Partition of Large Optimization Problems with One-Hot Constraint

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Take-home messages

Motivation:
Solving large optimization problems with the one-hot constraint efficiently.

Message1:
For difficult optimization problems with frustrations, the proposed methods are effective in improving solutions.

Message2:
One of the proposed methods releases us from adjusting \( \lambda \), which controls the strength of the one-hot constraint.
Agenda

1. Optimization of large problems using D-Wave
2. Proposed methods
3. Assessment of solution accuracy
4. Discussion on the results
5. Summary
1. Optimization of large problems using D-Wave
Limitations of the current D-Wave machine

- **Ising model of D-Wave machine**
  ① Number of qubits
  \[ \mathcal{H} = \sum_{(i,j) \in \text{Chimera}} J_{ij} \sigma_i \sigma_j + \sum_{i=1}^{N_q} h_i \sigma_i \]
  ② Restricted to Chimera graph

- **Practical optimization problem**
  ① Large number of variables
  \[ \mathcal{H} = \sum_{i<j}^{N_p} J_{ij} x_i x_j + \sum_{i=1}^{N_p} h_i x_i \]
  ② Between arbitrary variables

**Partitioning and embedding are required to solve practical optimization problems. In this talk, we focus on the partition of large optimization problems.**
Conventional tool: qbsolv

- Optimization process of qbsolv
  - Large problem
  - Partition into subproblems
  - Minor embedding

We propose efficient partitioning of large problems with the one-hot constraint.

We propose efficient partitions for the problems with one-hot constraint.

Example of a problem with one-hot constraint

< Traffic flow optimization by VW >

Select one route from three options for each taxi to minimize traffic congestion

F. Neukart, et. al., Front. ICT 4, 29 (2017)
2. Proposed methods
One-hot representation

<Original cost function>

\[ H_0 = \sum_{i<j} J_{ij} \delta(S_i, S_j) \]

\( S_i \in \{1, 2, ..., Q\} \)
variable with Q components

<Cost function with one-hot constraint>

\[ H_0 = \sum_{i<j} J_{ij} \sum_{q=1}^{Q} x_{qi} x_{qj} + \lambda \sum_{i=1}^{N} \left( \sum_{q=1}^{Q} x_{qi} - 1 \right)^2 \]

one-hot constraint

\( x_{qi} \in (0, 1) \)

\[ \begin{align*}
S_1 &= 2 \\
S_2 &= \dotsc \\
S_Q &= \dotsc \\
\end{align*} \]

Component 1
\[ \begin{align*}
\text{Component 1} & \quad \begin{array}{c}
0 \\
1 \\
\vdots \\
0
\end{array} \\
\text{Component 2} & \quad \begin{array}{c}
0 \\
1 \\
\vdots \\
0
\end{array} \\
\text{Component Q} & \quad \begin{array}{c}
0 \\
1 \\
\vdots \\
0
\end{array}
\end{align*} \]

Only Q of \( 2^Q \) states satisfy the one-hot constraint for each \( S_i \).

A fraction of states satisfy the one-hot constraint.
Simple example of bad partition

We should pay attention whether states satisfying the constraint are included or not.

< Current solution >

\[ S_1 = 3 \quad S_2 = 1 \quad S_3 = 4 \quad S_4 = 4 \]

Comp. 1

\[ 0 \quad 1 \quad 0 \quad 0 \]

Comp. 2

\[ 0 \quad 0 \quad 0 \quad 0 \]

Comp. 3

\[ 1 \quad 0 \quad 0 \quad 0 \]

Comp. 4

\[ 0 \quad 0 \quad 1 \quad 1 \]

one-hot constraint

①: currently selected component

< Candidates of transition destinations >

Extract as a subproblem

No destinations satisfy the one-hot constraint.

Better solutions cannot be searched by the optimization of the subproblem.
# Proposed methods

Two methods to extract subproblems including states that satisfy the constraint.

<table>
<thead>
<tr>
<th>Summary</th>
<th>Multivalued partition</th>
<th>Binary partition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Extract subproblems that contain current comp. for each variable</td>
<td></td>
<td>Extract a binary subproblem.</td>
</tr>
<tr>
<td>$S_1$</td>
<td>$S_2$</td>
<td>$S_3$</td>
</tr>
<tr>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
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Subproblem (more than two components)
1: currently selected component

<table>
<thead>
<tr>
<th>Pros</th>
<th>Multivalued partition</th>
<th>Binary partition</th>
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<tr>
<td>• Destinations satisfying the one-hot constraint exist for all variables.</td>
<td>• All states satisfy the constraint, and $\lambda$ disappears.</td>
<td></td>
</tr>
<tr>
<td>Cons</td>
<td>Multivalued partition</td>
<td>Binary partition</td>
</tr>
<tr>
<td>• Not all states satisfy the constraint.</td>
<td>• Only two components are considered at one time.</td>
<td></td>
</tr>
</tbody>
</table>

1: currently selected component

1: stay or transit binary variable: $y_i$
3.
Assessment of solution accuracy
Problem settings 1/2

■ Cost function

3D-4 components Potts models with 10x10x10 variables

\[ \mathcal{H}_0 = - \sum_{<i,j>} J_{ij} \delta S_i, S_j + \Delta_{ij} \]

\[ S_i \in (1, 2, 3, 4) \]

■ Problem graph

![Problem graph]

■ Parameters

<table>
<thead>
<tr>
<th>model</th>
<th>J_{ij}</th>
<th>\Delta_{ij}</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ferromagnetic model</td>
<td>-1</td>
<td>0</td>
</tr>
<tr>
<td>Anti-ferromagnetic model</td>
<td>+1</td>
<td>0</td>
</tr>
<tr>
<td>Potts glass model</td>
<td>+1(50%) or -1(50%)</td>
<td>0</td>
</tr>
<tr>
<td>Potts gauge glass model</td>
<td>-1</td>
<td>0(50%) or +1(25%) or -1(25%)</td>
</tr>
</tbody>
</table>

We evaluate solution accuracy for the several Potts models.
Problem settings 2/2

Simple examples of a ground state of the Potts models.

- **Ferromagnetic Potts model**
  - Interactions between same components exist.

- **Potts gauge glass model**
  - Interactions between different components exist.

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- **Ferromagnetic Potts model**
  - Components: Comp. 1, Comp. 2, Comp. 3, Comp. 4
  - Interactions: 
    - Between Comp. 1 and Comp. 2
    - Between Comp. 1 and Comp. 3
    - Between Comp. 1 and Comp. 4
    - Between Comp. 2 and Comp. 3
    - Between Comp. 2 and Comp. 4
    - Between Comp. 3 and Comp. 4
  - **One-hot constraint**
    - If one component is selected, all others are set to -J.

- **Potts gauge glass model**
  - Components: Comp. 1, Comp. 2, Comp. 3, Comp. 4
  - Interactions: 
    - Between Comp. 1 and Comp. 2
    - Between Comp. 1 and Comp. 3
    - Between Comp. 1 and Comp. 4
    - Between Comp. 2 and Comp. 3
    - Between Comp. 2 and Comp. 4
    - Between Comp. 3 and Comp. 4
  - **Frustration**
    - If all components are selected, the interactions cannot be satisfied simultaneously.

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**The ground states of the hard problem is non-trivial.**
Optimization process

We compare solution accuracy for three partitioning methods.
Results for the easy problems

Performance of normal and multivalued partitions are almost same. The energy obtained by binary partition differs from that of others.
Results for the hard problems

Performance of multivalued partition is better than that of normal one. The binary partition shows the best performance for the hard problems.
Discussion on the results
### Proposed methods

Two methods to extract subproblems including states that satisfy the constraint.

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<td>Extract subproblems that contain current solution for each variable</td>
<td>Extract a binary subproblem.</td>
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<tr>
<td></td>
<td></td>
<td>Randomly select two comps. in addition to current solutions</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Extract binary subproblem; “transit or not” binary variable: {y_{i}}</td>
</tr>
<tr>
<td></td>
<td>subproblem (more than two components)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>subproblem with two components</td>
</tr>
<tr>
<td></td>
<td>(1): current solution</td>
<td></td>
</tr>
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<td></td>
<td></td>
<td>(1): current solution</td>
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<tr>
<td>Pros</td>
<td>• Destinations satisfying the one-hot constraint exist for all variables.</td>
<td>• All states satisfy the constraint, and (\lambda) disappears.</td>
</tr>
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<td></td>
<td></td>
<td>• Large number of variables can be embedded.</td>
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<td>Cons</td>
<td>• Not all states satisfy the constraint.</td>
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Discussion: Binary partition for the ferromagnetic model

Question
Why is the performance of the binary partition remarkably bad for the ferromagnetic model?

Answer
Subproblems which can eliminate domain walls are rarely extracted.

<Current solution>
1D ferromagnetic Potts model with ten variables

comp. 1
\[
\begin{array}{cccccccc}
S_1 & S_2 & S_3 & S_4 & S_5 & S_6 & S_7 & S_8 & S_9 & S_{10} \\
1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0
\end{array}
\]

comp. 2
\[
\begin{array}{cccccccc}
0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1
\end{array}
\]

comp. 3
\[
\begin{array}{cccccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{array}
\]

comp. 4
\[
\begin{array}{cccccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{array}
\]

<Subproblem to align all variables to comp. 1>

\[
\begin{array}{cccccccc}
S_1 & S_2 & S_3 & S_4 & S_5 & S_6 & S_7 & S_8 & S_9 & S_{10} \\
1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0
\end{array}
\]

\[
\begin{array}{cccccccc}
0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1
\end{array}
\]

\[
\begin{array}{cccccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{array}
\]

\[
\begin{array}{cccccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{array}
\]

One of the first excited states which often appear.

The binary partition is not suitable for the ferromagnetic model.
Discussion: Binary partition for the anti-ferromagnetic model

Question
Why is the performance of the binary partition remarkably high for the anti-ferromagnetic model?

Answer
There exist many binary subproblems that reduce the energy.

<Current solution>

Suppose that we update the variable \( S_2 \).

\( S_2 \neq 1 \) reduce the energy.

<Binary subproblems to improve the current solution>

All binary subproblems can improve the current solution.

\[ \Rightarrow \text{Extracting only two components is sufficient.} \]

The existence of many low-energy transition destinations is essential.
Discussion: Binary partition for the hard problems

■ Question
Why is the performance of the binary partition high for the hard problems?

■ Answer
There exist many low-energy destinations caused by frustrations.

< Current solution >

Suppose that we update the variable $S_4$. Ground states satisfy three interactions.

There are two states that satisfy three interactions

$\Rightarrow$ Two of three binary subproblems can reduce the energy.

The binary partition is suitable for the problems with frustrations.
Summary of this talk

- **Summary**
  - We proposed two partitioning methods for problems with the one-hot constraint.
  - The binary partition shows best performance except for the ferromagnetic model.
  - The binary partition is suitable for problems with many low-energy destinations.
  - The binary partition contains only constraint-satisfying states, and we do not need to adjust the parameter $\lambda$.
  - We could not find problems for which the multivalued partition is suitable.

- **Future work**
  - Construct new algorithms to efficiently optimize the ferromagnetic model using the binary partition.
DENSO
Crafting the Core
Discussion: Normal partition for the easy problems

Question
Why is the performance of the multivalued partition is not superior to the normal one?

Answer
Transitions that violate the one-hot constraint can reduce the energy for the easy problems.

<Simple example of normal partition>
1D ferromagnetic Potts model
extract one-variable subproblem

<Energy of the subproblem>
\[
E(x = 1) = -2J + \lambda \\
E(x = 0) = 0
\]

If \( \lambda \) is not so large (\( \lambda < 2J \))
transitions violating the constraint can reduce the energy.

Multivalued partition is not so effective in improving solutions, if there exist states that satisfy many interactions simultaneously.