Solution Stability in Linear Programming Relaxations: Graph Partitioning and Unsupervised Learning

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Combinatorial Problems

Many ML problems take the form

\[(P1) \quad z^* := \arg\min_{z \in \mathcal{B}} w^\top z,\]

where

\begin{itemize}
  \item $\mathcal{B} \subseteq \{0, 1\}^n$: finite set of binary indicator vectors of length $n$.
\end{itemize}

\[\begin{array}{c}
1 \\
\vdots \\
0 \\
\end{array}
\begin{array}{c}
\vdots \\
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0 \\
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\begin{array}{c}
1 \\
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\begin{array}{c}
1 \\
\vdots \\
0 \\
\end{array}
\begin{array}{c}
\vdots \\
\downarrow \quad \text{w} \\
\end{array}
\begin{array}{c}
0 \\
1 \\
\end{array}
\]

\begin{itemize}
  \item Despite simplicity: very general model
\end{itemize}
Stability Analysis

Solution stability with respect to \( w \) for a single problem instance.

Why?

- \( w \) from noisy measurements: stable solutions → robust to noise
- \( w \) dependent on model parameters: stable solutions → trust in the model
- insight into data: multiple stable solutions can indicate different regimes
- parametrized solutions: solution paths, regularization paths, etc.

How?

- Linear programming analysis on LP relaxations
- Running example: graph partitioning
Example: Graph Partitioning / Clustering

- Graph \( G = (V, E) \), undirected, connected, simple
- \( z^* := \arg\min_{z \in B} w^T z \)
- Variables \( z \in \{0, 1\}^E \):
  - \( z_{i,j} = 1 \) “different partition”
  - \( z_{i,j} = 0 \) “same partition”
- Solutions \( B \subset \{0, 1\}^E \): all valid graph partitionings (multicut polytope)
- Weights \( w \in \mathbb{R}^E \):
  - \( w_{i,j} > 0 \) “prefer to be in the same partition”
  - \( w_{i,j} < 0 \) “prefer to be in different partition”
Example: Graph Partitioning / Clustering

- Graph $G = (V, E)$, undirected, connected, simple
- $\mathbf{z}^* := \text{argmin}_{\mathbf{z} \in \mathcal{B}} \mathbf{w}^\top \mathbf{z}$
- Variables $\mathbf{z} \in \{0, 1\}^E$,
  - $z_{i,j} = 1$ “different partition”,
  - $z_{i,j} = 0$ “same partition”,
- Solutions $\mathcal{B} \subset \{0, 1\}^E$: all valid graph partitionings (multicut polytope)
- Weights $\mathbf{w} \in \mathbb{R}^E$:
  - $w_{i,j} > 0$ “prefer to be in the same partition”,
  - $w_{i,j} < 0$ “prefer to be in different partition”.

$\pi(\cdot) = 1$
$\pi(\cdot) = 2$
$\pi(\cdot) = 3$
### Example (cont’)

Setting covers popular methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Weights</th>
</tr>
</thead>
<tbody>
<tr>
<td>Correlation Clustering</td>
<td>( w_{i,j} = \text{similarity ratings} )</td>
</tr>
<tr>
<td>Clustering Aggregation</td>
<td>( w(i,j) = \frac{1}{m} \sum_{k=1}^{m} (1 - 2r_{i,j}^k), \forall (i,j) \in V \times V ) (Expected similarity with proposal clusterings)</td>
</tr>
<tr>
<td>Modularity Clustering</td>
<td>( w(i,j) = \frac{1}{2</td>
</tr>
<tr>
<td>Relative Performance Clustering</td>
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<tr>
<td>Significance Clustering</td>
<td></td>
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<tr>
<td>Bias: diff. of cluster sizes</td>
<td>( \lambda \sum_{k,l=1}^{K} (</td>
</tr>
<tr>
<td>Bias: squared cluster sizes</td>
<td>( \lambda \sum_{k=1}^{K}</td>
</tr>
</tbody>
</table>
Linear Programming Relaxations

- $\mathcal{B}$ is a finite but large set
- Optimization over the convex hull $\text{conv}(\mathcal{B})$ is exact, i.e.

$$\arg\min_{z \in \mathcal{B}} w^\top z = \arg\min_{z \in \text{conv}(\mathcal{B})} w^\top z.$$
Linear Programming Relaxations (cont)

- $\mathcal{B}$ and thus $\text{conv}(\mathcal{B})$ is hard to describe
- Idea: approximate $\text{conv}(\mathcal{B})$ by a larger set $\hat{\mathcal{B}}$

$$\arg\min_{z \in \text{conv}(\mathcal{B})} \mathbf{w}^\top z \geq \arg\min_{z \in \hat{\mathcal{B}}} \mathbf{w}^\top z.$$
Facets and Valid Inequalities

Convex polytopes have two equivalent representations

- As a convex combination of extreme points
- As a set of facet-defining linear inequalities

A linear inequality with respect to a polytope can be

- valid, does not cut off the polytope,
- representing a face, valid and touching,
- facet-defining, representing a face of dimension one less than the polytope.
Solving Linear Relaxations

Delayed constraint generation

- Optimize over a subset of linear inequalities
- Identify violated inequalities over the full set

Returns solution and lower bound on the optimal objective

1. \( S \leftarrow [0, 1]^n \) \{Initial feasible set\}
2. \( \text{loop} \)
3. \( z \leftarrow \text{argmin}_{z \in S} w^T z \) \{Solve LP relaxation\}
4. \( S_{\text{violated}} \leftarrow \text{SEPARATEINEQUALITIES}(B, z) \)
5. \( \text{if no violated inequality found then} \)
6. \( \text{break} \)
7. \( \text{end if} \)
8. \( S \leftarrow S \cap S_{\text{violated}} \) \{Cut \( z \) from feasible set\}
9. \( \text{end loop} \)
10. \( \text{optimal} \leftarrow (z \in \{0, 1\}^n) \) \{Integrality check\}
11. \( (f, z^*) \leftarrow (w^T z, z) \)
Stability Range

Setting

- **optimal solution**
  \[ \mathbf{z}^* := \operatorname{argmin}_{\mathbf{z} \in \operatorname{conv}(\mathcal{B})} \mathbf{w}^\top \mathbf{z}, \]
- **perturbation vector** \( \mathbf{d} \in \mathbb{R}^n \),
- **modified weights** \( \mathbf{w}'(\theta) = \mathbf{w} + \theta \mathbf{d} \)

Stability Range

- **stability range**: \( \theta \)-interval
  \[ [\rho \mathbf{d}_-, \rho \mathbf{d}_+] \in (\{-\infty, \infty\} \cup \mathbb{R})^2 \text{ for which } \mathbf{z}^* \text{ remains optimal} \]
- **perturbed problem**
  \[ \min_{\mathbf{z} \in \operatorname{conv}(\mathcal{B})} \mathbf{w}'(\theta)^\top \mathbf{z}. \]
Stability Analysis (1)

- LP geometry: solution becomes suboptimal when \( w + \theta d \) leaves the cone of negative constraint normals at \( z^* \)
- Standard LP stability analysis: basis matrix approach
- Here: does not work, not all binding constraints at \( z^* \) are known, additionally degeneracy
Stability Analysis (2)

Idea from Jansen [7]

- explicitly search cone of constraint normals

\[
\begin{align*}
\min_{\alpha \in \mathbb{R}, z \in \mathbb{R}^n} & \quad w^T z + \alpha w^T z^* \\
\text{s.t.} & \quad \frac{1}{\alpha} z \in \text{conv}(B), \\
& \quad (d^T z^*)\alpha - d^T z = t : \lambda, \\
& \quad 0 \leq z_i \leq \alpha, \quad i = 1, \ldots, n.
\end{align*}
\]

- \( \left( \frac{1}{\alpha} z \right) \in \text{conv}(B) \) still linear \( (A(\frac{1}{\alpha} z) \leq b \iff Az - \alpha b \leq 0) \)
- Separation routine recycling: given \((z, \alpha)\) we can still separate from \(\text{conv}(B)\)
- Complexity: identical to canonical problem

Lagrange multiplier \( \lambda \) provides \( \rho_{d,-} \) for the left boundary \((t = -1)\) or \( \rho_{d,+} \) for the right boundary \((t = 1)\).
Stability Analysis (3)

Theorem (Stability Inclusion)

Let $z^*$ be the optimal solution of $P1$ for a given $B \subseteq \{0, 1\}^n$ and weights $w \in \mathbb{R}^n$. For a perturbation $d \in \mathbb{R}^n$, let $[\xi_d^-, \xi_d^+]$ be the true stability range for $\theta$ on $\text{conv}(B)$. If $\hat{B} \supseteq \text{conv}(B)$ is a polyhedral relaxation of $B$ using only facet-defining inequalities and if $z^*$ is a vertex of $\hat{B}$, then the stability range $[\rho_d^-, \rho_d^+]$ on $\hat{B}$, i.e., for the relaxation $\min_{z \in \hat{B}} w^T z$, is included in the true range: $[\rho_d^-, \rho_d^+] \subseteq [\xi_d^-, \xi_d^+]$.

Simply put

- estimated stability is conservative
- never overestimates the true stability
Multicut Polytope (1)

- Convex hull of the set of all partitionings of a graph: *multicut polytope*
- Extensive results in late eighties and early nineties [5, 6, 2, 3, 4].
- Classes of facet-defining inequalities known

Polynomial-time separable facet-defining inequalities for the multicut polytope

- Cycle inequalities
- Odd-wheel inequalities
Multicut Polytope: Cycle Inequalities

- generalize triangle inequalities,
- valid graph partitioning $z$ satisfies a *transitivity* relation: there is no all-zero path between any two adjacent vertices $i$, $j$ that are in different subsets of the partition.

For chord-free cycles $((i, j), p)$, $p \in \text{Path}(i, j)$, where $\text{Path}(i, j)$ is the set of paths between $i$ and $j$, we have the facet-defining inequalities

$$z_{i,j} \leq \sum_{(s,t) \in p} z_{s,t}, \quad (i, j) \in E, \quad p \in \text{Path}(i, j).$$

- Complete graphs: all cycles longer than three edges contain chords → reduces to triangle inequalities,
- Separation procedure: series of shortest path problems.
Multicut Polytope: Odd-wheel Inequalities

- A $q$-wheel is a connected subgraph $S = (V_s, E_s)$ with a central vertex $j \in V_s$ and a cycle of the $q$ vertices in $C = V_s \setminus \{j\}$,

- For each $i \in C$ there exists an edge $(i, j) \in E_s$.

Then, for every $q$-wheel, a valid partitioning $z$ satisfies

$$\sum_{(s, t) \in E(C)} z_{s,t} - \sum_{i \in C} z_{i,j} \leq \left\lfloor \frac{1}{2} q \right\rfloor,$$

- Polynomial-time separable [3, 2]
Experiment: Relaxation Tightness

Examine tightness of multicut polytope relaxation

- Maximize modularity objective on popular benchmark data sets [1, 8]
- Kernighan-Lin: popular graph-partitioning heuristic (VLSN)
- LP-C: LP relaxation with cycle-inequalities only
- LP-CO: LP relaxation with cycle- and oddwheel-inequalities

<table>
<thead>
<tr>
<th></th>
<th>Kernighan-Lin</th>
<th>LP-C</th>
<th>LP-CO</th>
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<tbody>
<tr>
<td>dolphins</td>
<td>0.5268</td>
<td>(0.5315)</td>
<td>4.2s</td>
</tr>
<tr>
<td></td>
<td>0.4s</td>
<td></td>
<td>0.5285</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>9.1s</td>
</tr>
<tr>
<td>karate</td>
<td>0.4198</td>
<td>0.4198</td>
<td>0.4198</td>
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<tr>
<td></td>
<td>0.1s</td>
<td>0.2s</td>
<td>0.2s</td>
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<tr>
<td>polbooks</td>
<td>0.5226</td>
<td>(0.5276)</td>
<td>147.4s</td>
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<tr>
<td></td>
<td>7.0s</td>
<td>0.5272</td>
<td>148.5s</td>
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<tr>
<td>lesmis</td>
<td>0.5491</td>
<td>(0.5609)</td>
<td>6.9s</td>
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<td></td>
<td>1.5s</td>
<td>0.5600</td>
<td>11.7s</td>
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<tr>
<td>att180</td>
<td>0.6559</td>
<td>(0.6633)</td>
<td>302.3s</td>
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<tr>
<td></td>
<td>14.5s</td>
<td>0.6595</td>
<td>1119.6s</td>
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- LP-CO achieves global optimum, LP-C only on smallest problem
- Heuristic fast but suboptimal
Experiment: Tracing Solution Path

- Stability quantifies when the perturbed solution becomes suboptimal
- → can be used to compute solution path

We can efficiently trace all solutions along a piecewise linear path in weightspace ("parametric programming").
Experiment: Tracing Solution Path

- Data: 26 classes of leaves, $w$: pairwise confusion rates from human experiments (courtesy of Frank Jäkel)
- Task: clustering leaves by human “confusion rates similarity”
- $d = 1$, uniform bias toward fewer/more clusters
- Trace solution path, identify stable solutions
Experiment: “Critical” Edges

In some cases, stability can be visualized in the input data.

- Social network data: edges indicate social contact
- Modularity clustering: grouping
- Question: which friendships are essential in that their removal would change the grouping?
- Answer: for each friendship between $i$ and $j$, check stability range for $d = w(E \setminus \{(i, j)\}) - w(E)$

Figure: Critical edges in karate social network.
Conclusions

- Proposed a general method to quantify solution stability for combinatorial optimization problems
  - Requires only separation oracle
  - Works for problems with exponentially many inequalities
- Computed stability is conservative
- Is exact if relaxation is \textit{locally exact}
- Allows computation of stability ranges and solution paths
# References

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  Sensitivity analysis in linear programming: Just be careful!  

  Finding and evaluating community structure in networks.  
LP-C/LP-CO tightness example

**Figure**: Example input graph with four vertices and edge weights as shown.

**Figure**: Fractional solution with $f(z^*) = -1.55$, obtained by the simple LP relaxation (without odd wheel inequalities).

**Figure**: Integer solution with $f(z^*) = -1.5$, obtained by adding the odd wheel inequality $z_{0,2} + z_{0,3} + z_{2,3} - z_{0,1} - z_{1,2} - z_{1,3} \leq 1$. 
Limitations of the Basis Matrix Approach: Example

Figure: Toy example input graph with signed edge weights shown. The optimal graph partitioning has an objective of $-1.6$ and produces the three sets as shown.
Limitations of the Basis Matrix Approach: Example

Figure: Per-edge weight sensitivities at the optimal solution, estimated by the basis matrix method.
Limitations of the Basis Matrix Approach: Example

Figure: Per-edge weight sensitivities at the optimal solution, exact by the auxiliary linear programming method.