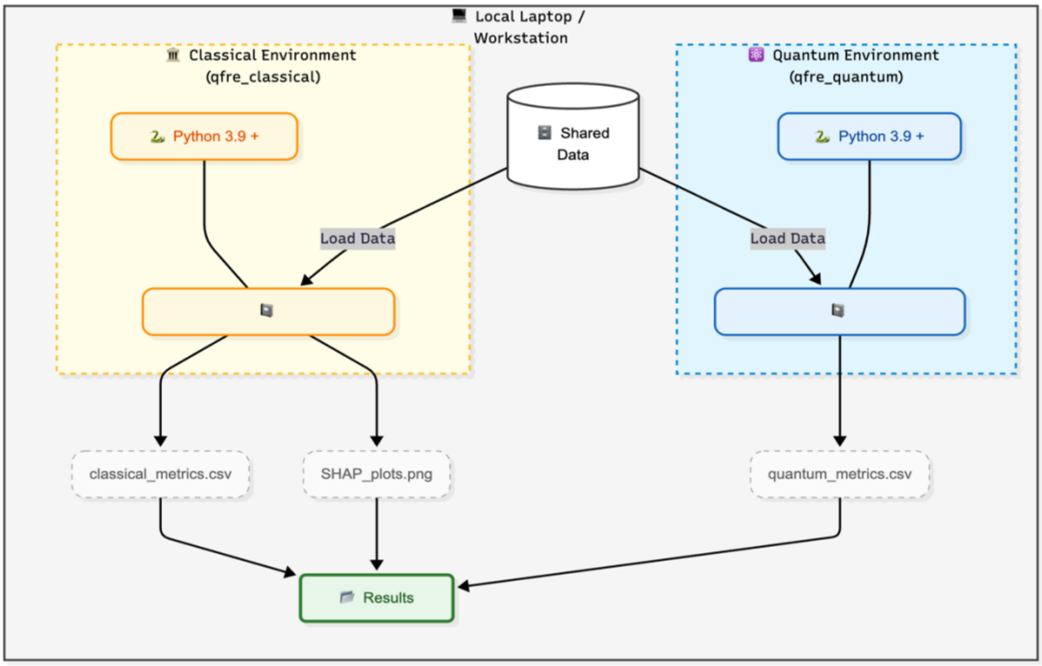

Figure 1: Dual-Environment Architecture Workflow

4 Installation and Configuration Steps

Step 1: Install Anaconda

1. Download the Anaconda distribution from https://www.anaconda.com/.
2. Run the installer following the on-screen instructions.
3. Once installed, open Anaconda Prompt (Windows) or Terminal (macOS/Linux).

Step 2: Configure the Quantum Environment

This environment is used only to execute quantum_ml_notebook.ipynb. It installs the Qiskit stack which is required for the Variational Quantum Classifier (VQC) and Quantum Neural Network (QNN).

1. **Create the environment:**

   conda create --name quantum_ml python=3.9

2. **Activate the environment:**

   conda activate quantum_ml

3. **Install the required libraries:**

   pip install qiskit==0.39.0 qiskit-machine-learning
   pip install pandas matplotlib seaborn scikit-learn imbalanced-learn
   pip install ipykernel

4. **Register this environment with Jupyter:**

   python -m ipykernel install --user --name=quantum_ml --display-name “Python (Q-FRE Quantum)”

Step 3: Configure the Classical Environment

This environment is used exclusively to execute classical_xai_notebook.ipynb. It installs specific versions of libraries SHAP and NumPy to ensure the explainer functions work correctly.

1. **Create the environment:**

   conda create --name classical_xai python=3.9

2. **Activate the environment:**

   conda activate classical_xai

3. **Install the required libraries (Note the specific numpy constraint):**

   pip install "numpy<2.0"
   pip install shap==0.41.0
   pip install scikit-learn pandas matplotlib seaborn imbalanced-learn
   pip install ipykernel

4. **Register this environment with Jupyter:**

   python -m ipykernel install --user --name=classical_xai --display-name “Python (Q-FRE Classical)”

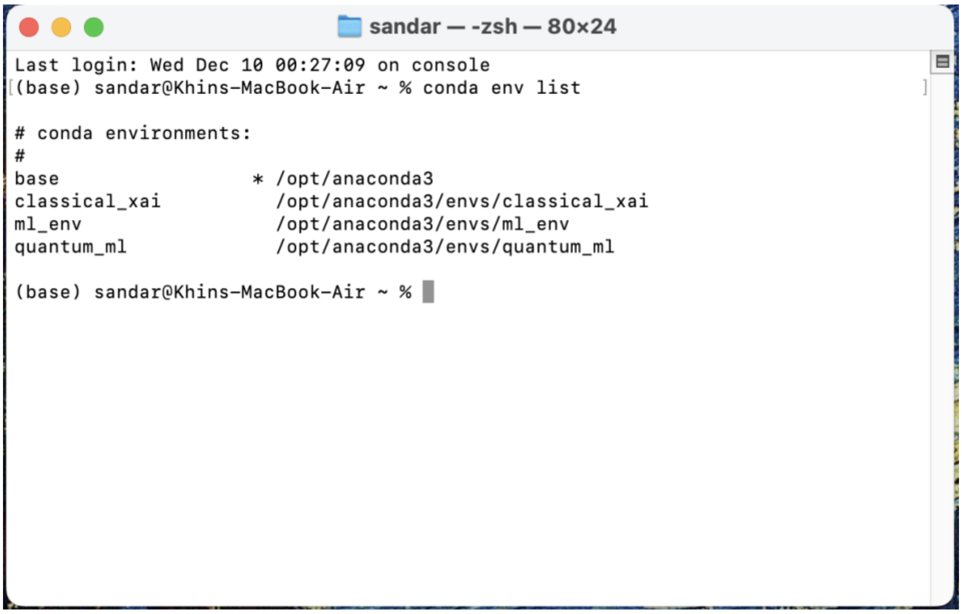

Figure 2: Verification of installed environments.

Step 4: Configure the Classical Environment

Before running full experiments, verify isolation by checking versions:

- **Quantum:** Run import qiskit inside quantum_ml. Expected Qiskit version: 0.39.0.
- **Classical:** Run import shap inside classical_xai. Expected NumPy version: < 2.0.

5 Project Directory Structure

To ensure the code executes without path errors, arrange your project folder exactly as follows: Note: The results/ folder is created automatically when the script is run if it does not already exist.

```
Q-FRE_Project_Root/
├── data/
│   └── WA_Fn-UseC_-HR-Employee-Attrition.csv
│       (IBM HR Analytics Dataset, sourced from Kaggle)
│
├── notebooks/
│   ├── quantum_ml_notebook.ipynb
│   │   (Executed within the quantum_ml environment)
│   └── classical_xai_notebook.ipynb
│       (Executed within the classical_xai environment)
│
└── results/
    ├── classical_metrics.csv
    ├── quantum_metrics.csv
    └── Visual outputs (e.g., confusion matrices, SHAP plots)
```

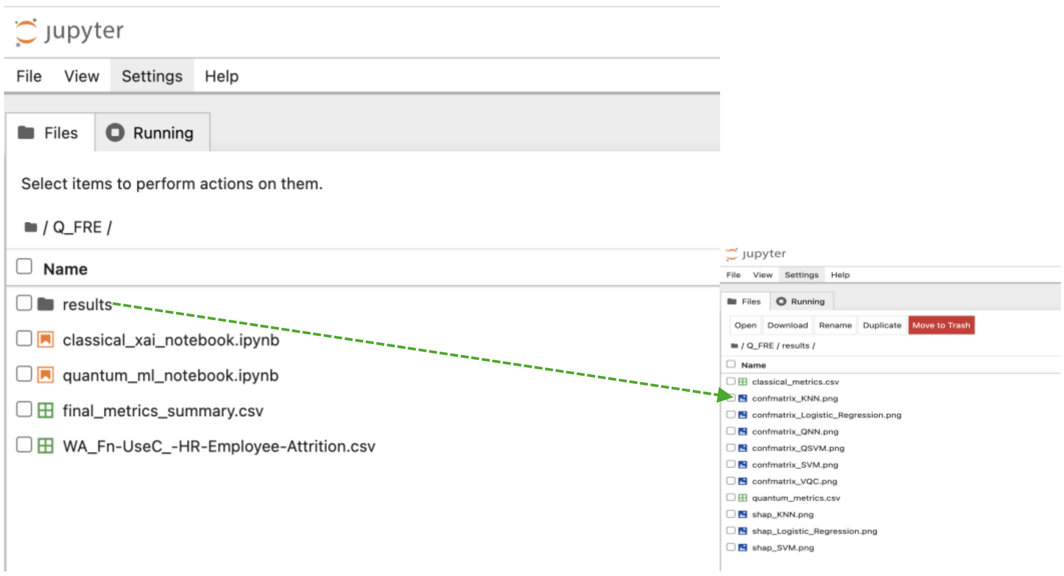

Figure 3: Actual Project Directory Structure.

6 Execution Guide

6.1 Phase A: Running the Quantum Models

1. Launch Jupyter Notebook:

   jupyter notebook

2. Open quantum_ml_notebook.ipynb from the project folder.
3. CRITICAL STEP: Go to the Menu Bar → Kernel → Change Kernel → Select Python (Q-FRE Quantum).

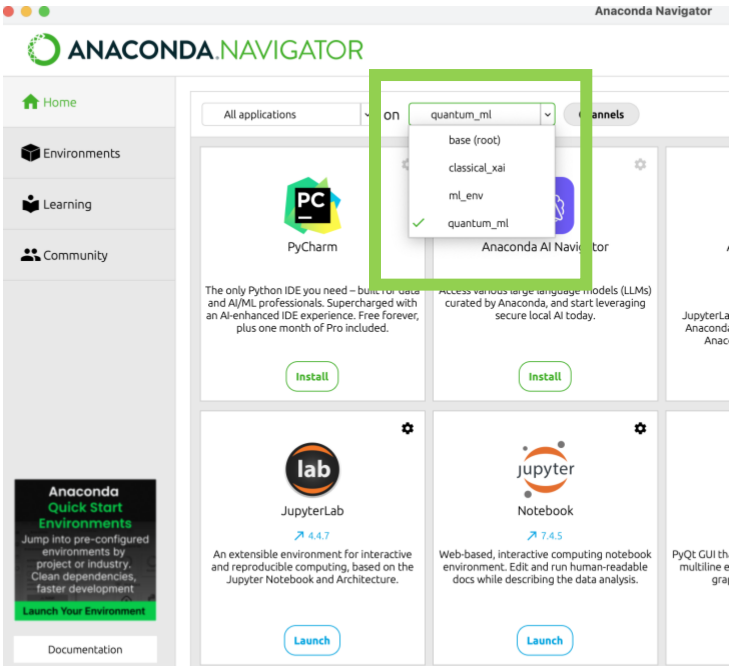

Figure 4: Selecting the correct kernel for quantum execution.

4. Run all cells.

   i. Process → The notebook performs PCA, defines the Z-Feature Map, and trains the VQC and QNN using the COBYLA optimizer (100 iterations).

   ii. Output → Generates quantum_metrics.csv and confusion matrix images in the results/ folder.

6.2 Phase B: Running Classical Models & SHAP

1. Open classical_xai_notebook.ipynb from the project folder.
2. CRITICAL STEP: Go to the Menu Bar → Kernel → Change Kernel → Select Python (Q-FRE Classical).

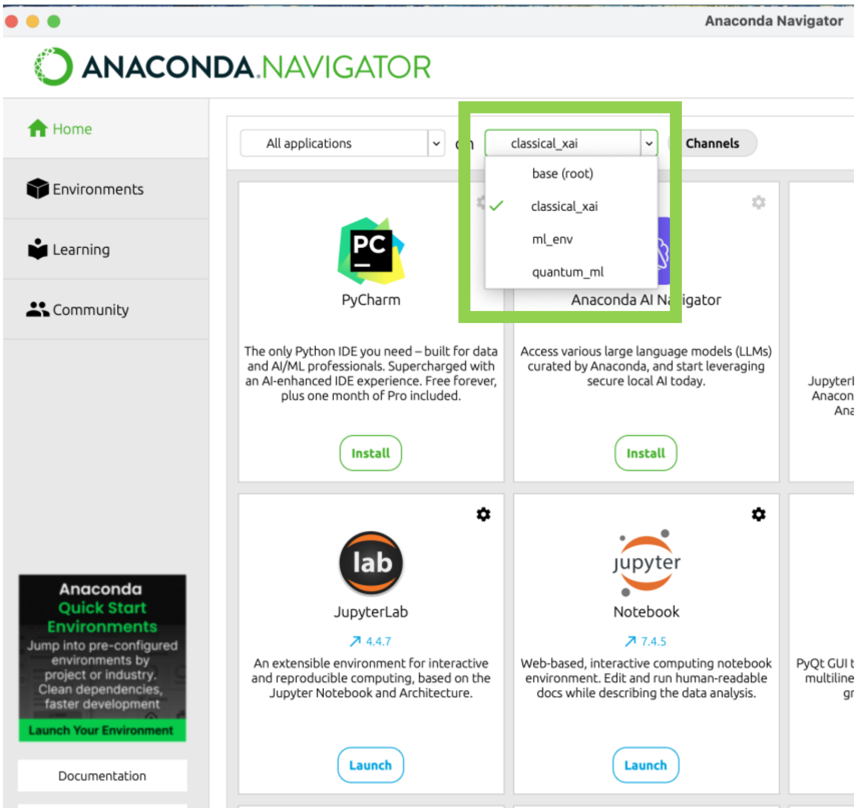

Figure 5: Selecting the correct kernel for quantum execution.

3. Run all cells.

   i. Process → Trains Logistic Regression, SVM, and KNN. Then, runs the SHAP KernelExplainer to generate feature importance plots.

   ii. Output → Generates classical_metrics.csv and SHAP summary plots in the results/ folder.

Note on Reproducibility: To ensure reproducibility, fixed random seeds (e.g., random_state=42) are used for splitting dataset and initialization of model where applicable. Minor numerical variations can still occur as a result of the stochastic nature of quantum simulation on classical hardware.

7 Troubleshooting

Issue	Probable Cause	Solution
ImportError: Numba needs NumPy 1.21...	Wrong Kernel	You are likely running SHAP code in the Quantum environment. Switch the kernel to Q-FRE Classical.
ModuleNotFoundError: No module named 'qiskit'	Wrong Kernel	You are likely running Quantum code in the Classical environment. Switch the kernel to Q-FRE Quantum.
Long Runtime (>1 hour)	Simulation Overhead	Quantum simulation is CPU-intensive. To speed up testing, reduce the maxiter parameter in the COBYLA optimizer from 100 to 20 inside quantum_ml_notebook.ipynb.
FileNotFoundError	Path Issue	Ensure the dataset is located inside a folder named data within the project root, as described in Section 5.

8 References

IBM (n.d.) *HR Analytics Employee Attrition & Performance*. Available at: https://www.kaggle.com/datasets/pavansubhasht/ibm-hr-analytics-attrition-dataset [Accessed 1 August 2025].