QUANTUM ANNEALING: AN INSIGHT INTO ITS CURRENT POTENTIAL

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Introduction

The research question of my investigation is “To what extent do current quantum annealers outperform classical computers?”. Quantum annealing is an emerging technology that promises important progress in the quantum computing sector. The possible applications it has are problems where low-energy states are required. For instance, optimisation problems or probabilistic sampling problems. In this investigation I focused on formulating optimisation problems and solving them in D-Wave Systems’ quantum annealer to give an insight into the various real-world applications that quantum annealing has. Concretely, I have solved two new problems of chess, that had not been solved with quantum annealing before, and a common travelling salesman problem, that gives some insight into the potential real-world applications of quantum computing. Furthermore, the main focus of the investigation is the implementation of a support vector machine algorithm in D-Wave System’s annealer. The first step was to formulate the problem as a quadratic unconstrained binary optimisation (QUBO) problem using a specific encoding. Several adaptations had to be made in order to overcome issues of physical embedding and connectivity limitations of D-Wave’s Chimera architecture. These implied the use of sampling techniques, so, in the end, my proposal of a quantum support vector machine was a combination of optimisation and sampling. Finally, the classification performance of this new quantum approach was extremely successful and it will probably outperform classical algorithms sooner than we expect. After this investigation, I genuinely believe that this new upcoming field of quantum information opens another perspective to the computational problems that will exceed the classical computer’s performance.

Hypothesis

Given the potential of the current D-Wave System’s annealer in terms of number of qubits, I expect that the algorithm will be efficient regarding the time of computation, thanks to quantum parallelism, and will produce satisfactory classification results, as the QUBO formulation proposed fulfils many of the conditions of the classical support vector machine algorithm.

Objectives

The objectives of this investigation are the formulation of two own chess problems, mainly for divulgation and illustrative purposes, and the formulation and implementation of a support vector machine algorithm in a quantum annealer, as well as the comparison of its classification performance with that of the classical algorithm executed with two real datasets.

Methodology

The support vector machine (SVM) is a supervised machine learning algorithm used mainly for binary classification, although it can be extended to multi-class classification. The classifier separates the data points of each class with an optimal hyperplane. The training of an SVM is expressed as an unconstrained optimisation problem of Lagrangian multipliers, which are real values, from which you can calculate the equation of the separating hyperplane. Knowing that, new points can be classified with a decision rule. With the testing data, the SVM model can predict all the data points belonging to this set and compare the predictions with the actual labels, the actual class of each point, and evaluate the performance of the SVM. I followed this process for both the classical approach and the quantum approach.

To formulate the problem of minimisation for training the SVM as a QUBO, I had to make an encoding so that the Lagrangian multipliers could be represented by binary variables, the qubits. Moreover, since the actual quantum computer of D-Wave has limitations in the number of qubits and their connectivity, I had to use less samples for training the model and use some sampling techniques to overcome issues and fulfil some constraints. When pursuing the sampling solution to the physical limitations, I had to optimise the size of samples of data trained at a time in order to embed the configuration into the Chimera topology of the annealer, as seen in Figure 1. I will not get into the details of my proposal of the quantum support vector machine but I do want to comment on its performance with two datasets I tested, as explained in the following section.

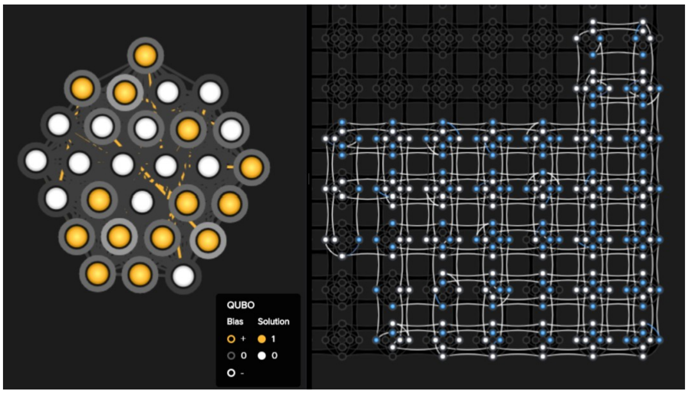

Figure 1: Physical embedding of a sample of data

Results

I used a breast cancer dataset [11] to classify tumours as benign or malign and a pulsar dataset [12] to classify stars as pulsars or non-pulsars. I executed both the classical SVM and the quantum SVM and compared their performance and surprisingly both models were outstandingly good. Their classification metrics were really high, higher than 0.8 in all cases, in both datasets and for the breast cancer dataset the quantum SVM actually outperformed the classical model slightly so it is completely satisfactory. Still, there remains room for improvement and changes to be made to the quantum model so that it reaches the point of exceeding the classical computer's performance, but I genuinely believe that in a near future this will be achieved.

Conclusions

In my exploration, through the proposal of a quantum support vector machine algorithm, not only have I proven that it is indeed possible to perform this machine learning algorithm in a quantum annealer but I have also proven that its classification performance is outstandingly successful.

Programs

The chess problems that I have solved are the knight's tour (https://github.com/carlacarov/d-wave-projects/blob/master/the-knights-tour-pos.py) and the n-queens problem . Also, I have developed an application for the n-queens problem, found at https://n-queens-dwave.herokuapp.com/. Also, I have programmed a travelling salesman problem, for which I also created an application https://travelling-salesman-dwave.herokuapp.com/. You can also see the code for the SVMs in https://github.com/carlacarov/d-wave-projects/blob/master/quantum-svm.py.

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