Direct Mapping of Some Problems to Ising Models with Three-Valued Coupling Coefficients

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2015/12/08 Lab seminar

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Agenda

- Introduction
- Graph coloring problem
- Graph isomorphism problem
- Maximum clique problem
- Conclusions

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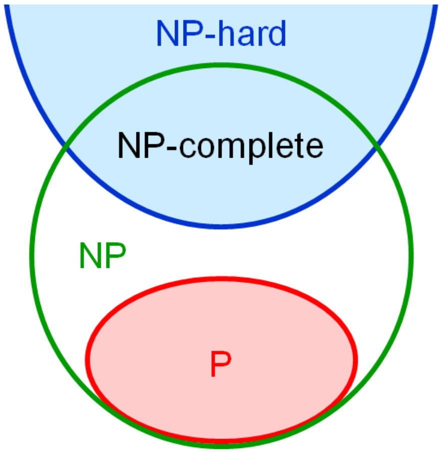
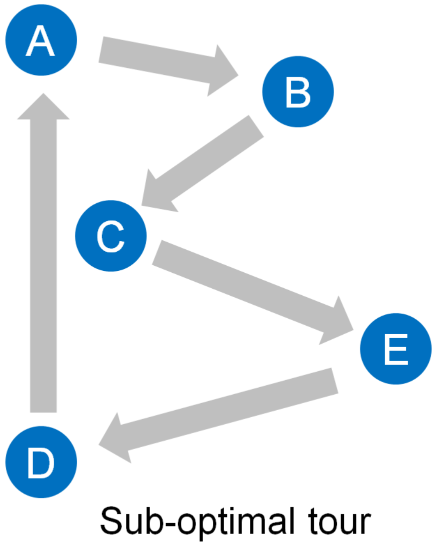
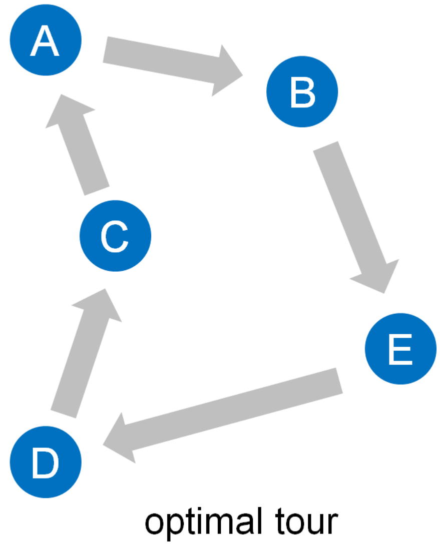
P and NP

- Decision problem: Yes-or-no question
    - **P**: Polynomial-time
    - **NP**: Non-deterministic polynomial-time
        - *Yes*-instances can be verified in polynomial time.
- **NP-hard**: Any NP problem can be reduced to this in polynomial-time.
- **NP-complete**: Intersection of NP-hard and NP



NP-hard and NP-complete



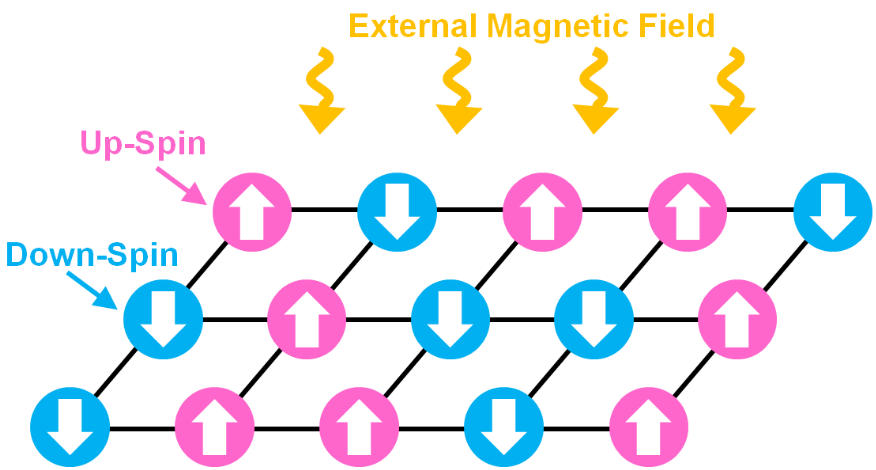


- Question A: "What is the minimum cost tour?"
  - **NP-hard** optimization problem
- Question B: "Can we make a tour with cost less than 100?"
  - **NP-complete** decision problem

Exponential time?

- Exponential time: $\mathrm{O}(2^{\mathrm{poly}(n)})$ ex. 2^n
- Sub-exponential time: $\mathrm{O}(2^{\mathrm{o}(n)})$ ex. $2^{\sqrt{n}}$
- Any NP problem can be solved *at most* exponential time.
  - NP $\subseteq$ PSPACE $\subseteq$ EXPTIME
- 3-SAT problem is believed to require **exponential time**.
  - Exponential time hypothesis (ETH) (Impagliazzo & Paturi, 1999)
- For some other NP-complete problems, **sub-exponential time** algorithms are known.
  - ex.) Hamiltonian cycle problem on planar graphs (Deineko, et al., 2006)

Ising model



- Spins: $s_i \in \{1, -1\}$
- Hamiltonian

$$H = -\sum_{i,j} J_{ij} s_i s_j - \sum_i h_i s_i.$$

- Finding a ground state (minimum energy state) of an Ising model is **NP-hard** (Barahona, 1982).

Alternative representation

- Spins: $x_i \in \{0, 1\}$
- QUBO (Quadratic unconstrained binary optimization)

$$H = \sum_{i,j} Q_{ij} x_i x_j.$$

- Since $x_i = x_i^2$, we can include the effect of the external field into the weights of self-loops Q_{ii} .
- The two representations, based on {-1,1}-spins and {0,1}-spins, can be **mutually transformed into each other** by the relation $s_i = 2x_i - 1$.
  - Precisely, we need to add or subtract some constant, but this does not change the optimal configuration.

Conversion

- QUBO to Ising model

$$J_{ij} \leftarrow -Q_{ij},$$
$$h_i \leftarrow -\sum_k (Q_{ik} + Q_{ki}).$$

- Ising model to QUBO

$$Q_{ij} \leftarrow -J_{ij} + \frac{\delta_{ij}}{2}\left(\sum_k (J_{ik} + J_{ki}) - h_i\right).$$

Ising model solvers

Recently, several special hardwares or physical systems for solving Ising models have been proposed.

1. D-Wave machines
   - D-Wave One (2011, 128 qubits)
   - D-Wave Two (2013, 512 qubits)
   - D-Wave 2X (2015, 1 152 qubits)
   - Based on quantum annealing (Boixo, et al., 2014)
2. Ising chip by Hitachi, Ltd. (Yamaoka, et al., 2015; Yoshimura, et al., 2015)
   - 20 480 spins
3. **Coherent Ising Machine**

Coherent Ising Machine

- **Laser network** (Utsunomiya, et al., 2011; Takata, et al., 2012; Takata and Yamamoto, 2014; Utsunomiya, et al., 2015)
  - N slave lasers
  - Right or left circular polarizations
  - Extension to XY model is easy.
- **DOPO (degenerate optical parametric oscillator) network** (Z. Wang, et al., 2013; Marandi, et al., 2014; Haribara, et al., 2015)
  - N pulses in a ring cavity
  - 0 or π phases
  - Better scalability

Constraints on coupling coefficients

- On November 13th, Prof. Aihara asked some of us to suggest possible applications of CIMs with each of the following four conditions:

	Number of connections	Weight type
1	2 000 x 2 000	**{-1, 0, 1}-valued**
2	10 000 x 10 000	**{-1, 0, 1}-valued**
3	160 x 160	real-valued
4	1 600 x 1 600	real-valued

- Problem is that most problems worth solving cannot be directly represented by using the thee-valued weights.

Literature search

- D-Wave machines
  - Lattice model for protein folding (Perdomo-Ortiz, et al., 2012)
  - Hamiltonian path problem and graph coloring problem (Rieffel, et al., 2015)
  - Graph isomorphism problem (Zick, et al., 2015)
- Ising chips
  - Max-cut problem (Yamaoka, et al., 2015)
- Coherent Ising machines
  - Max-cut problem (Z. Wang, et al., 2013; Haribara, et al., 2015)

Purpose

- Fortunately, I found a nice review that describes how to map many famous NP or NP-hard problems to Ising models (Lucas, 2014).
- Among the listed problems, I found some can be represented even if $J_{ij} \in \{-1, 0, 1\}$.
- In this talk, I will introduce three problems which also have tight relation to real-world applications.
    - **Graph coloring problem**
    - **Graph isomorphism problem**
    - **Maximum clique problem**

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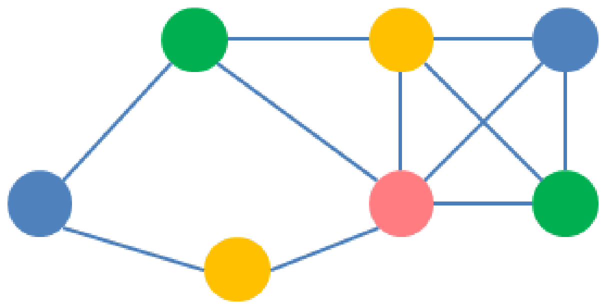
Graph coloring problem

- Question: "Can we color n-vertices with k-colors such that all adjacent vertices are colored differently?"



- NP-complete
- Planar graphs are always colorable by four colors.
- Related problem "what is the minimum number of colors?" (NP-hard) is difficult to directly map to the restricted CIMs.
- Applications: register allocation (Chaitin, 1982), flight level allocation (Barnier & Brisset, 2004), etc.

Related studies

- Review paper (Galinier, et al, 2013)
- Exact algorithms (Malaguti, et al., 2011)
  - Even a 125-vertex problem is intractable.
- Simulated quantum annealing (Titiloye and Crispin, 2011)
  - Achieved best-known solutions up to 1000 vertices.
- Independent sets (Hao and Wu, 2012)
  - Good for problems of a few thousand vertices
- Greedy methods (Brelaz, 1979; Leighton, 1979; Hasenplaugh, et al., 2014)
  - Millions of vertices

Preliminaries

- Spin representing vertex *i* is assigned color *c*: $x_{i,c} \in \{0, 1\}$
- Spin number = vertex number (*n*) x color number (*k*)
- Adjacency matrix: $A = \{a_{ij}\}$
  - 1: connected, 0: not connected

Mapping

- Hamiltonian (Lucas, 2014; Rieffel, et al., 2015)

$$H = \sum_{i=1}^{n} \left(1 - \sum_{c=1}^{k} x_{i,c}\right)^2 + \sum_{i<j} \sum_{c=1}^{k} a_{ij} x_{i,c} x_{j,c} \ .$$

- The 1st term represents the constraint that all vertices are assigned exactly 1 color.
- The 2nd term represents the constraint that if two nodes are connected, we cannot give the same color to them.
- If $H = 0$ is achieved, we know the graph is *k*-colorable.

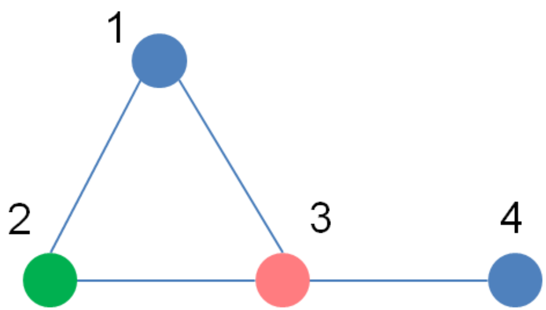
Expansion

- The 1st term

$$
\begin{aligned}
H_1 &= \sum_{i=1}^{n} \left(1 - \sum_{c=1}^{k} x_{i,c} \right)^2, \\
&= \sum_{i=1}^{n} \left(1 - 2 \sum_{c=1}^{k} x_{i,c} + \sum_{c=1}^{k} x_{i,c} \sum_{d=1}^{k} x_{i,d} \right), \\
&= \sum_{i=1}^{n} \left(1 - 2 \sum_{c=1}^{k} x_{i,c} x_{i,c} + \sum_{c=1}^{k} \sum_{d=1}^{k} x_{i,c} x_{i,d} \right), \\
&= \sum_{i=1}^{n} \left(1 - \sum_{c=1}^{k} x_{i,c} x_{i,c} + \sum_{c \neq d} x_{i,c} x_{i,d} \right).
\end{aligned}
$$

- Self-loop weights are -1, and weights between spins for the same vertex and different colors are 1.

Example



Num. of vertices $n = 4$
Num. of colors $k = 3$
Num. of spins $4 \times 3 = 12$

	1 1	1 2	1 3	2 1	2 2	2 3	3 1	3 2	3 3	4 1	4 2	4 3
1 1	-1	1	1	1	0	0	1	0	0	0	0	0
1 2	1	-1	1	0	1	0	0	1	0	0	0	0
1 3	1	1	-1	0	0	1	0	0	1	0	0	0
2 1	0	0	0	-1	1	1	1	0	0	0	0	0
2 2	0	0	0	1	-1	1	0	1	0	0	0	0
2 3	0	0	0	1	1	-1	0	0	1	0	0	0
3 1	0	0	0	0	0	0	-1	1	1	1	0	0
3 2	0	0	0	0	0	0	1	-1	1	0	1	0
3 3	0	0	0	0	0	0	1	1	-1	0	0	1
4 1	0	0	0	0	0	0	0	0	0	-1	1	1
4 2	0	0	0	0	0	0	0	0	0	1	-1	1
4 3	0	0	0	0	0	0	0	0	0	1	1	-1

the 1st constraint
the 2nd constraint

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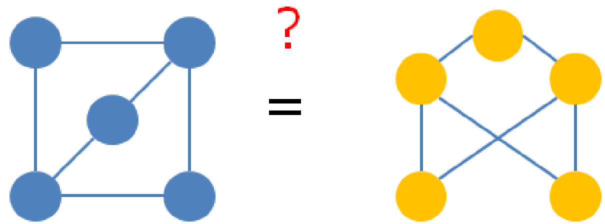
Graph isomorphism problem

- Question: "Are two graphs topologically the same?"



- This belongs to NP. NP-completeness is not known.
- Last month, it was claimed that a **quasi-polynomial time** algorithm exists (Babai, 2015).
- Applications: verification of integrated circuit layouts, identification of chemical compounds, etc.

Preliminaries

- Spin representing the mapping from vertex *i* of the original graph to vertex *u* of the target graph: $x_{u,i} \in \{0, 1\}$
- Number of spins: n^2
    - *n* is the number of vertices.
    - This is the worst case. In most cases, it can be reduced to $n \log_2(n)$ (Zick, et al., 2015).
- Original graph's adjacency matrix: $A = \{a_{ij}\}$
- Target graph's adjacency matrix: $B = \{b_{uv}\}$

Mapping

- Hamiltonian (Zick, et al., 2015)

$$H = \sum_u \left(1 - \sum_i x_{u,i}\right)^2 + \sum_i \left(1 - \sum_u x_{u,i}\right)^2 + \sum_{i,j,u,v,i \neq j} (1 - a_{ij}) b_{uv} x_{u,i} x_{v,j} + \sum_{i,j,u,v,u \neq v} a_{ij} (1 - b_{uv}) x_{u,i} x_{v,j}.$$

- The 1st and 2nd terms represent the constraint that mapping is one-to-one.
- The 3rd term represents the constraint that if two nodes are not connected at the original graph, they cannot be connected at the target graph as well.
- The 4th term is similar.
- If $H = 0$ is achieved, we know the two graphs are isomorphic.

Expansion

- The 1st term

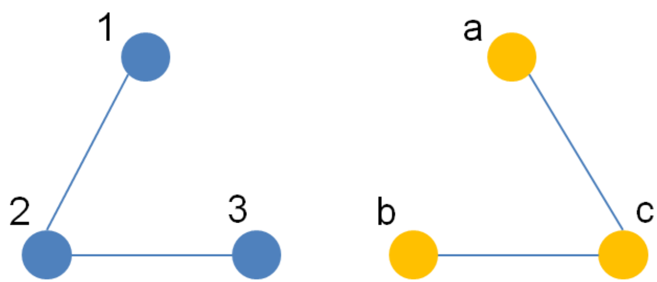
$$
\begin{aligned}
H_1 &= \sum_u \left(1 - \sum_i x_{u,i}\right)^2, \\
&= \sum_u \left(1 - 2\sum_i x_{u,i} + \sum_i x_{u,i} \sum_j x_{u,j}\right), \\
&= \sum_u \left(1 - 2\sum_i x_{u,i} x_{u,i} + \sum_i \sum_j x_{u,i} x_{u,j}\right), \\
&= \sum_u \left(1 - \sum_i x_{u,i} x_{u,i} + \sum_{i \neq j} x_{u,i} x_{u,j}\right).
\end{aligned}
$$

- Self-loop weights are -1, and weights between spins for the same target vertex and different original vertices are 1.
- After adding the 2nd term, self-loop weights become -2.

Transformation

- Weight matrix
  - Diagonal elements: -2
  - Non-diagonal elements: 0 or 1
  - Symmetric
- Transformation to make the weight matrix three-valued (Zick, et al., 2015):
  - Reduce diagonal elements to half.
  - Keep only one side of non-diagonal elements and all values on the other side are reset to 0.

Example



Number of vertices $n = 3$
Number of spins $3^2 = 9$

	1a	1b	1c	2a	2b	2c	3a	3b	3c
1a	-1	1	1	1	1	0	1	0	1
1b	0	-1	1	1	1	0	0	1	1
1c	0	0	-1	0	0	1	1	1	1
2a	0	0	0	-1	1	1	1	1	0
2b	0	0	0	0	-1	1	1	1	0
2c	0	0	0	0	0	-1	0	0	1
3a	0	0	0	0	0	0	-1	1	1
3b	0	0	0	0	0	0	0	-1	1
3c	0	0	0	0	0	0	0	0	-1

Self-loop
Vertex constraint (one-to-one)
Edge constraint

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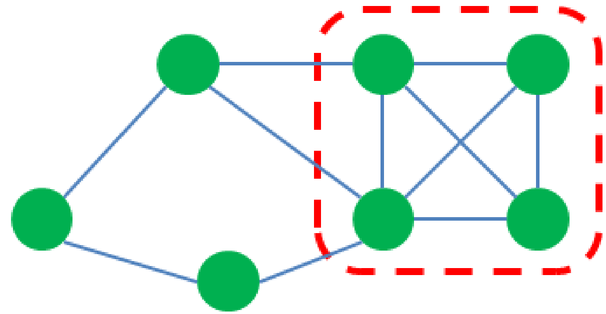
Maximum clique problem

- Question: "What is the maximum subgraph in which every pair of nodes is connected?"



- NP-hard
- Related problem "does this graph have a clique of size *k*?" (NP-complete) can be answered by solving the optimization problem.

Precisely, a clique is a subset of nodes. Edges are not included.

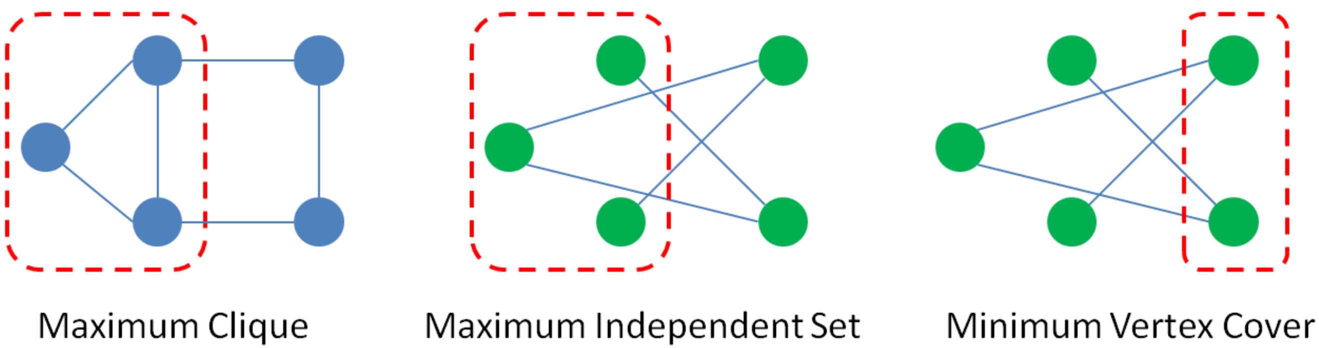
Applications

- Determination of lower-bound for graph coloring problem
- Protein structure alignment (Strickland, et al., 2005, Zhu and Weng, 2005, Malod-Dognin, et al., 2010)

- Note that the notion of *clique* is usually too stringent for community detection in practice.

Equivalent problems

- Maximum clique problem is essentially equivalent to:
  - **Maximum independent set (MIS)**
  - **Minimum vertex cover**
  - **Maximum set packing**
- Also, **3-SAT** with *m*-clause can be mapped to MIS with *3m* vertices (Lucas, 2014).



Mapping

- Spin representing vertex *i*: $x_i \in \{0, 1\}$
- Number of spins = Number of vertices (*n*)
- Adjacency matrix: $A = \{a_{ij}\}$
- Hamiltonian (Lucas, 2014)

$$H = \sum_{i \neq j} (1 - a_{ij}) x_i x_j - \sum_i x_i.$$

- The 1st term represents the constraint that we cannot select node pairs which are not connected.
- The 2nd term represents the objective that we are trying to select as many nodes as possible.

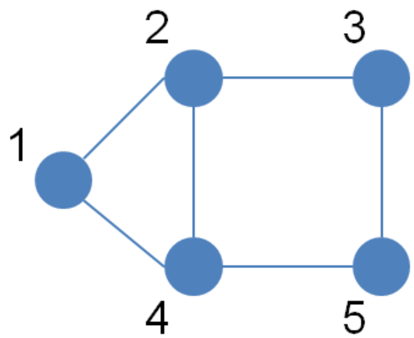
Is the constraint always satisfied?

- Hamiltonian

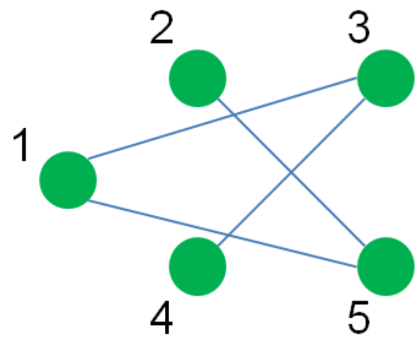
$$H = \sum_{i \neq j} (1 - a_{ij}) x_i x_j - \sum_i x_i.$$

- Assume that a pair of spins violate the constraint. Then, if we change one of them from 1 to 0, following occurs.
  - The 2nd term increases by 1.
  - The 1st term decreases by at least 2 because of the symmetry with respect to switching *i* and *j*.
  - In total, the energy decreases.
- Therefore, any configuration that fails to satisfy the constraint cannot be a minimum energy state.

Example



Original graph



Complement graph

$$\begin{array}{c|c}
 & \begin{matrix} 1 & 2 & 3 & 4 & 5 \end{matrix} \\
\begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{matrix} & \begin{bmatrix} -1 & 0 & 1 & 0 & 1 \\ 0 & -1 & 0 & 0 & 1 \\ 1 & 0 & -1 & 1 & 0 \\ 0 & 0 & 1 & -1 & 0 \\ 1 & 1 & 0 & 0 & -1 \end{bmatrix}
\end{array}$$

Self-loop
Constraint

Num. of vertices $n = 5$
Num. of spins 5

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Summary

Problems mappable to Ising models with three-valued weights

Problem name	Problem type	Class	Spin type	Num. of spins
Graph coloring	decision	NP-complete	$\{0,1\}$	$n \times k$
Graph isomorphism	decision	NP	$\{0,1\}$	n^2
Max. clique	optimization	NP-hard	$\{0,1\}$	n
Max. independent set	optimization	NP-hard	$\{0,1\}$	n
Min. vertex cover	optimization	NP-hard	$\{0,1\}$	n
Max. set packing	optimization	NP-hard	$\{0,1\}$	Num. of subsets
3-SAT	decision	NP-complete	$\{0,1\}$	$3m$
Hamiltonian path	decision	NP-complete	$\{0,1\}$	n^2
Max-cut	optimization	NP-hard	$\{-1,1\}$	n

Other approaches

This page originally included some unpublished ideas, which are excluded in this version.

- **Weight decomposition** method
  - Proposed by Prof. Kawarabayashi
  - Numerically tested by Mr. Haribara

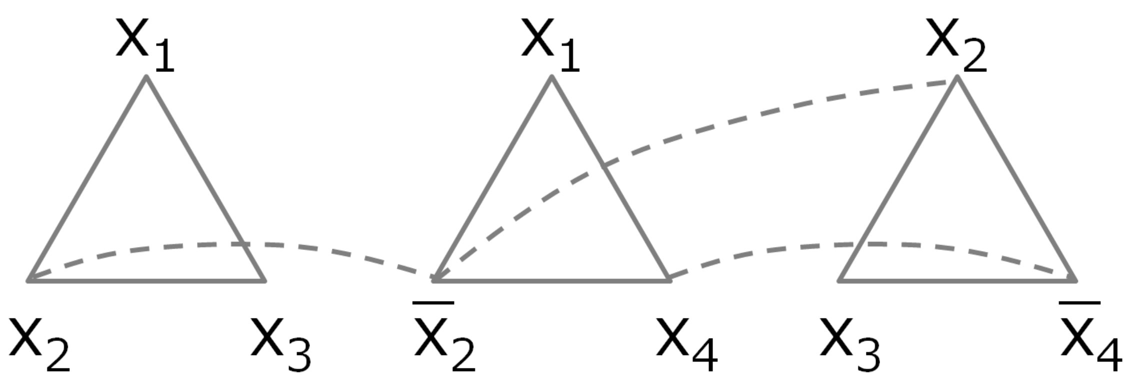
Future works

- Prof. Yamamoto recommended to focus on **graph coloring problem** and pointed out that we need to know more about:
  - Status of state-of-the-art heuristic algorithms
  - Problem size required in real-world applications

Appendix

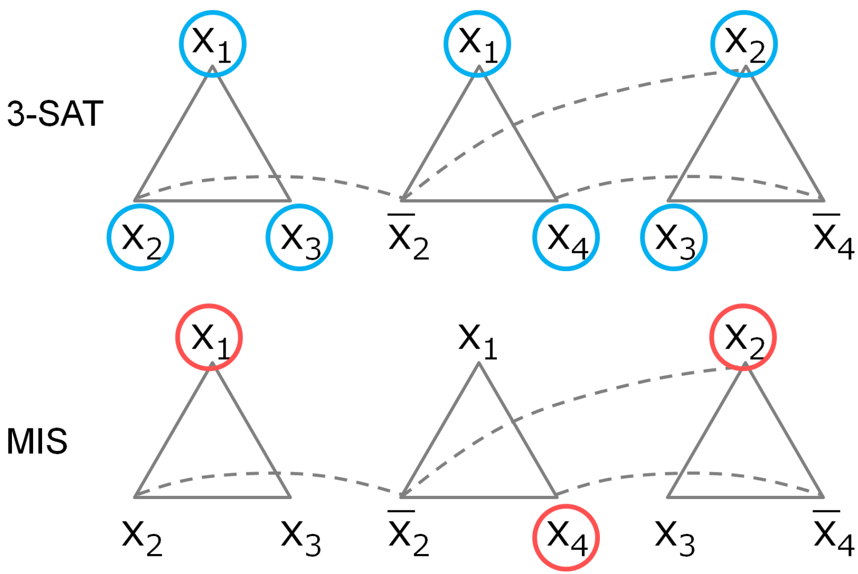
Mapping from 3-SAT to MIS

- 3-SAT: $\Psi(x_1, \ldots, x_n) = C_1 \wedge \ldots \wedge C_m$
  - ex.) $\Psi = (x_1 \vee x_2 \vee x_3) \wedge (x_1 \vee \overline{x}_2 \vee x_4) \wedge (x_2 \vee x_3 \vee \overline{x}_4)$
- Conversion
  1. Convert clauses to triangles.
  2. Add links between contradicting (x_i and $\overline{x}_i$) literals.



3-SAT and MIS

- 3-SAT solution exists => MIS solution of size *m* exists
  - Keep 1 literal in each triangle and remove others.
- MIS solution of size *m* exists => 3-SAT solution exists
  - Select all nodes whose literals appear in MIS solution at least once. Select x_i if neither x_i nor $\overline{x}_i$ appears.



Many-body interaction

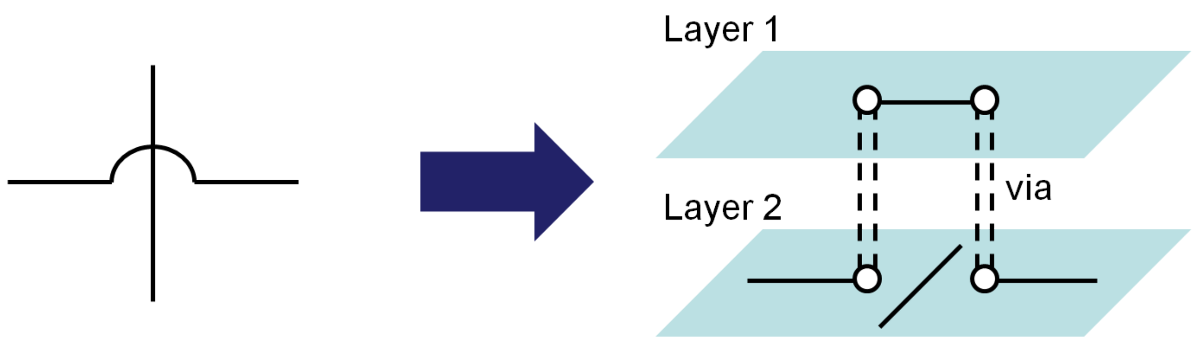
- If we are allowed to use real-valued coupling coefficients, **many-body interaction** can be implemented by adding auxiliary spins (Perdomo-Ortiz, et al., 2012).
- For example, if the Hamiltonian contains a term $x_1 x_2 x_3$, where $x_i \in \{0, 1\}$, add **a new variable** $y \in \{0, 1\}$ and replace the term with $y x_3$.
- This is safe as long as $y = x_1 x_2$. To achieve this, **penalty term *E*** should be added to the Hamiltonian.

  $$E = c(3y + x_1 x_2 - 2y x_1 - 2y x_2) \ .$$

  where $c > 0$ is a parameter. We can see that $E = 0$ for $y = x_1 x_2$ and $E > c$ for $y \neq x_1 x_2$.
- By using this technique, 3-SAT with *n*-variables and *m*-clauses can be mapped to QUBO with *n*+*m* spins.

Application of Max-cut

- VLSI design (Barahona, et al., 1988).
    - Crossing wires must be assigned to different layers.
    - By optimally assigning components to each layer, we want to minimize the number of via holes.
    - This problem can be mapped to Max-cut problems having both positive and negative weights.

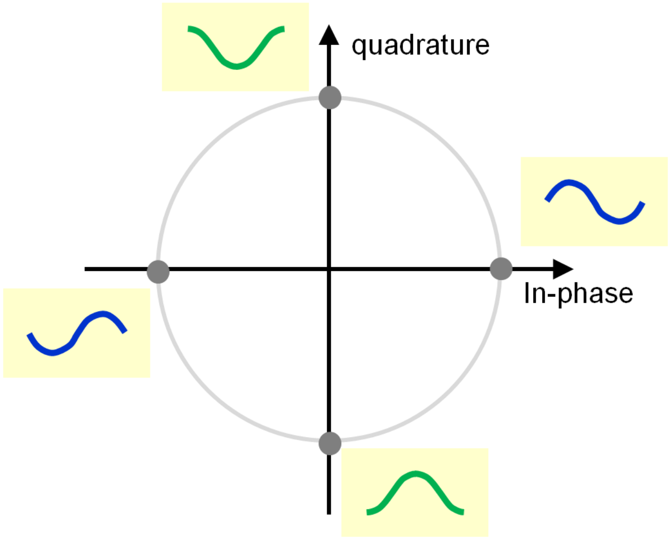


In-phase and quadrature

- Reference signal: $\sin(x)$
- Phase- and amplitude-modulated signal:

$$\begin{aligned} A\sin(x+\phi) &= A\sin(x)\cos(\phi) + A\cos(x)\sin(\phi), \\ &= I\sin(x) + Q\cos(x). \end{aligned}$$

  - In-phase component: $I\sin(x)$
  - quadrature component: $Q\cos(x)$



Quantum annealing and AQC

- **Quantum annealing** (Kadowaki and Nishimori, 1998)

  $$H(t) = H_P + \Gamma(t) H_T.$$

  - H_P : Hamiltonian associated with the problem
  - H_T : Transverse field
  - $\Gamma(t)$: Amplitude of H_T that is gradually decreasing

- **Adiabatic quantum computation (AQC)** (Farhi, et al., 2001)

  $$H(t) = \left(1 - \tfrac{t}{T}\right) H_0 + \tfrac{t}{T} H_P.$$

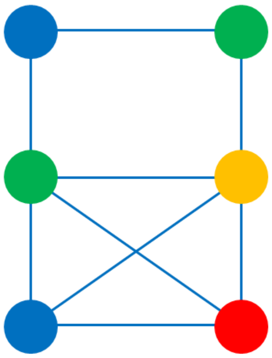
  - H_0 : Initial Hamiltonian
  - T : Total running time
  - *Adiabatic theorem* gives the necessary length of T for certainly finding an optimal solution.

Simple coloring

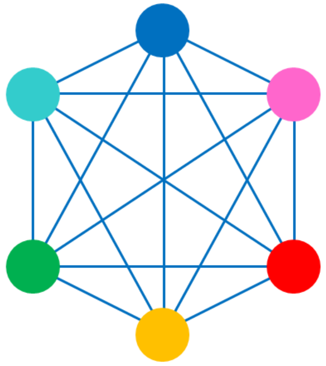
- A graph G having maximum degree Δ is $\Delta + 1$-colorable.
  1. Select a vertex v.
  2. Repeatedly select a vertex from the remaining that is adjacent to any vertex previously selected.
  3. Assign colors to the vertices in the opposite order (lastly selected one is firstly colored). **This requires only Δ colors** except v.
     - In each step, at least one neighbor is uncolored.
     - Thus, at most $\Delta - 1$ neighbors are colored.
  4. At last, if v has unfortunately Δ neighbors and all are differently colored, assign a new color to it.
- The last point determines whether G is Δ-colorable.

Brooks' theorem

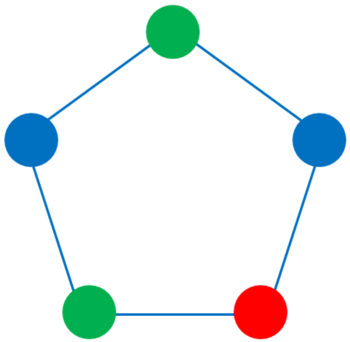
- A graph G having maximum degree Δ is Δ-colorable unless it is a complete graph or a cycle graph of odd length.



Δ-colorable



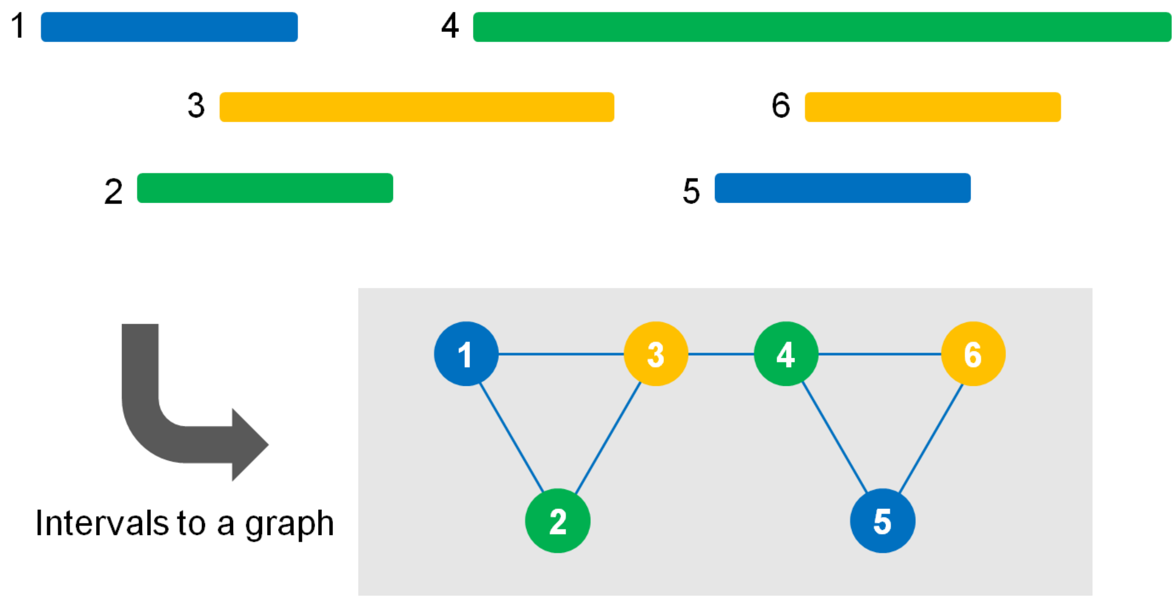
not Δ-colorable



not Δ-colorable

Interval graph coloring

- Interval graphs can be optimally colored in polynomial time.
- Algorithm is simple. Just sort the intervals according to their *start* time, and assign colors to the intervals from the beginning.



MIS and related problems

- Maximum independent set (MIS)
  - Question: "What is the maximum size of node subset among which no edge exists?"
- Minimum vertex cover
  - Question: "What is the minimum size of node subset that contains at least one endpoint of every edge?"
- Maximum set packing
  - U : Set of all items
  - $S_i \subseteq U$: Subsets of items
  - Question: "What is the maximum number of subsets in which no item is selected more than once?"

MIS and MVC

- Maximum independent set (MIS) problem and minimum vertex cover (MVC) problem are essentially equivalent.
- Intuitively, this can be seen from the following lemma:

  "For any vertex cover (not necessarily minimum), its complement vertex set is independent."

  - By definition, the cover set contains at least one endpoint of every edge.
  - Assume that an edge exists between vertices in the complement set.
  - If so, both of the endpoints are not in the cover set, resulting in contradiction.
  - Thus, the complement set is independent.

Related problems

type	Covering problem	Packing problem
set	(A) minimum set cover	(B) maximum set packing
vertex	(C) minimum vertex cover	(D) maximum independent set
edge	(E) minimum edge cover	(F) maximum matching

- (A), (B), (C), and (D) are NP-hard.
- (E) and (F) are polynomial-time optimization problems.
- (A) is equivalent to minimum hitting set.
- (B), (C), (D), and maximum clique are all equivalent.
- (A) is generalization of (C) to hypergraphs.
- (F) can be solved by blossom algorithm in polynomial time.
- (E) can be reduced to (F) in polynomial time.