**Classical Pre-processing: Overview of the Hyperparameter Optimisation Algorithm**

**Avner Bensoussan, Elena Chachkarova, Karine Even-Mendoza, Sophie Fortz, Connor Lenihan**

**King's College London, Faculty of NMES**

**June 2024**

The provided algorithm optimises hyperparameters for a quantum problem by leveraging a Regularising Gradient Boosting Regression (XGBoost), divided into three stages: data preparation, model training, and hyperparameter optimisation.

**Data Preparation:** We add opensource commonly used molecular Hamiltonians (H2O, LiH, BeH2, Hc and H chain) and combine them with the provided Hamiltonians of 20 qubits or less, run the wrapper in classical mode while giving a randomly generated set of hyperparameters each time, and record the energy level as the score. We repeat it. As a result, we have a data array to train a Regularising Gradient Boosting Regression (XGBoost). We store generated data—consisting of hyperparameter vectors (Xs) and their corresponding energy levels (Ys)—for further processing.

**Model Training:** Our algorithm uses an XGBoost model to predict the best hyperparameters. Before training, it ensures all data vectors are of consistent length by padding them as needed. We split the padded data array into training and testing sets. We then train, test and evaluate the model's performance.

**Hyperparameter Optimisation:** With the XGBoost model trained, the algorithm proceeds to predict the optimal hyperparameters for a given Hamiltonian of 28 qubits. It generates a series of hyperparameter vectors and uses the XGBoost model to predict their performance. We return the vector with the minimum score (predicted energy level) as the optimal set of hyperparameters. Finally, the algorithm runs adapt-QSCI with the optimised hyperparameters.