A Quantum Annealing Approach to Biclustering

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12-13 December, 2016 – TPNC 2016, Sendai (Japan)

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Introduction

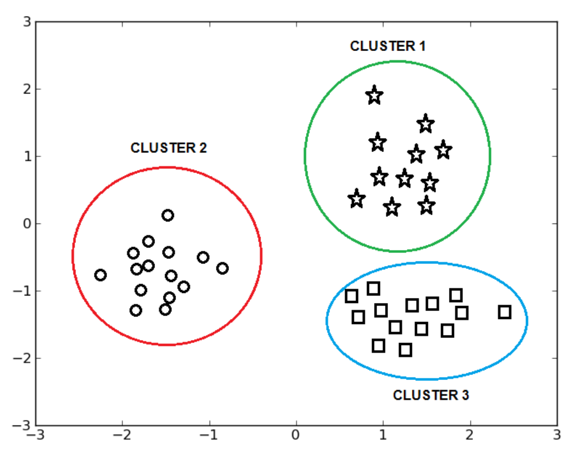
Motivation

- Problems in Artificial Intelligence are typically intractable.
- Heuristics, greedy approaches etc are used instead of exact algorithms.
- Can the D-Wave quantum annealing hardware be helpful?
- No final answer at this stage.
- We investigate this for the biclustering problem

Biclustering

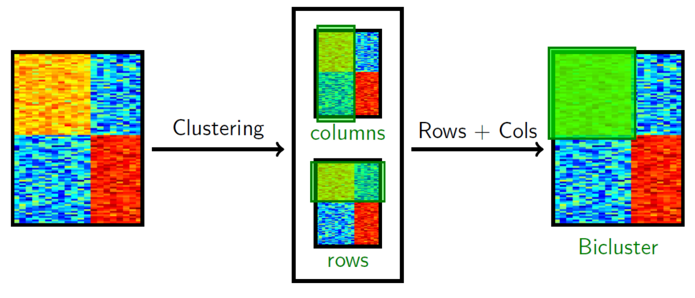
Clustering

Partition into groups a set of objects based on the concept of similarity



Biclustering

Perform **simultaneous** clustering of rows and columns of a given data-matrix

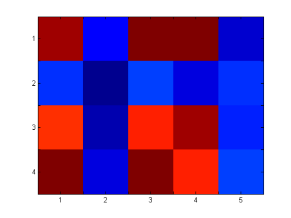


Biclustering

- Used in different scenarios, the most important is **expression microarray data analysis**
  - Rows and columns represent genes and experiments respectively
  - Biclustering can provide invaluable information to biologist
- We focus on the **One-Bicluster** problem
  - Standard technique where biclusters are extracted one by one
  - We extract the largest bicluster
  - The other biclusters can be retrieved by masking the previous ones

Biclustering

- **Input:** real-valued matrix. Each entry $a_{i,j}$ represents the activation level of gene i under the experimental condition j



- **Output:** binary matrix that represents which elements belong to the bicluster

$$\begin{pmatrix} 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 & 0 \end{pmatrix}$$

- Bicluster elements must comply a **topological constraint**

Valid configuration

$$\begin{pmatrix} 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 & 0 \end{pmatrix} \longrightarrow \begin{pmatrix} 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

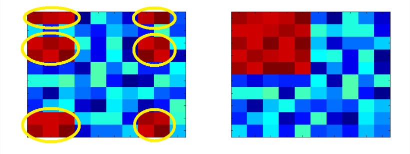
Invalid configuration

$$\begin{pmatrix} 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 1 & 0 \end{pmatrix}$$

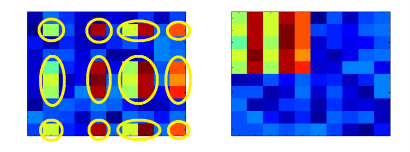
Biclustering

- The similarity between elements is defined by a coherence measure
- We used two types of coherence:

Constant coherence $O_{i,j,t,k} = w|a_{i,j} - a_{t,k}|$



Additive coherence $O_{i,j,t,k} = w(a_{i,j} + a_{t,k} - a_{t,j} - a_{i,k})^2$



Quantum Annealing

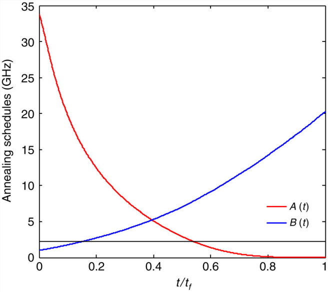
Quantum Annealing

- Conjectured in 1984 as an improvement of simulated annealing
- QA is typically achieved by the Ising Hamiltonian:

$$H(t) = A(t)H_X + B(t)H_P, \;\; t \in [0, t_f].$$

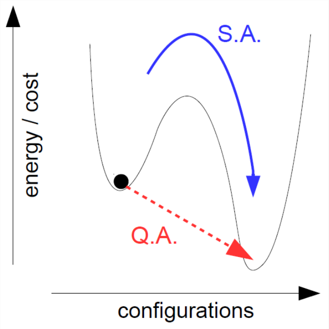
- The solution to an optimisation problem is encoded in the ground state of H_P:

$$H_P = \sum_{i \in \mathcal{V}} h_i \sigma_i^z + \sum_{(i,j) \in \mathcal{E}} J_{ij} \sigma_i^z \sigma_j^z$$



Quantum Tunneling

- Quantum fluctuations can help "tunneling" through barriers
- Numerical and experimental results have suggested that quantum tunnelling can be more effective than thermal fluctuation for reaching the ground state.
- This is still the subject of active scrutiny



QUBO

Quadratic Unconstrained Binary Optimization (QUBO)

- Often it is more convenient to model with 0/1-valued variables than the $1/-1$-valued Ising variables.
- This results in an equivalent formulation of the Ising energy minimisation problem as a QUBO problem.
- QUBOs are Ising models where the spin variables $s_i \in \{+1, -1\}$ are transformed to binary-valued variables $x_i \in \{0, 1\}$.
- This transformation is easily realised through $s_i = 2x_i - 1$.

Quadratic Unconstrained Binary Optimization (QUBO)

Goal

Find the assignment to a set of binary variables $x_1 \ldots x_n$ so as to minimize the function:

$$O(x_1, \ldots, x_n) = \sum_{i=1}^{n} a_i x_i + \sum_{1 \leq i < j \leq n} b_{i,j} x_i x_j$$

Every instance of a QUBO can be represented by a graph

Example

$$O(x_1, x_2) = 2x_1 - x_2 + x_1 x_2$$

QUBO Model for One-Bicluster problem

Objective function:

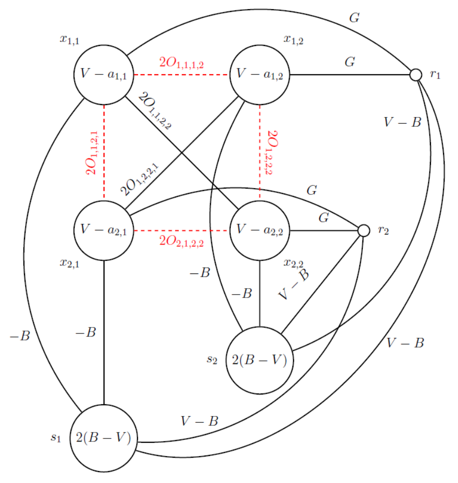
$$\arg\max_{(c_{1,1},\cdots,c_{N,M})}\left(\sum_{i,j} a_{i,j}c_{i,j} - \sum_{i,j,t,k} O_{i,j,t,k}c_{i,j}c_{t,k} + \sum_{i<t} B_{i,t}\right)$$

Complete model for a 2x2 data-matrix

$N \times M$ matrix

$\Downarrow$

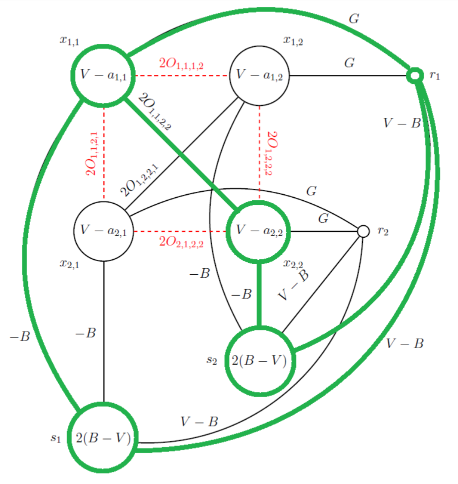
$N \times M + N + M$ nodes



QUBO Model for One-Bicluster problem

Non-valid configuration

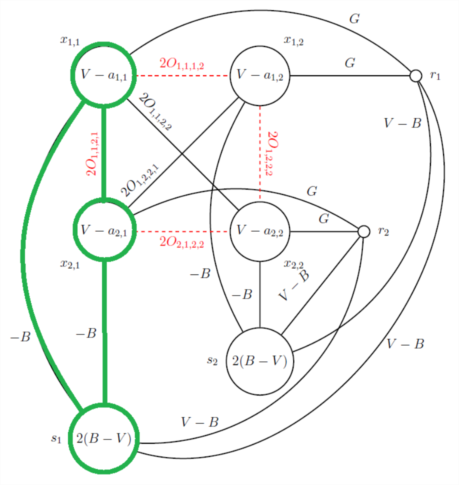
$$\sum = G > 0$$



QUBO Model for One-Bicluster problem

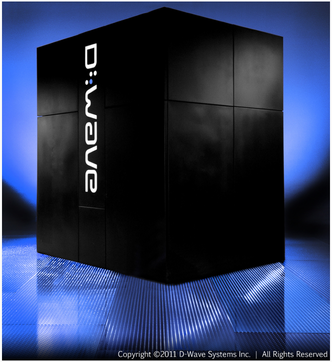
Valid configuration
$\sum = 0$

Model validity
For all valid assignments, the extra constraints provide a null contribution to the objective function. For all other configurations the contribution is > 0.



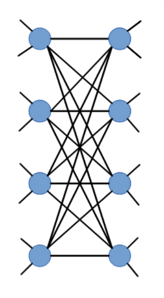
D-Wave

- First commercially available quantum annealer
- Two have been sold:
    - Lockheed Martin
    - Google - NASA
- Finds the ground state of **Ising spin glass models** or equivalently solves **Quadratic Unconstrained Binary Optimization** (QUBO) problems



Minor Embedding

- The D-Wave has a well defined **fixed architecture**
- Create a **logical model** and map it into the D-Wave architecture
- Chimera is not a **complete graph**
- A single logical qubit may need more than one **physical qubit** to be represented
- The **minor embedding** technique finds the sets of physical nodes that represent the logical ones



Minor Embedding

We performed the minor embedding using the **official D-Wave libraries** provided by J. Cai, B. Macready and A. Roy

Results of our experimental analysis

	(D-Wave 2)	(D-Wave 2X)	(Future ?)
Qubits	**512**	**1152**	**2048**
Max data-matrix size	5×6	7×7	8×8

The model proposed is very accurate but has a high space complexity:

- $\mathcal{O}(n^2 m^2)$ edges (quadratic terms)

Suitability of Quantum Annealing

Criteria for problems that are suitable for treatment with a quantum annealer:

Landscape Analysis

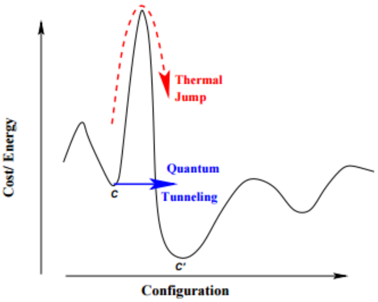
Solutions to the problem are valuable or interesting.

Runtime Advantages

Must exhibit a significant speed-up compared to other (classical) algorithms used for that problem.

Landscape Analysis

- The energy landscape must have tall and narrow barriers
- Frustration of the system implies that the energy landascape becomes extremely rugged (tall and narrow barriers)
- The biclustering Hamiltonian (both logic and embedded) gives rise to a frustrated system.



Quantum Speed-up?

- Based on the current results, one cannot claim a quantum speedup for D-Wave 2X, as this would require that the quantum processor in question outperforms the best known classical algorithm.

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Conclusion

Conclusions and Future Work

Conclusions

- The model proposed allows us to solve the biclustering problem with high accuracy
- Space complexity of the model + current D-Wave architecture do not allow to address big matrices

Future Work

- Study new techniques in order to decompose big instances into smaller ones