

Partially Optimal Cubic Subspace Clustering

Research Project Machine Learning

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- 1 Introduction
- 2 Partial Optimality for Cubic Clique Partition Problem
- 3 Cubic Subspace Instance Construction
- 4 Experiments and Evaluation
- 5 Conclusion

Problem Statement (1)

Finite sample set S , cost function $c: \binom{S}{3} \rightarrow \mathbb{R}$.

Instance of the **Cubic Clique Partition Problem**:

$$\min_{y: \binom{S}{2} \rightarrow \{0,1\}} \sum_{abc \in \binom{S}{3}} c_{abc} y_{ab} y_{bc} y_{ac}$$

subject to $y_{ab} + y_{bc} - 1 \leq y_{ac}$ for all distinct $a, b, c \in S$.

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Find a **partially optimal solution**, i.e. fix some labels y_{ab} for distinct $a, b \in S$

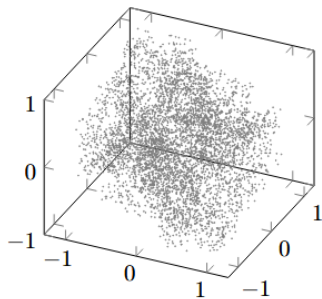
$$\begin{cases} y_{ab} = 1 & \text{join } a, b \\ y_{ab} = 0 & \text{cut } a, b \\ y_{ab} = ? & \text{unknown} \end{cases}$$

in such way that there still exists an optimal solution.

Problem Statement (2)

Subspace Instances of the Cubic Clique Partition Problem

Samples S : points $S \subset \mathbb{R}^3$



(a) Samples S

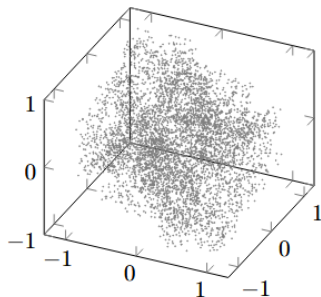
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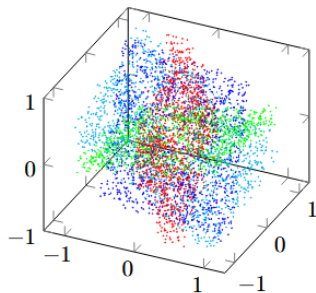
Samples S : points $S \subset \mathbb{R}^3$

Point generation: 3 distinct planes containing the origin, noise σ

Optimal labeling y^* : original planes



(a) Samples S



(b) Optimal labeling y^*

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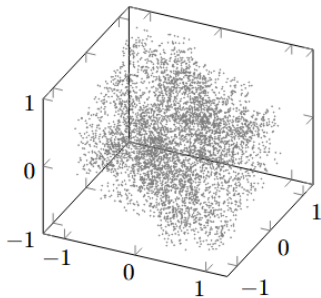
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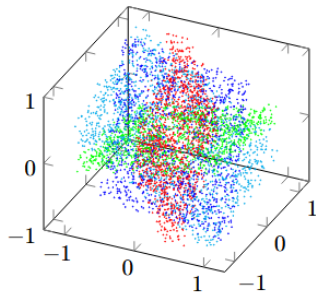
Point generation: 3 distinct planes containing the origin, noise σ

Optimal labeling y^* : original planes

Cost function c ? (no concrete plane information given)



(a) Samples S



(b) Optimal labeling y^*

Related Work:

- Stein, Di Gregorio, and Andres, "Partial Optimality in Cubic Correlation Clustering"
- Lange, Karrenbauer, and Andres, "Partial Optimality and Fast Lower Bounds for Weighted Correlation Clustering"
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Tasks and Solutions:

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→ implementation in C++

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- 3 Apply algorithm to the subspace instances, assess partial optimality, accuracy and computation time
→ experiments and evaluation

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Partial Optimality for Cubic Clique Partition Problem

Extended cost function $c: \binom{S}{3} \cup \binom{S}{2} \cup \emptyset \rightarrow \mathbb{R}$

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Instance of the extended cubic clique partition problem:

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subject to $y_{ab} + y_{bc} - 1 \leq y_{ac}$ for all distinct $a, b, c \in S$.

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Let $Y \neq \emptyset$, $\phi: Y \rightarrow \mathbb{R}$ and $\sigma: Y \rightarrow Y$. σ is an **Improving Map** for the problem $\min_{y \in Y} \phi$ if for every $y \in Y$: $\phi(\sigma(y)) \leq \phi(y)$.

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Moreover, let $Q \subseteq Y$ and σ an improving map. If for every $y \in Y$, $\sigma(y) \in Q$, then there is an optimal solution $y^* \in Q$. to $\min_{y \in Y} \phi$.

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Let $Y \subseteq \{\text{feasible } y \mid y: \binom{S}{2} \rightarrow \{0,1\}\}$, $\phi_c: Y \rightarrow \mathbb{R}$ and σ an improving map. If for every $y \in Y$: $\sigma(y)_{ab} = \beta$, $ab \in \binom{S}{2}$, $\beta \in \{0,1\}$, then there is an optimal solution y^* to $\min_{y \in Y} \phi_c$ such that $y^*_{ab} = \beta$.

Pair-CUT Partial Optimality Condition

Let $ij \in \binom{S}{2}$. If there exists $R \subseteq S$ such that $i \in R \wedge j \notin R$ and

$$c_{ij}^+ \geq \sum_{p \in R \wedge q, r \notin R \vee p, q \in R \wedge r \notin R} c_{pqr}^- + \sum_{p \in R \wedge q \notin R} c_{pq}^-$$

then there is an optimal solution y^* to $\min_{y \in Y} \phi_c$ such that $y_{ij}^* = 0$.

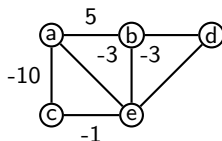
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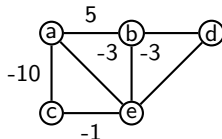
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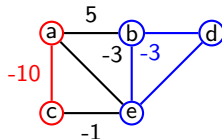
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a-b Min-Cut



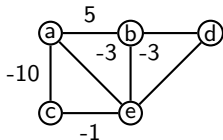
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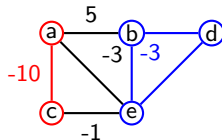
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Improving map $\sigma : Y \rightarrow Y$ for $y \in Y$ and $pq \in \binom{S}{2}$:

$$\begin{cases} \sigma(y)_{pq} = 0 & y_{ij} = 1 \wedge |\{p, q\} \cap R| = 1 \\ \sigma(y)_{pq} = y_{pq} & \text{otherwise} \end{cases}$$

Partial Optimality Conditions:

- ① Subproblem-CUT-condition (cut subset from its complement)
- ② CUT-conditions (cut pairs and triples)
- ③ JOIN-conditions (join subsets, pairs and triples)

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CUT-conditions can be applied simultaneously.

JOIN-conditions must be applied iteratively!

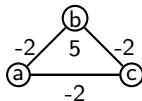
$Q_1, Q_2 \in Y$: if there exists an optimal $y_1^* \in Q_1$ and there exists an optimal $y_2^* \in Q_2 \nrightarrow$ there is an optimal $y^* \in Q_1 \cap Q_2$:

$$\min_{y \in Y} \phi_c = -2$$

$$Q_1 = \{y \in Y \mid y_{ab} = 1\}$$

$$Q_2 = \{y \in Y \mid y_{ac} = 1\}$$

$$\rightarrow Q_1 \cap Q_2 = \{y \in Y \mid y_{ab} = 1 \wedge y_{ac} = 1\} \nrightarrow$$



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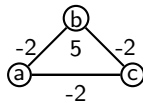
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Apply partial optimality conditions \rightarrow solve subproblems!



Partial Optimality Algorithm

Partial Optimality Algorithm:

Input: labeling y without fixed labels

while condition applied **do**

 apply subproblem-CUT-condition exhaustively

 apply one of JOIN-conditions (in effective order)

end while

apply CUT-conditions exhaustively

Output: partially optimal labeling y with some fixed labels

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- 1 Subproblem-CUT-condition: fix 0-labels for element pairs from different sample subsets; solve each subset as an independent problem; accumulate the results in c_\emptyset ;
- 2 JOIN-Conditions: fix 1-labels for elements of the sample subset; add the join-cost to c_\emptyset ; solve the problem where the subset is considered as one sample;

Subproblem-CUT and Subset-JOIN

Subproblem-CUT: cut sample subsets R_1, R_2, \dots, R_k that are only connected via non-negative costs (applied if $k > 1$)

Subproblem-CUT and Subset-JOIN

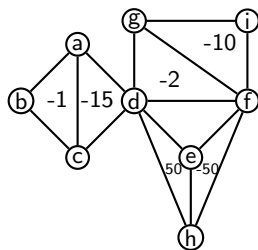
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(the worst bipartition joining cost \approx min-cut)

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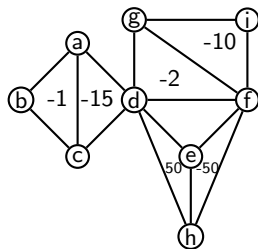


$$c_{\emptyset} = 0$$

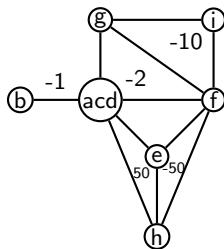
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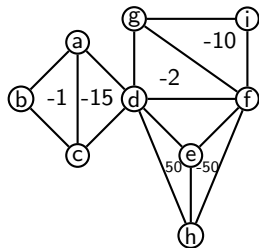


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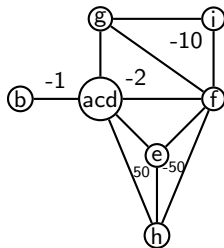
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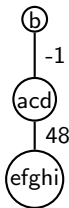
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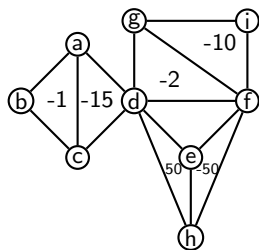


$$c_{\emptyset} = -75$$

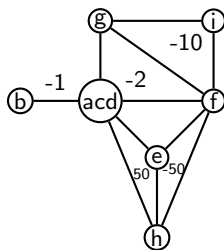
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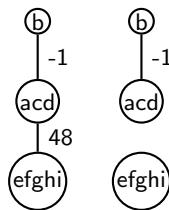
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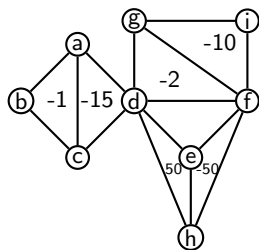


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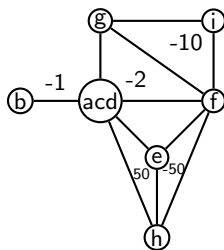
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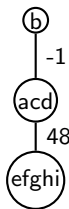
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$$c_{\emptyset} = 0$$



$$c_{\emptyset} = -15$$



$$c_{\emptyset} = -75$$



$$c_{\emptyset} = -76$$



Other JOIN-conditions

Pair-JOIN-1: join samples $ij \in \binom{S}{2}$ if their overall joining reward \geq the sum of rewards and penalties for joining some subset R with $i \in R \wedge j \notin R$ with \bar{R} (\approx i-j min-cut)

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Pair-JOIN-2: join samples $ik \in \binom{S}{2}$ if there exist $ijk \in \binom{S}{3}$ that fulfills 3 conditions (\approx i-jk min-cut, \approx ij-k min-cut, 1 explicit condition)

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Pair-JOIN-3: join samples $ij \in \binom{S}{2}$ if $c_{ij} \leq$ the sum of reward costs for joining pairs and triples containing i or j

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Pair-JOIN-3: join samples $ij \in \binom{S}{2}$ if $c_{ij} \leq$ the sum of reward costs for joining pairs and triples containing i or j

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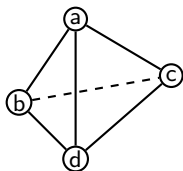
Pair-JOIN-4: join samples $ik \in \binom{S}{2}$ if there exists $ijk \in \binom{S}{3}$ such that 7 explicit conditions hold

Triple-JOIN: join samples $ijk \in \binom{S}{3}$ if the condition holds (similar to Pair-JOIN-1) (\approx i-jk min-cut)

Pyramid Instance and CUT-conditions

$$c_{bcd} = 10$$

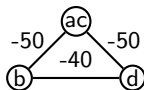
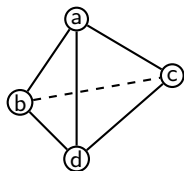
$$c_{abc} = c_{abd} = c_{acd} = -50$$



Pyramid Instance and CUT-conditions

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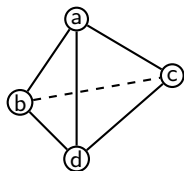


Pair-JOIN-2

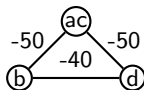
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Subset-JOIN

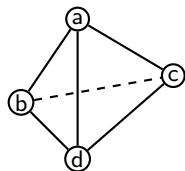


$$c_{\emptyset} = -140$$

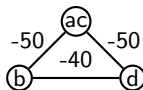
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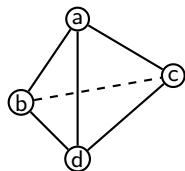
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Pair-CUT: cut samples i, j if the direct joining penalty \geq the sum of rewards for joining some subset R with $i \in R \wedge j \notin R$ with \bar{R} (\approx i-j min-cut)

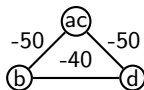
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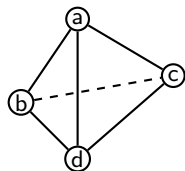
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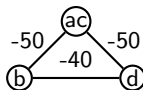
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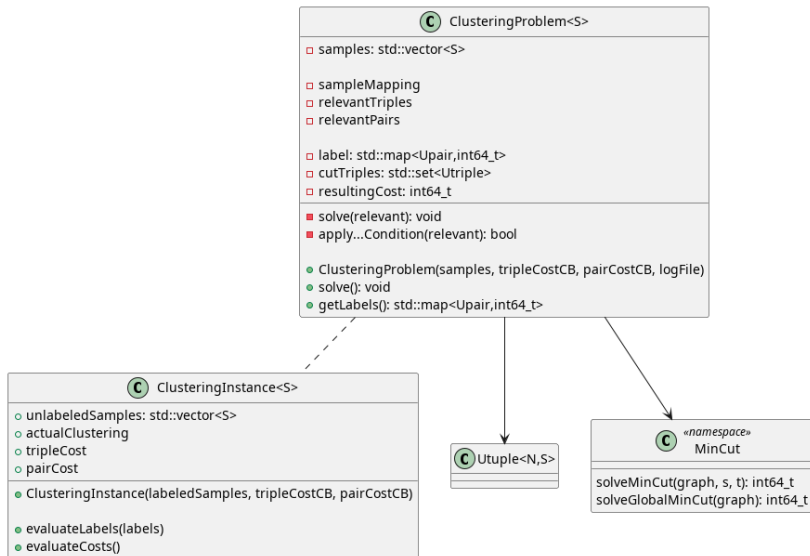
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Samples in the pyramid with $c_{bcd} = 100$ are unjoinable!
Triple-CUT is applied to the triple bcd

Program Structure

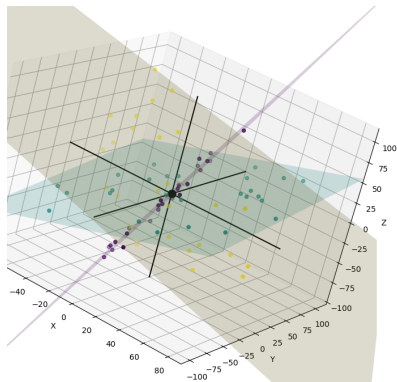


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Plane and Point Generation

Plane Generation:

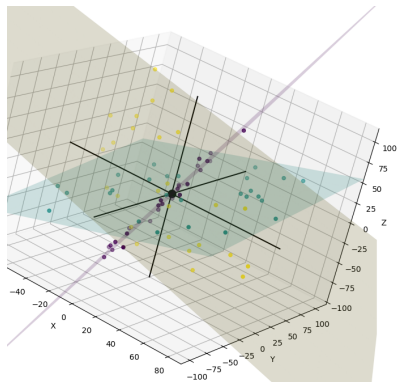
- generate 3 planes
as distinct normal vectors
 $\vec{n}_1, \vec{n}_2, \vec{n}_3$ (normalized)



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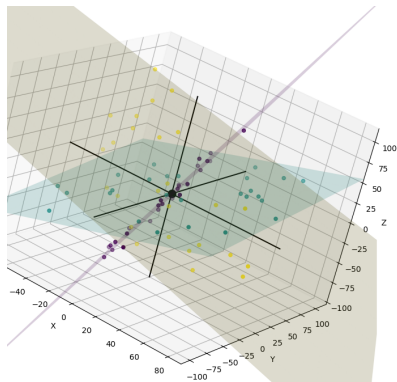
- generate 3 planes as distinct normal vectors $\vec{n}_1, \vec{n}_2, \vec{n}_3$ (normalized)
- compute a $\vec{r}_{i,1}$ (normalized) orthogonal to \vec{n}_i ($i \in \{1, 2, 3\}$)



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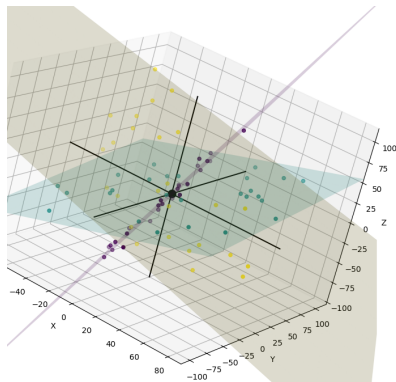
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Point Generation on the plane $(\vec{n}, \vec{r}_1, \vec{r}_2)$, parameters (D, σ) :

- random variables $k_1, k_2 \in [-D, D]$ (uniform distribution)
- random variable k_n (normal distribution based on σ)
- generate point $p = k_1 \vec{r}_1 + k_2 \vec{r}_2 + k_n \vec{n}$

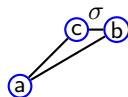
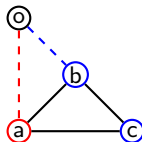
Cost Function (1)

Triangle $abc \in \binom{S}{3}$

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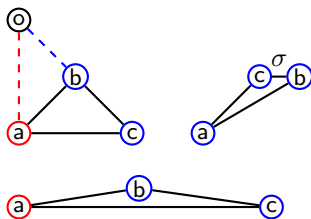
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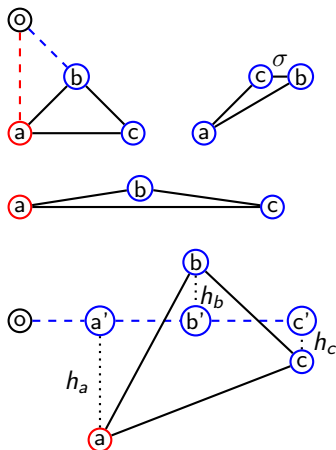
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(3) h_a, h_b, h_c : distances
to the best fitted plane
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$$h_a + h_b + h_c > 3\sigma + 10^{-6}$$

$$\rightarrow c_{abc} = \frac{(h_a + h_b + h_c) - (3\sigma + 10^{-6})}{3D}$$



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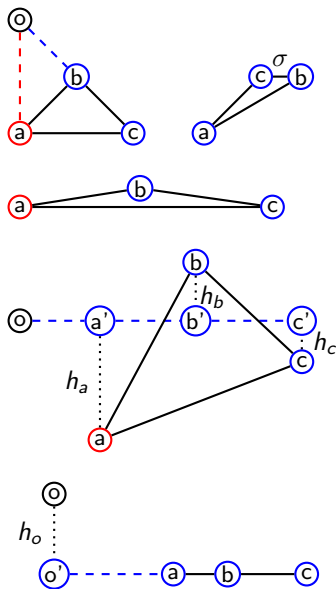
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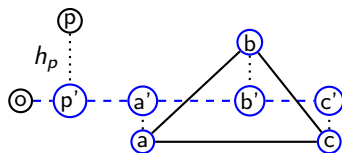
$$h_o > \frac{10}{\#points}\sigma + 10^{-6}$$

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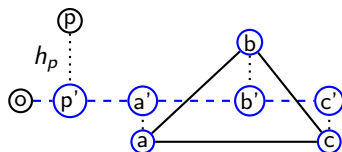
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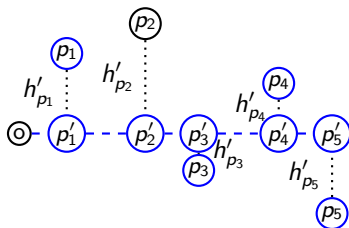
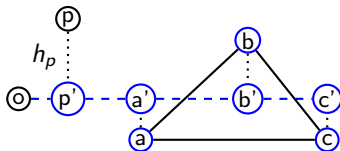
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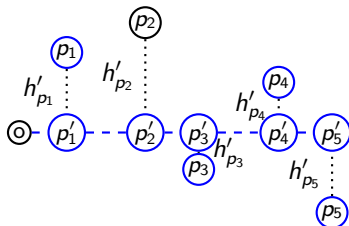
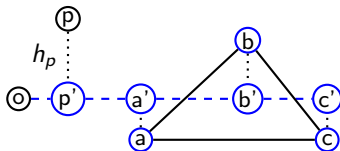
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$$\delta_p := \frac{hp' - (\sigma + 10^{-6})}{D}$$

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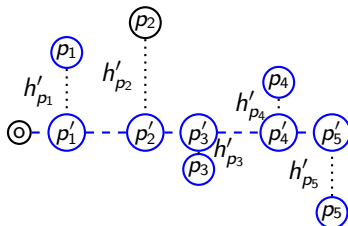
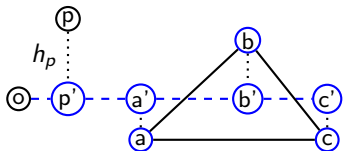
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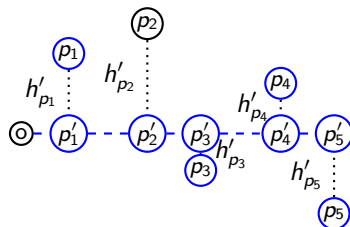
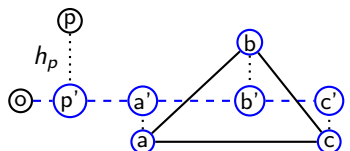
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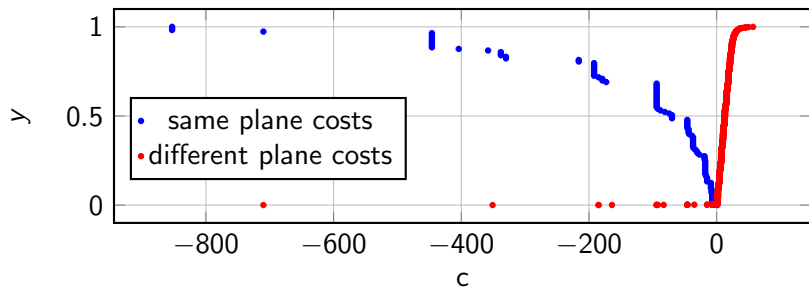
$$|M| \leq 3 \rightarrow c_{abc} = 0$$

$$\rightarrow c_{abc} = 2^{|M|-4} \cdot \sum_{p \in M} \delta_p$$

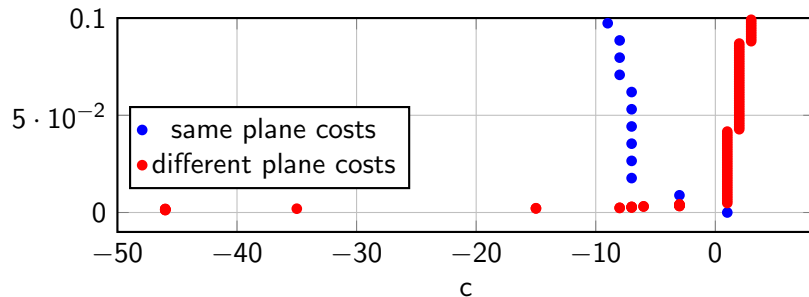
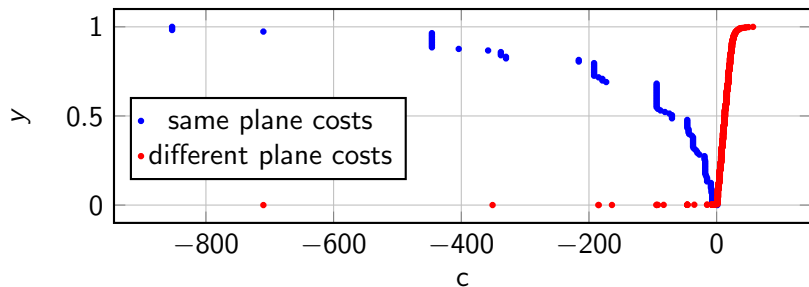


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Cost Function Evaluation (3x15 points, $\sigma = 1$)



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- Apply the algorithm to the random cubic subspace instances with $D = 100$ and fixed $\sigma = 0, 1, 2, 3, 4, 5$:
 - 3x7 points (solve 15 instances)
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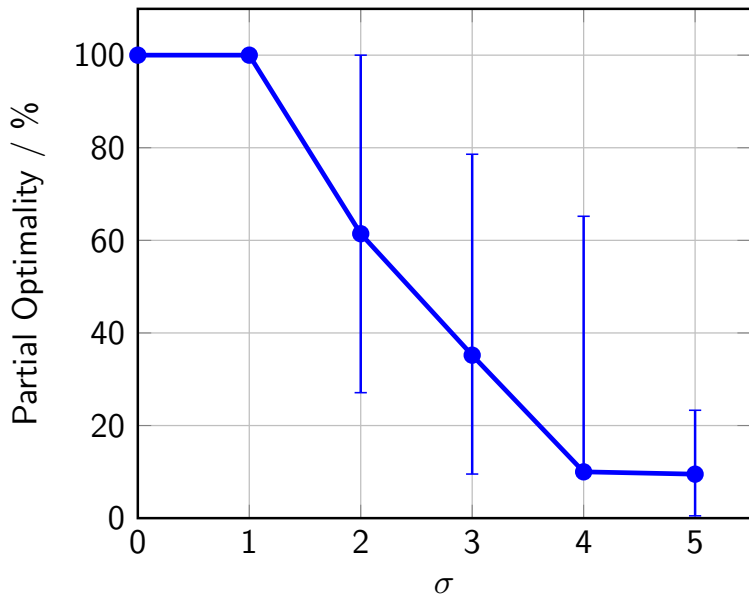
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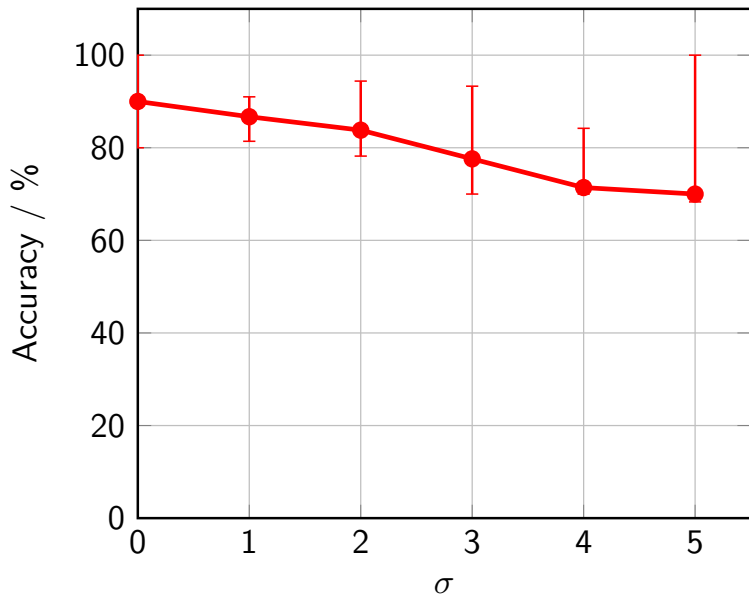
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- Capture
 - 1.quartile (Q1)
 - median (Q2)
 - 3.quartile(Q3)
 - the worst computation time

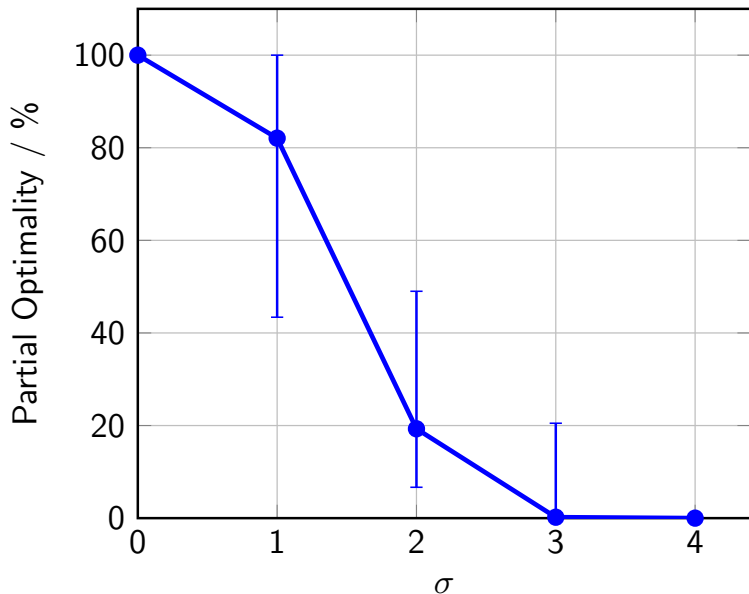
Partial Optimality (3x7 points)



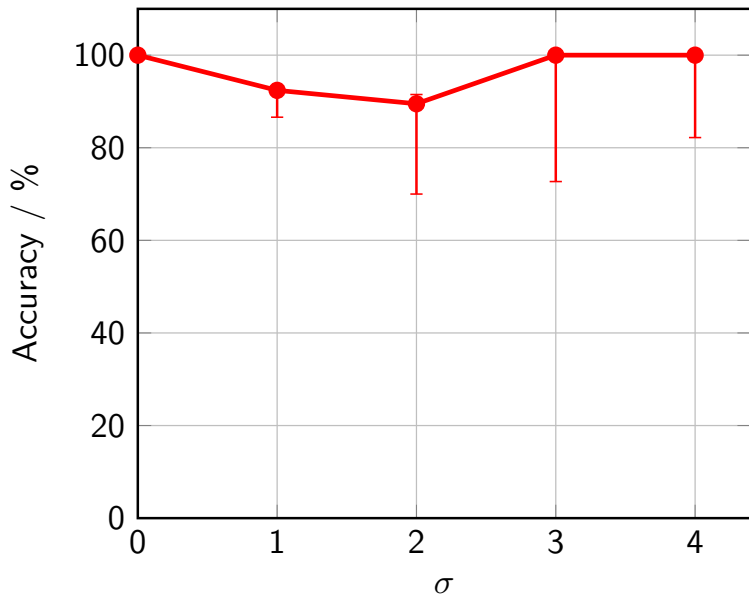
Accuracy (3x7 points)



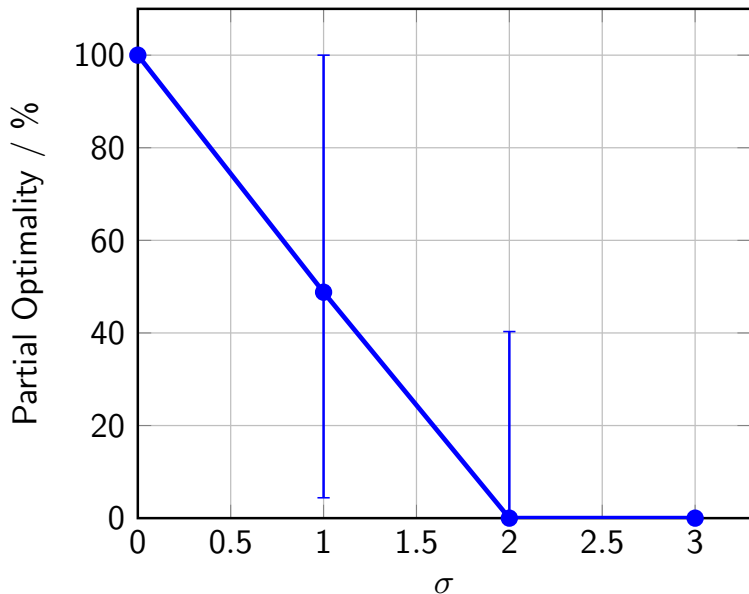
Partial Optimality (3x10 points)



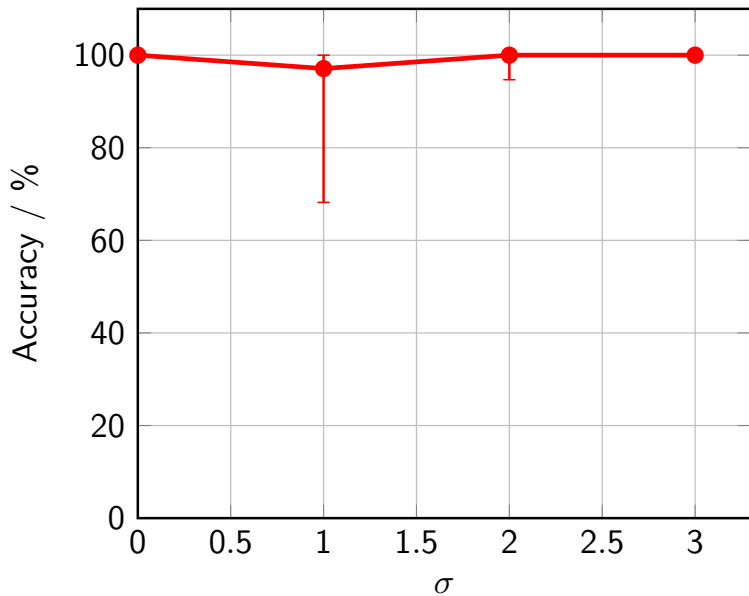
Accuracy (3x10 points)



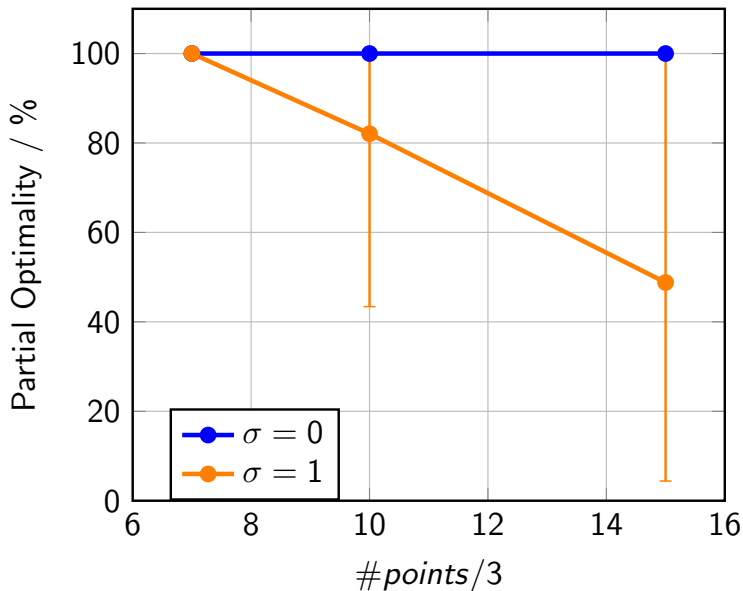
Partial Optimality (3x15 points)



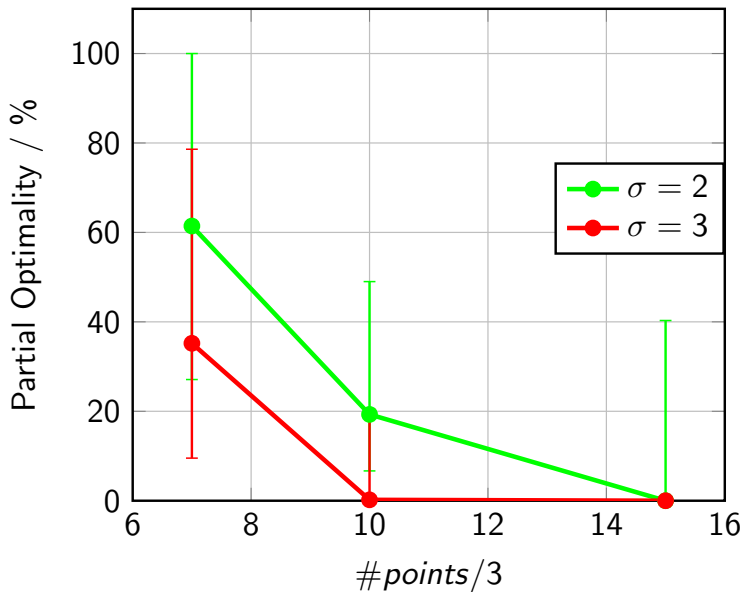
Accuracy (3x15 points)



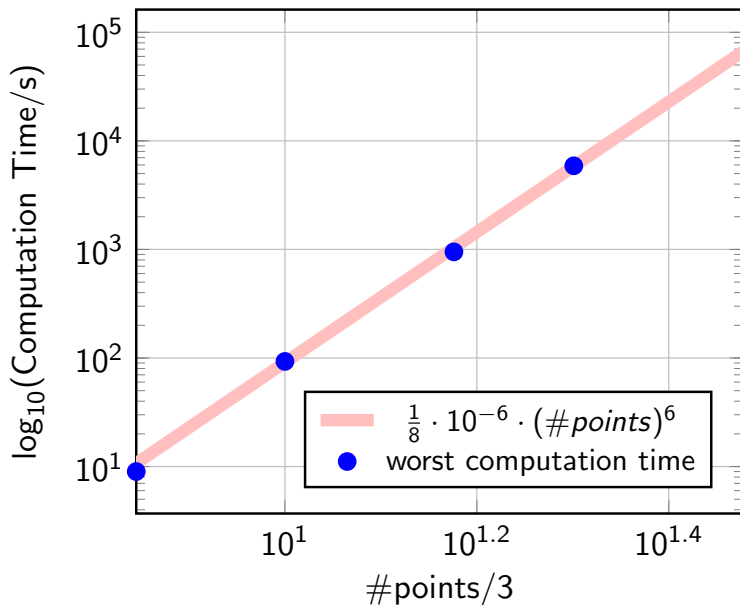
Partial Optimality



Partial Optimality



Computation Time (worst case)



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 - pair labeling and triple cuts
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Future Work:

- optimize and parallelize the algorithm
- overcome the partial optimality loss for c
- determine better parameters for c
- update c with advanced criteria

My program, scripts and presentation:

<https://github.com/Vovsanka/ResearchProjectML>

Bibliography:

-  Lange, Jan-Hendrik, Bjoern Andres, and Paul Swoboda. “Combinatorial persistency criteria for multicut and max-cut”. In: *CVPR* (2019).
-  Lange, Jan-Hendrik, Andreas Karrenbauer, and Bjoern Andres. “Partial Optimality and Fast Lower Bounds for Weighted Correlation Clustering”. In: *ICML* (2018).
-  Stein, David, Silvia Di Gregorio, and Bjoern Andres. “Partial Optimality in Cubic Correlation Clustering”. In: *ICML* (2023).