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QUBO FORMULATIONS FOR THE SNAKE-IN-THE-BOX AND COIL-IN-THE-BOX PROBLEMS

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CONTENT

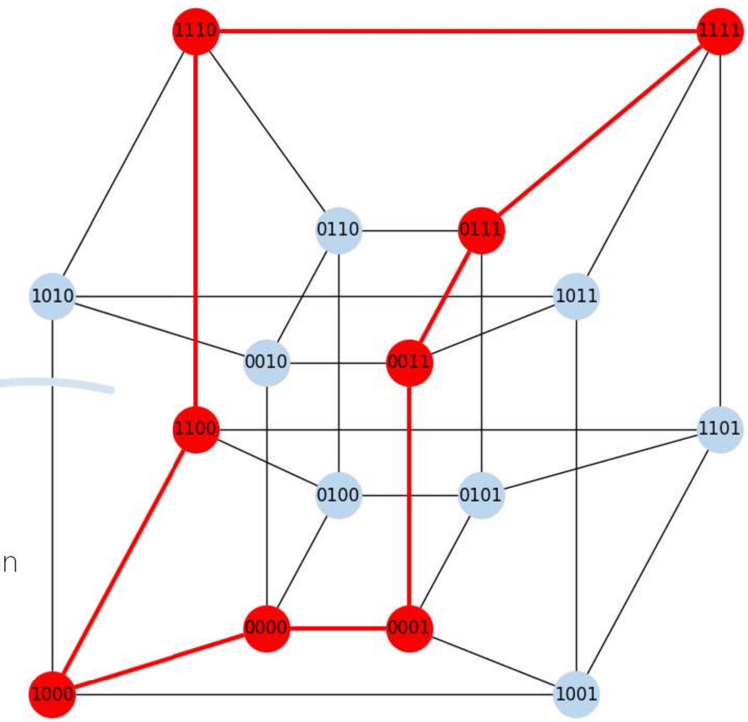
- Snake-in-the-box and Coil-in-the-box problems
- QUBO formulations and Quantum Annealers
- Formulations of the problems
- Results

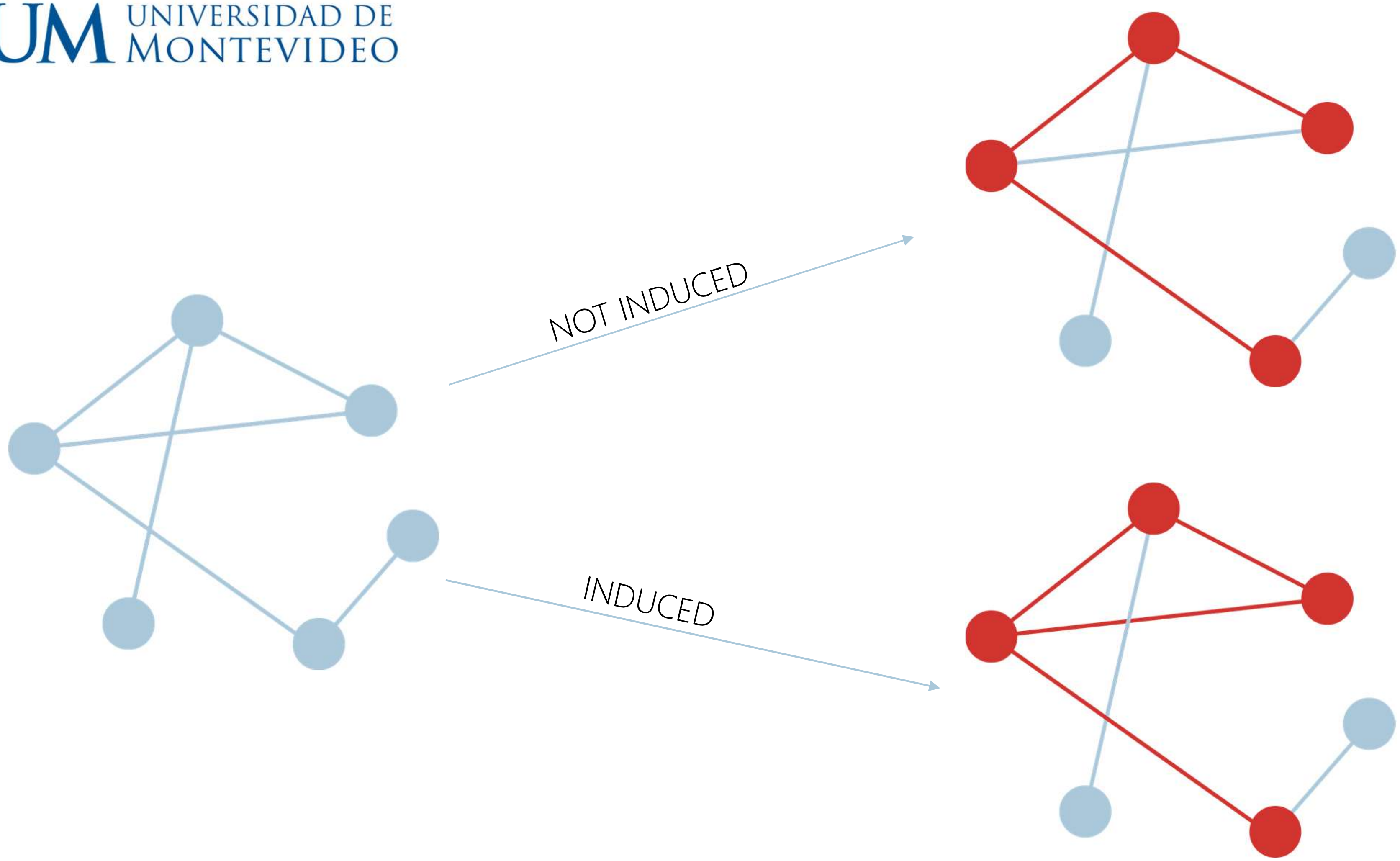
SNAKE-IN-THE-BOX AND COIL-IN-THE-BOX PROBLEMS

- The Snake-in-the-box problem (SITB) involves finding the máximum length of an hypercube of n dimensions Q_n.

- The Coil-in-the-box problem (CITB) involves finding the máximum length of an induced cycle of an hypercube of n dimensions Q_n.

For n = 4 the máximum length of an induced cycle is at least 8

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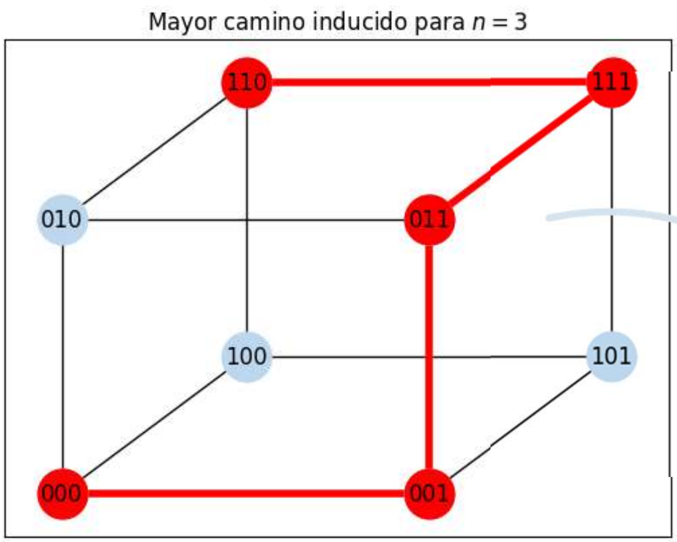
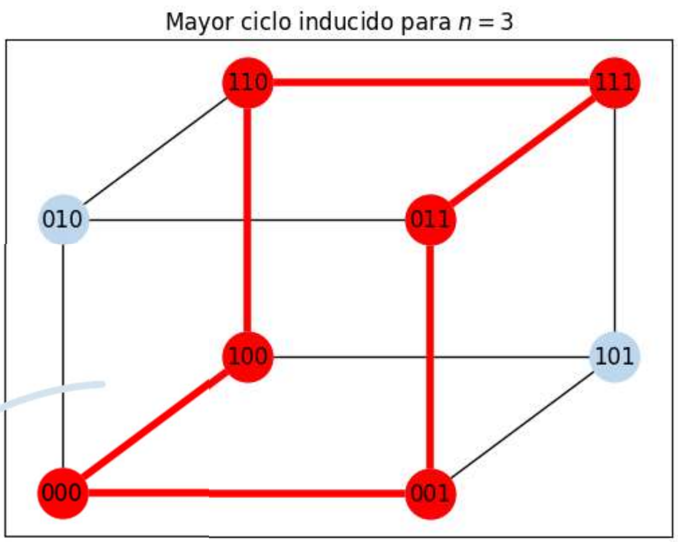
EXAMPLES FOR DIMENSION 3



For n = 3 the longest induced path has length 4



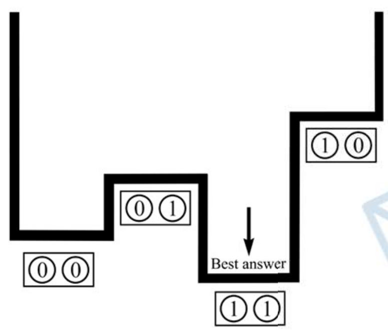
For n = 3 the máximum induced cycle has length 6

BEST VALUES

Dimension	SITB	CITB	Proven to be the best value?
1	1	0	Sí
2	2	4	Sí
3	4	6	Sí
4	7	8	Sí
5	13	14	Sí
6	26	26	Sí
7	50	48	Sí
8	98	96	Sí
9	190	188	No
10	370	366	No
11	712	692	No
12	1373	1344	No
13	2687	2594	No

QUBO FORMULATION AND QUANTUM ANNEALERS

- QUBO (Quadratic Unconstrained Binary Optimization) is a mathematical model for optimization problems.The objective is to minimize a binary quadratic form. Therefore we want to find the mínimum value of a function $Q: \{0,1\}^n \rightarrow \mathbb{R}$ of the form $\mathrm{Q}(\mathrm{x}) = \sum_{i,j} \alpha_{i,j} x_i x_j$
- Quantum Annealers are a type of quantum computer used to solve optimization problems. They are specifically designed to find the lowest energy configuration of a system.
- D-Wave is the pioneering company in the manufacturing of Quantum Annealers.



QUBO FORMULATION FOR THE INDUCED SUB-GRAPH PROBLEM

- The induced subgraph problem consists of determining whether $G_1 = (V_1, E_1)$ is an induced subgraph of $G_2 = (V_2, E_2)$, given two graph G_1 and G_2.
- G_1 is an induced graph of G_2 if and only if there exists an injective function $\phi: V_1 \to V_2$ such that $\{u, v\} \in E_1$ if and only if $\{\phi(u), \phi(v)\} \in E_2$.
- For the QUBO formulation define the binary variables $x_{u,i}$ for $u \in V_1,\ i \in V_2$ such that $x_{u,i} = 1$ only if $\phi(u) = i$. We also define s_i for $i \in V_2$ such that $s_i = 1$ if and only if there exists some $u \in V_1$ that maps to i.

$$Q = H_A + H_B$$

$$H_A = \sum_{u \in V_1} \left(1 - \sum_{i \in V_2} x_{u,i}\right)^2 + \sum_{i \in V_2} \left(s_i - \sum_{u \in V_1} x_{u,i}\right)^2$$

← ϕ is injective

$$H_B = \sum_{uv \in E_1} \sum_{ij \notin E_2} x_{u,i} x_{v,j} + \sum_{uv \notin E_1} \sum_{ij \in E_2} x_{u,i} x_{v,j}$$

← ϕ is structure preserving

QUBO FORMULATION FOR THE MAXIMUM COMMON INDUCED SUB-GRAPH PROBLEM

- The maximum common induced subgraph problem consists of finding a subgraph of the largest possible order that is induced in both $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$, given two graphs G_1 and G_2.
- This is equivalent to finding the set $A \subset V_1$ with the maximum number of elements such that there exists an injective function $\phi: A \to V_2$ that preserves the graph structure.
- We also define p_u for $u \in V_1$ such that $p_u = 1$ if and only if $u \in A$.

$$Q = \alpha H_A + \beta H_B + \gamma H_O$$

$$H_O = -\sum_{u \in V_1} p_u$$

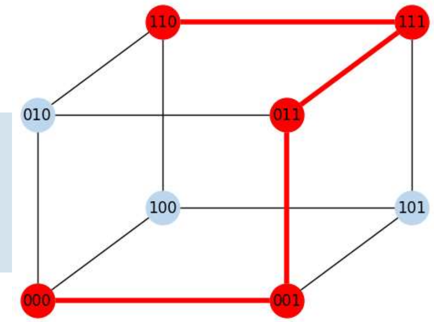
Maximice the number of elements of A.

$$H_A = \sum_{u \in V_1} \left(p_u - \sum_{i \in V_2} x_{u,i} \right)^2 + \sum_{i \in V_2} \left(s_i - \sum_{u \in V_1} x_{u,i} \right)^2$$

ϕ is injective

$$H_B = \sum_{uv \in E_1} \sum_{ij \notin E_2} x_{u,i} x_{v,j} + \sum_{uv \notin E_1} \sum_{ij \in E_2} x_{u,i} x_{v,j}$$

ϕ is structure preserving



QUBO FORMULATION FOR THE SITB PROBLEM

- For the Snake-in-the-box problem we can solve the maximum induced subgraph problem with $G_1 = P_{2^n}$ y $G_2 = Q_n$, adding a restriction to ensure that the selected subgraph is a path.
- This is the same (only if $G_1 = P_{2^n}$) to ensure that the selected subgraph is connected.
- We use the same formulation, adding a term H_C that ensures this.

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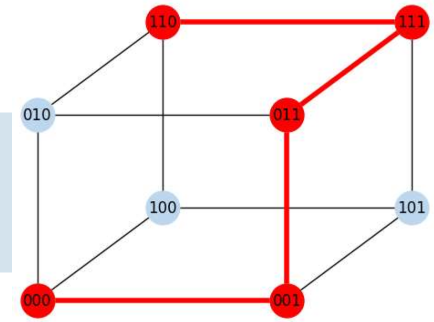

QUBO FORMULATION FOR THE SITB PROBLEM

- The formulation uses $|V_1||V_2| + |V_1| + |V_2| = 2^{2n} + 2^{n+1}$ binary variables

$$Q = \alpha H_A + \beta H_B + \gamma H_O + \delta H_C$$

$$H_O = -\sum_{u \in V_1} p_u$$

$$H_A = \sum_{u \in V_1} \left(p_u - \sum_{i \in V_2} x_{u,i} \right)^2 + \sum_{i \in V_2} \left(s_i - \sum_{u \in V_1} x_{u,i} \right)^2$$

Maximum common induced subgraph formulation

$$H_B = \sum_{uv \in E_1} \sum_{ij \notin E_2} x_{u,i} x_{v,j} + \sum_{uv \notin E_1} \sum_{ij \in E_2} x_{u,i} x_{v,j}$$

$$H_C = (1 - p_{v_0})^2 + \sum_{uv \in E_1} (p_u - p_v)^2$$

Ensures that the subgraph is a path

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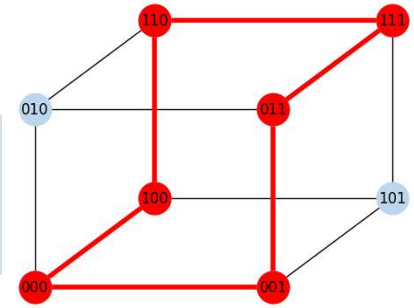
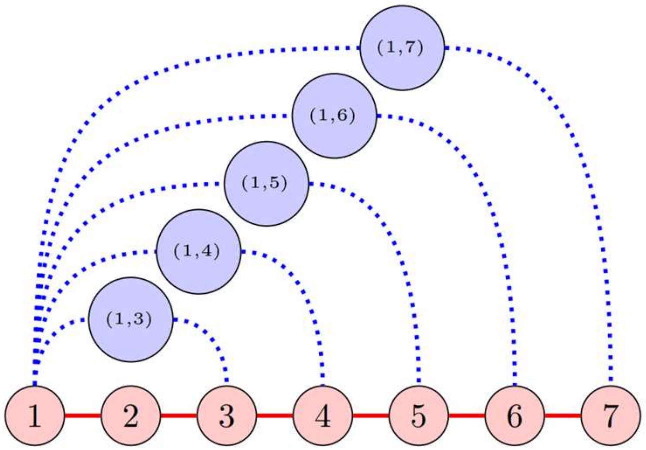
FORMULACIÓN QUBO PARA EL PROBLEMA DEL CITB

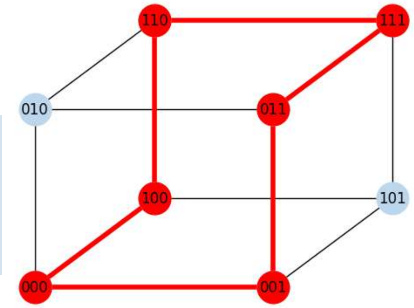


- El problema del Coil-in-the-box es equivalente a resolver el problema del máximo subgrafo inducido común donde G_1 es un grafo conteniendo todos los posibles ciclos (longitud 3 hasta 2^n) y $G_2 = Q_n$, agregando la restricción de que el subgrafo elegido sea un ciclo.
- Igual que en el caso anterior, se deben agregar términos extra para asegurar que el subgrafo elegido es un ciclo
- Se usa la misma formulación que para el problema del máximo subgrafo inducido común, agregando dos términos H_C y H_R que aseguran que el subgrafo elegido es un ciclo.

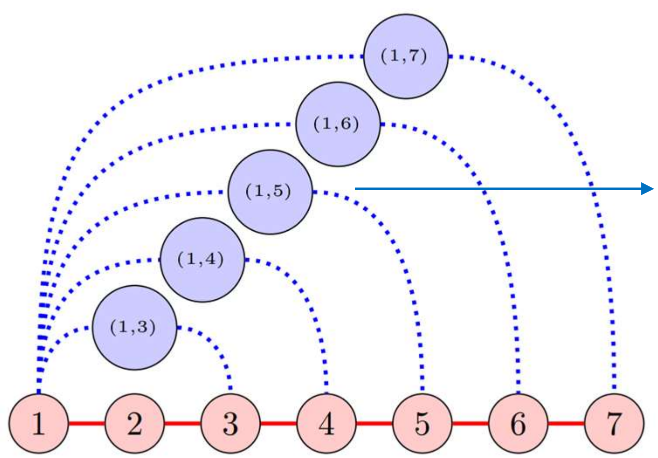
Grafo G_1 para n = 3

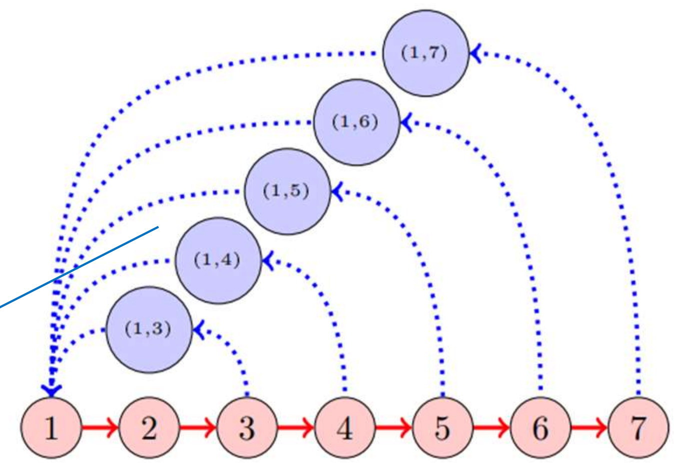


QUBO PARA EL PROBLEMA DEL CITB

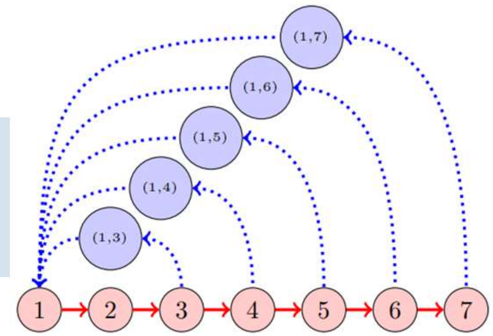


- Definimos a partir de G_1 un grafo dirigido. Denotamos cada arista (u, v) de este grafo dirigido cómo $u \to v$, para $u, v \in V_1$.
- Diferenciamos los vértices de V_1 cómo $V_1 = V_{path} \cup V_{cycle}$
- $V_{path} = \{1, 2, \ldots, 2^n - 1\}$
- $V_{cycle} = \{(1,3), (1,4), \ldots, (1, 2^n - 1)\}$





QUBO FORMULATION FOR THE COIL IN THE BOX PROBLEM



- The formulation uses $|V_1||V_2| + |V_1| + |V_2| = 2^{2n+1} - 2^n - 4$ binary variables.

$$Q = \alpha H_A + \beta H_B + \gamma H_O + \delta H_C + \epsilon H_R$$

$$H_O = -\sum_{u \in E_1} p_u$$

$$H_A = \sum_{u \in V_1}\left(p_u - \sum_{i \in V_2} x_{u,i}\right)^2 + \sum_{i \in V_2}\left(s_i - \sum_{u \in V_1} x_{u,i}\right)^2$$

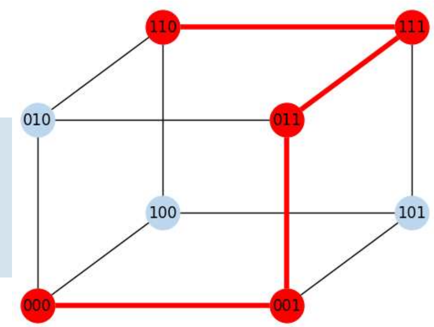
$$H_B = \sum_{uv \in E_1}\sum_{ij \notin E_2} x_{u,i}x_{v,j} + \sum_{uv \notin E_1}\sum_{ij \in E_2} x_{u,i}x_{v,j}$$

Maximum common induced subgraph formulation

$$H_C = \left(1 - \sum_{u \in V_{cycle}} p_u\right)^2$$

$$H_R = \sum_{u \in V_{path}}\left(p_u - \sum_{v:\, u \to v \in \overrightarrow{E_1}} p_v\right)^2$$

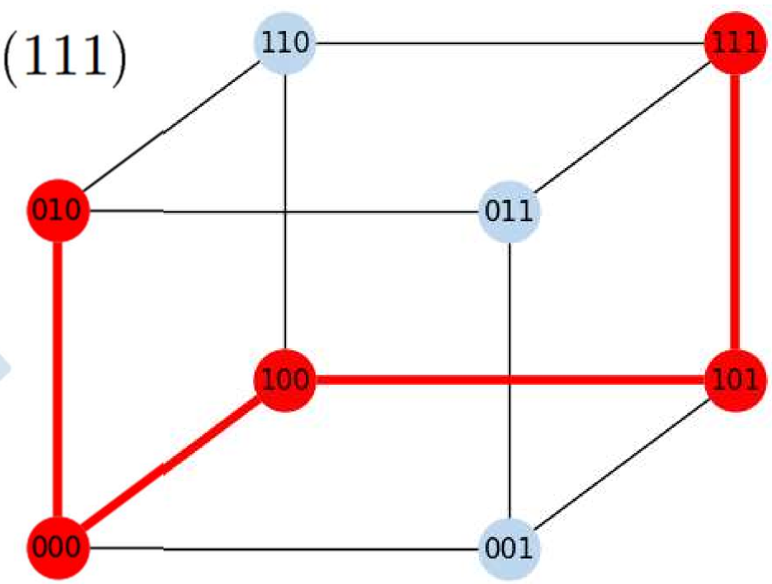
Ensures that the subgraph is a cycle



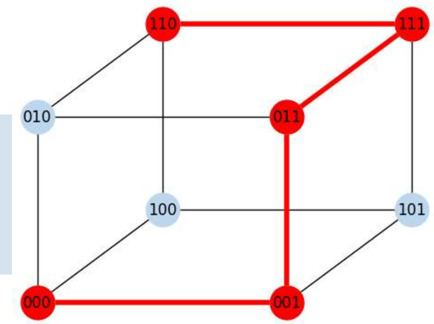
RESULTS SITB

- Best solution for n = 3 using DWave Quantum Annealers.

$$(010) \rightarrow (000) \rightarrow (100) \rightarrow (101) \rightarrow (111)$$



RESULTS SITB



- Using hybrid solvers and simulated annealing we found the optimal solution for n = 5

$$(10100) \to (00100) \to (00101) \to (01101) \to (01111) \to (11111) \to (10111) \to (10011) \to (00011) \to (00010) \to (01010) \to (11010) \to (11000) \to (11001)$$

$$(11001) \to (10001) \to (10000) \to (10100) \to (00100) \to (01100) \to (01000) \to (01010) \to (01011) \to (00011) \to (00111) \to (10111) \to (11111) \to (11110)$$

Hybrid solver

Paths of length 13

Simulated annealing

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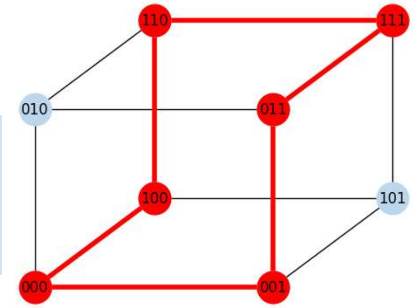
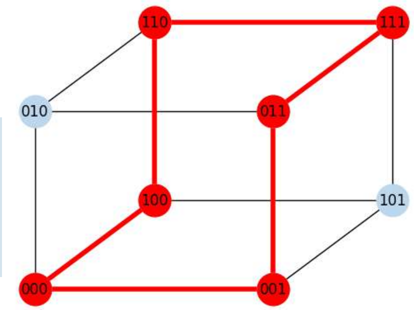


RESULTS CITB

- Best soluition for dimension 2 using Dwave Quantum Annealers.

$$(11) \to (01) \to (00) \to (10)$$

RESULTS CITB



- Using hybrid solvers and simulated annealing we found the optimal solution for n = 5

$$(00101) \to (00111) \to (10111) \to (11111) \to (11101) \to (11100) \to (10100) \to (10000) \to (10010) \to (11010) \to (01010) \to (01011) \to (01001) \to (00001)$$

$$(10111) \to (10110) \to (00110) \to (00100) \to (01100) \to (01000) \to (11000) \to (10000) \to (10001) \to (00001) \to (00011) \to (01011) \to (11011) \to (11111)$$

Cycles of length 14

Hybrid solver

Simulated annealing

THANK YOU!

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