A STUDY OF SCALARISATION TECHNIQUES FOR MULTI-OBJECTIVE QUBO SOLVING*

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ABSTRACT

In recent years, there has been significant research interest in solving Quadratic Unconstrained Binary Optimisation (QUBO) problems. Physics-inspired optimisation algorithms have been proposed for deriving optimal or sub-optimal solutions to QUBOs. These methods are particularly attractive within the context of using specialised hardware, such as quantum computers, application specific CMOS and other high performance computing resources for solving optimisation problems. Examples of such solvers are D-wave’s Quantum Annealer and Fujitsu’s Digital Annealer. These solvers are then applied to QUBO formulations of combinatorial optimisation problems. Quantum and quantum-inspired optimisation algorithms have shown promising performance when applied to academic benchmarks as well as real-world problems. However, QUBO solvers are single objective solvers. To make them more efficient at solving problems with multiple objectives, a decision on how to convert such multi-objective problems to single-objective problems need to be made. In this study, we compare methods of deriving scalarisation weights when combining two objectives of the cardinality constrained mean-variance portfolio optimisation problem into one. We show significant performance improvement (measured in terms of hypervolume) when using a method that iteratively fills the largest space in the Pareto front compared to a naïve approach using uniformly generated weights.

Keywords Digital Annealer, QUBO, Multi-objective optimisation, Adaptive Scalarisation

Keywords Multi-objective, Quadratic Unconstrained Binary Optimisation, Cardinality Constrained Mean-Variance Portfolio Optimisation Problem, Digital Annealer, Scalarisation

1 Introduction

In recent years, there has been significant research interest in solving Quadratic Unconstrained Binary Optimisation (QUBO) formulations of optimisation problems. This is a common formulation used by hardware solvers classified as quantum or quantum-inspired machines. They have been shown to achieve a speed up compared to classical optimisation algorithms implemented on general purpose computers Ayodele [2022a]. Ising machines such as Fujitsu’s

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Digital Annealer (DA) Hiroshi et al. [2021] and D-wave’s Quantum Annealer McGeoch and Farré [2020] are single objective solvers. Many optimisation problems however have more than one objective, e.g. the Cardinality Constrained Mean-Variance Portfolio Optimisation Problem (CCMVPOP) Chang et al. [2000] considered in this study entails selecting assets that maximise returns while minimising the associated risks. Typically, multi-objective problems are converted to single objective problems before the Ising machines are applied to them. For example, the $c$-constraint approach was used in the Quantum Annealer to solve a portfolio optimisation problem Phillipson and Bhatia [2021]. Scalarisation has also been used when solving multi-objective QUBO in previous work Zhou et al. [2018], Ayodele et al. [2022]. One of the main challenges to using scalarisation is how to define a set of weights resulting in a diverse set of solutions on the Pareto front (PF). A common approach is to generate weights uniformly using, for example, the simplex lattice design Zhou et al. [2018]. However, a uniform choice of weights does not necessarily translate to a diverse set of Pareto-optimal solutions Liefooghe et al. [2015], Zhou et al. [2018]. Previous studies have therefore also considered iterative method which uses a dichotomic procedure to derive new weights perpendicular to two solutions that have the largest distance between them Dubois-Lacoste et al. [2011], Liefooghe et al. [2015]. In this study, we propose a method for deriving scalarisation weights which targets less explored regions of the PF. The proposed method utilises the weights used during previous scalarisations in addition to the relative position of the corresponding solutions in the PF and relies less on the weights and fitness being perfectly correlated.

The following section presents the problem description of the CCMVPOP. Methods of generating scalarisation weights used in this study are described in Section 3. Results and conclusions are presented in Sections 4 and 5.

2 Cardinality Constrained Mean-Variance Portfolio Optimisation Problem

Portfolio Optimisation entails selecting assets that maximise returns while minimising the associated risks. In the CCMVPOP Chang et al. [2000], cardinality constraints on the number of asset types to be considered are imposed. Given the number of asset types to consider ($n$), the fixed number of assets a portfolio must contain ($K$), the expected return of asset $i$ ($\mu_i$) and the covariance between assets $i$ and $j$ ($\sigma_{i,j}$), the minimum ($\epsilon_i$) and maximum ($\delta_i$) proportion of a chosen asset $i$, we aim to find the proportion of each asset $i$ to hold ($w_i \in [0, 1]$). Binary variables $z_i$ are used to indicate whether an asset $i$ is selected or not. The CCMVPOP is formally defined as follows.

\[
\text{minimise} \quad \lambda_1 \left( \sum_{i=1}^{n} \sum_{j=1}^{n} w_i w_j \sigma_{i,j} \right) + \lambda_2 \left( - \sum_{i=1}^{n} w_i \mu_i \right) \\
\text{subject to} \quad \sum_{i=1}^{n} w_i = 1, \quad \sum_{i=1}^{n} z_i = K \\
\epsilon_i z_i \leq w_i \leq \delta_i z_i, \quad z_i \in \{0, 1\}, \quad i = 1, \ldots, n
\]

The first objective is the first term in Eq. (1) and minimises the risk (sum of covariance between all pairs $i,j$ of chosen assets) of the chosen assets of the portfolio. The second objective is the second term in Eq. (1) and maximises returns (sum of expected return of each asset $i$) of chosen assets. A negative sign is appended to the second objective to convert it to a minimisation problem. $\lambda = (\lambda_1, \lambda_2)$ is a set of scalarisation weights. The cardinality constraint (Eq. 2) forces the number of chosen assets to be equal to $K$, and Eq. (3) ensures the proportion of a chosen asset $w_i$ to be within given bounds. The QUBO formulation of the CCMVPOP ($K = 10$, $\epsilon_i = 0.01 \delta_i = 1$) used is based on the binary representation presented in Parizy et al. [2022].

3 Scalarisation Methods

In Ayodele et al. [2022], a scalarisation framework, Scalarisation Based DA (SB-DA), was proposed for obtaining multiple non-dominated solutions for the bi-objective quadratic assignment problem formulated as QUBO. A CPU implementation of the 1st generation DA algorithm Aramon et al. [2019] was used in that study. However, in this study, we use the 3rd generation DA Hiroshi et al. [2021] which is designed to be faster and more efficient than previous generations of the DA, it also benefits from hardware speedup Hiroshi et al. [2021]. For simplicity, we use DA to refer to 3rd generation DA in the rest of this work.

We propose two extensions of the SB-DA, which we call SB-DAs and SB-DAi (Alg. 1). Parameters $B$, $D$ and $G$ are QUBO matrices representing the first objective, second objective and constraint functions, respectively. The number of scalarisation weights is denoted by $k$ and time is the total time allowed for all DA executions. To allow more solutions to be considered for non-dominance, $n_{top}$ is a parameter used to define the number of top solutions (solutions with the lowest energies) to be returned during each DA execution. In this study, we compared three
Algorithm 1 SB-DA Algorithm

Require: $B$, $D$, $k$, $time$, $n_{top}$, s_type
1: $\Lambda \leftarrow \{(0, 1), (1, 0)\}$
2: if $s_{type}$ in [random, uniform] then Mode $\leftarrow$ static else Mode $\leftarrow$ iterative
3: if $s_{type}$ is random then add $k - 2$ sets of random weights to $\Lambda$
4: if $s_{type}$ is uniform then $\Lambda \leftarrow SLD(H = k, m = 2)$
5: if Mode is static then $A \leftarrow$ execute SB-DAs else $A \leftarrow$ execute SB-DAi
6: return all non-dominated solutions from archive $A$

Algorithm 2 SB-DAi

Require: $B$, $D$, $k$, $time$, $n_{top}$, $\Lambda$
1: $A \leftarrow \emptyset, W \leftarrow \emptyset$ $\triangleright$ Initialise archive and mapping between weights and solutions
2: for each $i \in \{1, \ldots, k\}$ do
3: if $i \leq 2$ then
4: $\lambda = (\lambda_1, \lambda_2) \leftarrow \Lambda$; $R, S \leftarrow B, D$
5: else
6: $R, S \leftarrow rescale(B, D)$
7: $\lambda \leftarrow \emptyset, max_d \leftarrow 0$ $\triangleright$ Initialise weights and maximum distance
8: for $j \in [1, i - 2]$ do
9: $d \leftarrow Distance(W_j, W_{j+1})$ $\triangleright$ Manhattan distance
10: $(\lambda_{sol1}^1, \lambda_{sol2}^1), sol1]$, $((\lambda_{sol1}^2, \lambda_{sol2}^2), sol2] \leftarrow W_j, W_{j+1}$
11: $\lambda_{temp} \leftarrow (avg(\lambda_{sol1}^1, \lambda_{sol2}^1), avg(\lambda_{sol1}^2, \lambda_{sol2}^2))$
12: if $(d > max_d)$ and $(\lambda_{temp} \notin W)$ then $\lambda \leftarrow \lambda_{temp}, max_d \leftarrow d$
13: end for
14: if $\lambda = \emptyset$ then $\lambda \leftarrow$ Random weights $\triangleright$ each set of weights sums to 1
15: end if
16: $Q \leftarrow (\lambda_1 \cdot R + \lambda_2 \cdot S) + \alpha \cdot G$
17: $Y \leftarrow ExecuteDA(Q, n_{top}, time\_limit = \frac{T}{k})$, add all solutions in $Y$ to $A$
18: $W_j \leftarrow [\lambda, Y_0]$ $\triangleright$ save weight and best solution in $Y$
19: end for
20: return $A$

methods of deriving scalarisation weights, s_type set to random, uniform or iterative. Where s_type is set to random, k sets of randomly generated weights are pre-computed. For each set of weights $\lambda = (\lambda_1, \lambda_2)$, $\lambda_1$ is a random value between range $[0, 1]$ while $\lambda_2 = 1 - \lambda_1$. For s_type set to uniform method, k sets of evenly distributed weights are pre-computed. In this study, we use the the Simplex Lattice Design (SLD) (Line 4 of Alg. 1) to generate evenly distributed weights. Where s_type is iterative, weights are derived with the aim of finding solutions that fall within the less crowded region of the Pareto front. To achieve this aim, a mapping between each set of weights and the best solution found by the DA using such set of weights are stored as $W$. $W$ is sorted in ascending order of $\lambda_1$. For any two adjacent solutions in $W$, the manhattan distance between the solutions are recorded. Solutions $sol1$ and $sol2$ that correspond to the largest gap in the Pareto front are saved. A set of scalarisation weights used to derive $sol1$ and $sol2$ are $\lambda_{sol1} = (\lambda_{sol1}^1, \lambda_{sol1}^2)$ and $\lambda_{sol2} = (\lambda_{sol2}^1, \lambda_{sol2}^2)$ respectively. An average of $\lambda_{sol1}$ and $\lambda_{sol2}$ becomes the scalarisation weights used in the new iteration (Lines 9-11). The new set of weights is however only used if this has not been used in previous iterations (Line 12). If there is no unique set of weights that can be derived using this procedure, randomly generated weights are used.

SB-DA can be executed in one of two modes. It is executed in static mode (SB-DAs: Alg. 3), if s_type is random or uniform and in iterative mode (SB-DAi: Alg. 2) if s_type is set to iterative. In SB-DAs, scalarisation weights are pre-computed while in SB-DAi, a set of scalarisation weights at a given iteration is influenced by the set of scalarisation weights used in previous iterations. An iteration of SB-DA refers to a run of the DA with a given set of scalarisation weights. In both modes of the SB-DA, each objective is optimised independently ($\lambda = (0, 1)$ and $\lambda = (1, 0)$) before other weights are used. This is because QUBO matrices $B$ and $D$ are rescaled using information about the Lower Bound (LB) and Upper Bound (UB). These bounds are achieved by minimising each objective independently. LB of $B$ (or $D$) is derived by minimising $B$ (or $D$) independently. Conversely, UB of $B$ (or $D$) is derived by minimising $D$ (or $B$) independently. The LB or UB are updated if smaller or larger energies are found for any individual objective at any iteration of the SB-DA. In Line 4 of Alg. 3 and Line 6 of Alg. 2, $rescale(B, D)$ is computed such that $R = \max_{1 \leq i \leq k}(UB_i)/(UB_1 \cdot LB_1) \cdot B$ and $S = \max_{1 \leq i \leq k}(UB_i)/(UB_2 \cdot LB_2) \cdot D$. This is done to
reduce bias towards any of the objectives, allowing the algorithm to control the bias using the scalarisation weights only. QUBO matrix $Q$ (Alg. 3: Line 5, Alg. 2: Line 16) is an aggregate of QUBO matrices representing the objectives and constraint, penalty weight ($\alpha$) is set using Maximum change in Objective function divided by Minimum Constraint function of infeasible solutions (MOMC) originally proposed in Ayodele [2022]. ExecuteDA (Alg. 3: Line 6, Alg. 2: Line 17) runs DA on $Q$ for $time\_limit$ seconds, returning the non-dominated solutions found amongst the best $n\_top$ solutions. Note that SB-DA proposed in Ayodele et al. [2022] is equivalent to the proposed extended SB-DA when executed with $s\_type$ set to uniform and $n\_top = 1$.

4 Results

To generate the results presented in this section, default parameters of the DA are used. Table 1 shows that the uniform method consistently found the highest number of non-dominated solutions while the iterative method consistently found the lowest number of non-dominated solutions across all problem instances. However, using the proposed iterative method consistently led to the highest hypervolume. Higher hypervolume values were reached because the iterative method was able to find weights that allowed the algorithm to focus on harder and more extreme regions of the search space.

To illustrate the difference between the behaviour of the methods, we show an example of a single run on the CCMVPOP instances in Figures 1 and 2. This shows that the iterative method allowed the algorithm to concentrate on regions of the Pareto front that are harder to reach. To show that this behaviour is consistent across multiple runs, we also present comparison of iterative and uniform using the empirical attainment surface [López-Ibáñez et al., 2010] in Figures 3 and 4 (darker regions show parts where one method is better than the other). This is a visualisation of the Empirical Attainment Function (EAF). The EAF of an algorithm is the probability, estimated from multiple runs, that the non-dominated set produced by a single run of the algorithm dominates a particular point in the objective space. The visualisation of the EAF [Grundert da Fonseca et al., 2001] has been shown as a suitable graphical interpretation of the quality of the outcomes returned by local search methods. The visualisation of the differences between the EAFs of two alternative algorithms indicates how much better one method is compared to another in a particular region of the objective space [López-Ibáñez et al., 2010]. The EAF visualisations were done using the eaf R package.\(^2\) In

\(^2\)http://lopez-ibanez.eu/eaftools

Table 1: Average and standard deviation number of non-dominated solutions and hypervolume across 20 runs of the DA (stopping criteria: 0.05$n$, Number of weights: 10). Hypervolume values have been divided by $10^{25}$. Reference points used for computing the hypervolume values are the sum of all positive QUBO coefficients in $B$ and $D$ ($\sum_{i=1}^{m} \sum_{j=1}^{m} \max\{0, B_{ij}\}, \sum_{i=1}^{m} \sum_{j=1}^{m} \max\{0, D_{ij}\}$). Best values presented in bold (student t-test used for test of significance).

| Problem Instance (n) | Scalarisation Method | Mean ±Stdev Non-dominated solutions | Mean ±Stdev Hypervolume | Mean ±Stdev Non-dominated solutions | Mean ±Stdev Hypervolume |
|----------------------|----------------------|------------------------------------|-------------------------|------------------------------------|-------------------------|
| Port1 (248)          | Random               | 324 ±50                            | 37.06 ±14.38            | 628 ±132                          | 121.64 ±25.30           |
|                      | Uniform              | 354±39                             | 28.71 ±9.50             | 866±51                            | 94.27 ±1.90             |
|                      | Iterative            | 250±25                             | 60.37±0.22              | 417±71                            | 136.46±1.45             |
| Port2 (680)          | Random               | 514±82                             | 159.92±7.79             | 552±112                           | 117.79±25.35            |
|                      | Uniform              | 676±61                             | 155.38±0.86             | 798±49                            | 116.73±1.23             |
|                      | Iterative            | 275±50                             | 164.44±0.92             | 398±49                            | 136.42±2.25             |

\(^{2}\)http://lopez-ibanez.eu/eaftools
Figure 1: Comparing Scalarisation Methods (stopping criteria: 0.05n seconds, Number of weights: 10). plots show the best solution(s) produced by each method (left plot: n_top = 1 and annotated by weights that resulted in the corresponding best solution, right plot: n_top = 1000)

Figure 2: Comparing Scalarisation Methods (stopping criteria: 0.05n seconds, Number of weights: 10). plots show the best solution(s) produced by each method (left plot: n_top = 1 and annotated by weights that resulted in the corresponding best solution, right plot: n_top = 1000)

Figure 3 and 4, we particularly see more darker regions (indicating better performance) using the iterative method on 'Port1' and 'Port3' instances compared to the uniform method.

5 Conclusions

This study compared three simple methods of generating scalarisation weights within the context of bi-objective QUBO solving. The methods were applied to QUBO formulation of the CCMVPOP. We show that considering more
Some areas of future work include, 1. comparing approach on different problems. 2. comparing approach on problems with more than two objectives.

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