On the hardness of quadratic unconstrained binary optimization problems

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QUBO problems

Many discrete optimization problems can be reformulated as QUBO problems with the following cost function [1]

$$C(x_1, \dots, x_N) = \sum_{i,j} Q_{i,j} x_i x_j \qquad (1)$$

where $x_i = 0,1$ and $Q_{i,j} = Q_{j,i}$ is a symmetric $N \times N$ matrix.

A more convenient and equivalent form, i.e., in terms of an Ising model, is defined by the Hamiltonian

$$H = \sum_{1=i<j=N} J_{i,j} S_i S_j + \sum_{i=1}^{N} h_i S_i \qquad (2)$$

where $S_i = \pm 1$.

We investigate three different classes of QUBO problems.

2-Satisfiability problems

A 2SAT problem is specified by N binary variables x_i and a conjunction of M clauses defining a binary-valued cost function

$$C(x_1, \dots, x_N) = (L_{1,1} \cup L_{1,2}) \cap (L_{2,1} \cup L_{2,2}) \cap \cdots \cap (L_{M,1} \cup L_{M,2})$$

where the literal $L_{\alpha,j}$ stands for either $x_{i(\alpha,j)}$ or its negation $\bar{x}_{i(\alpha,j)}$ for $\alpha = 1, \dots, M$ and $j = 1, 2$.

The corresponding formulation of Ising Hamiltonian is given by [2]

$$H_{2SAT} = \sum_{\alpha=1}^{M} h_{2SAT}(\varepsilon_{\alpha,1} S_{i(\alpha,1)}, \varepsilon_{\alpha,2} S_{i(\alpha,2)})$$

where $\varepsilon_{\alpha,j} = +1(-1)$ if $L_{\alpha,j}$ stands for x_i ($\bar{x}_i$) and $h_{2SAT}(S_l, S_m) = (S_l - 1)(S_m - 1)$.

Fully-connected spin glass (RAN)

The spin glass model is defined by the Hamiltonian Eq. (2). The values of all the parameters $J_{i,j}$'s and h_i's are assigned by uniform random numbers in the range $[-1,1]$. Computing the ground state configuration of the spin glass model is, in general, very hard and is proven to be NP-hard.

Fully-connected regular spin glass (REG)

This class of problems is defined by assigning the parameters in Eq. (2) with the following equations

$$J_{i,j} = 1 - \frac{i + j - 2}{N - 1}, \qquad h_i = 1 - \frac{2(i - 1)}{N - 1}$$

Methods

QUBO22:

A computer code that uses GPUs and/or CPUs to solve QUBOs, PUBOs, and Exact cover problems [3]. QUBO22 simply enumerates all 2^N possible configurations while keeping track of those that yield the lowest, next to lowest cost. QUBO22 obviously always finds the true ground state. With the current computer resources, QUBO22 can be applied to solve applications with problem size up to $N = 58$.

Heuristic methods:

For larger problems, heuristic methods of qbsolv and D-Wave Hybrid solver provided by D-Wave are used to find the lowest states.

D-Wave Advantage 5.1 quantum annealer:

A real quantum annealing device is used to solve all the problems mentioned above [4]. The success probability of finding the ground state is calculated by using the state obtained by qbsolv.

Hamming distance

The Hamming distance between the low-lying energy states and the ground state is calculated by exact enumeration for small systems. Representative results for $N = 20$ problem taken from the three problem classes are shown below.

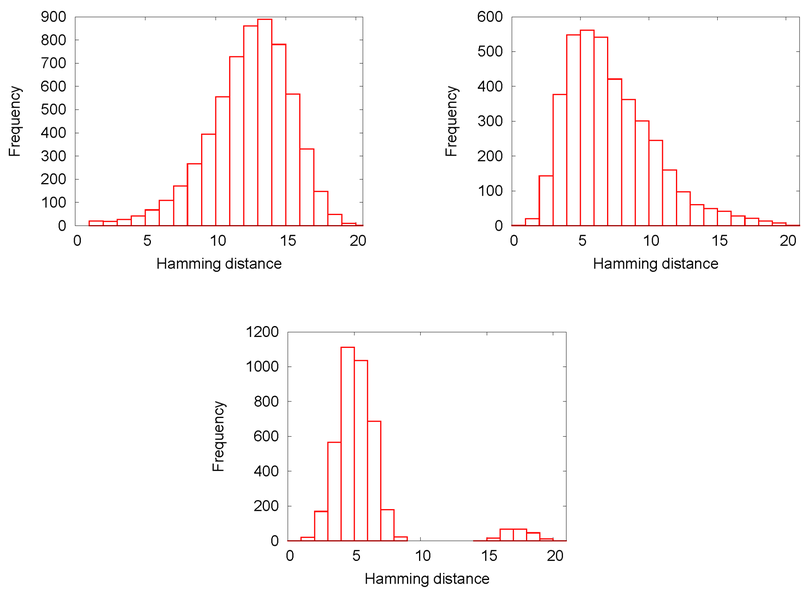

Fig. 1 Top left: 2SAT. Top right: RAN. Bottom: REG.

Quantum annealing experiments

Large problems up to $N = 170$ are created and submitted to the D-Wave Advantage 5.1 quantum annealer located at JSC, FZJ, Germany. The scaling of the most interesting measure, i.e., the success probability of the ground state, as a function of the problem size, is shown below.

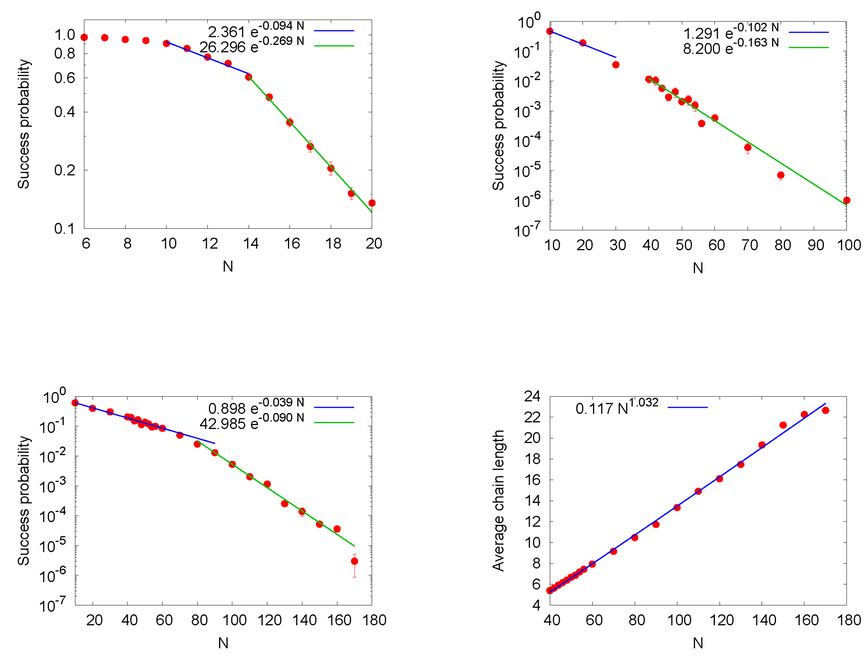

Fig. 2 Top left: 2SAT. Top right: RAN. Bottom Left: REG. Bottom right: REG, Embedding.

Summary and outlook

We performed spectral analysis and quantum annealing experiments on three classes of QUBO problems. Our results demonstrate that the exponents characterizing the scaling of the success probability of the D-Wave annealer to solve a QUBO correlate very well with the predictions based on the Hamming distance computed for small QUBO instances.

It is of interest to use simulated annealing for solving the three sets of problems to study if the Hamming distance distributions for small problem instances also predict the effectiveness of simulated annealing.

References:

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