Partially Optimal Cubic Subspace Clustering

Research Project Machine Learning

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Technische Universität Dresden

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Problem Statement (1)

Finite sample set S, cost function $\mathrm{c}\colon \binom{S}{3} \to \mathbb{R}$.
Instance of the **Cubic Clique Partition Problem**:

$$\min_{\mathrm{y}\colon \binom{S}{2} \to \{0,1\}} \sum_{abc \in \binom{S}{3}} \mathrm{c}_{abc}\, \mathrm{y}_{ab}\, \mathrm{y}_{bc}\, \mathrm{y}_{ac}$$

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

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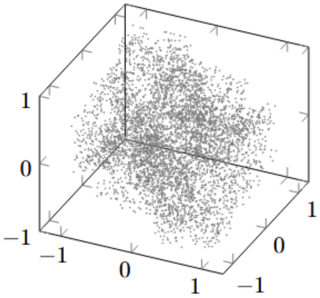
Find a **partially optimal solution**, i.e. fix some labels y_{ab} for distinct $a, b \in S$

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

in such way that there still exists an optimal solution.

Subspace Instances of the Cubic Clique Partition Problem

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



(a) Samples S

Problem Statement (2)

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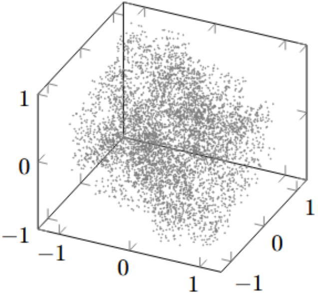
Samples S: points $S \subset \mathbb{R}^3$

Point generation: 3 distinct planes containing the origin, noise σ
Optimal labeling y^*: original planes



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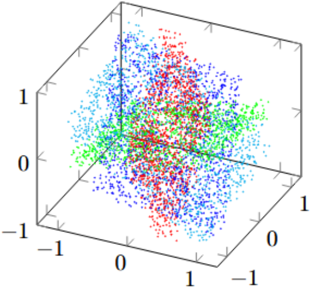

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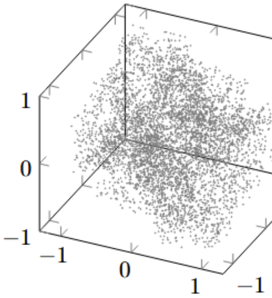
Cost function c? (no concrete plane information given)



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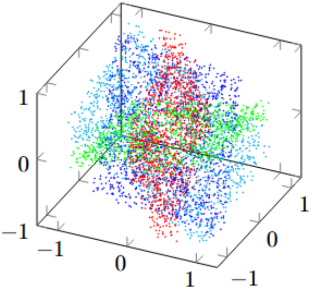

(b) Optimal labeling y^*

Research Goals and Contributions

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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   $\rightarrow$ implementation in C++

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   $\rightarrow$ point generation, appropriate **cost function** c
3. Apply algorithm to the subspace instances, assess partial optimality, accuracy and computation time
   $\rightarrow$ experiments and evaluation

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

Partial Optimality for Cubic Clique Partition Problem

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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 $Y \neq \emptyset$, $\phi\colon Y \to \mathbb{R}$ and $\sigma\colon Y \to Y$. σ is an **Improving Map** for 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 $Y \subseteq \{\text{feasible } y \mid y\colon \binom{S}{2} \to \{0,1\}\}$, $\phi_c\colon Y \to \mathbb{R}$ 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 $i \in R \land j \notin R$ and

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

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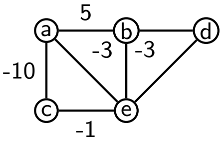

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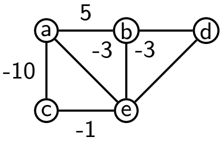
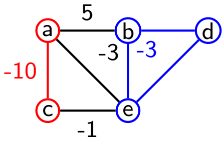


a-b Min-Cut



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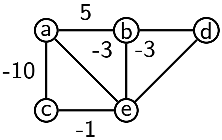

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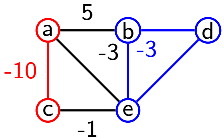

Improving map $\sigma : Y \to Y$ for $y \in Y$ and $pq \in \binom{S}{2}$:

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

Partial Optimality Conditions:

1. Subproblem-CUT-condition (cut subset from its complement)
2. CUT-conditions (cut 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 $\mathrm{y}_1^* \in Q_1$ and there exists an optimal $\mathrm{y}_2^* \in Q_2 \nrightarrow$ there is an optimal $\mathrm{y}^* \in Q_1 \cap Q_2$:

$$\min_{\mathrm{y}\in Y} \phi_\mathrm{c} = -2$$
$$Q_1 = \{\mathrm{y} \in Y \mid \mathrm{y}_{ab} = 1\}$$
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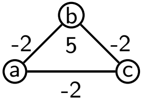
$$\rightarrow Q_1 \cap Q_2 = \{\mathrm{y} \in Y \mid \mathrm{y}_{ab} = 1 \wedge \mathrm{y}_{ac} = 1\} \lightning$$



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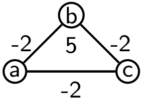

Apply partial optimality conditions → solve subproblems!

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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Reduction to subproblems:

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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 $R_1, R_2, \ldots, R_k$ that are only connected via non-negative costs (applied if $k > 1$)

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Subset-JOIN: join sample subset R with only non-positive costs if its worst bipartition joining cost is less than or equal to the reward of joining R with $\overline{R}$ (applied if $|R| > 1$)
(the worst bipartition joining cost $\approx$ min-cut)

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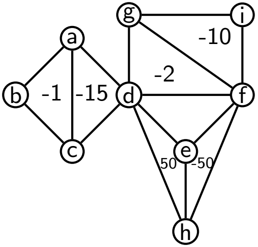

$c_\emptyset = 0$

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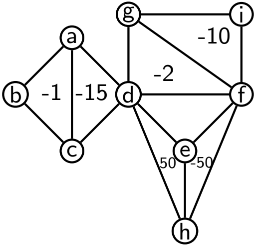

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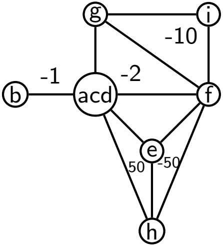

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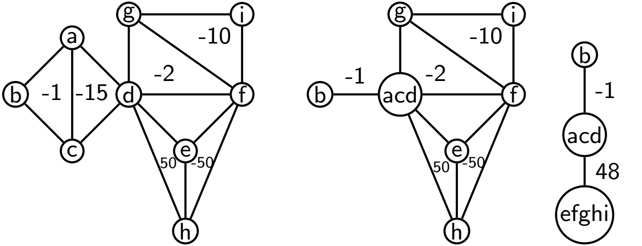

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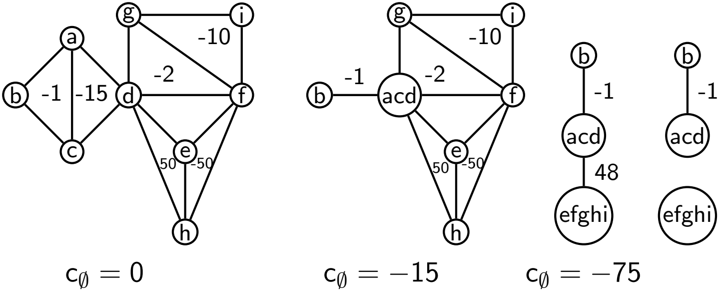

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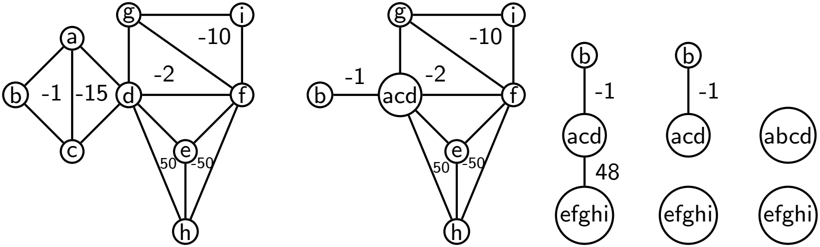

$c_\emptyset = 0$ $\quad$ $c_\emptyset = -15$ $\quad$ $c_\emptyset = -75$ $\quad$ $c_\emptyset = -76$

Other JOIN-conditions

Pair-JOIN-1: join $ij \in \binom{S}{2}$ 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 $\overline{R}$ ($\approx$ i-j min-cut)

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Pair-JOIN-2: join $ik \in \binom{S}{2}$ 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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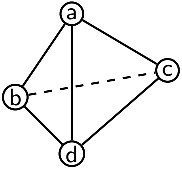
Triple-JOIN: join $ijk \in \binom{S}{3}$ if a condition holds (similar to Pair-JOIN-1) ($\approx$ i-jk min-cut)

Pyramid Instance and CUT-conditions

$c_{bcd} = 10$

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



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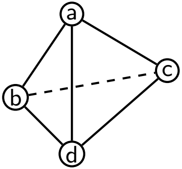

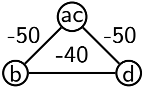

Pair-JOIN-2

Pyramid Instance and CUT-conditions

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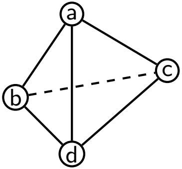

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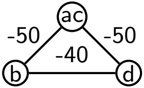
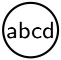


Subset-JOIN



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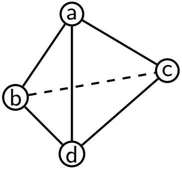

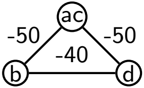

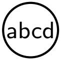

Pair-JOIN-2 Subset-JOIN $c_{\emptyset} = -140$

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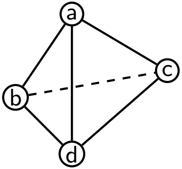

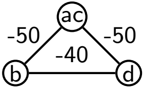

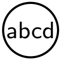

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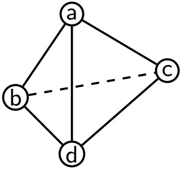

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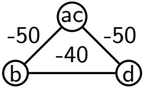

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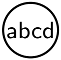

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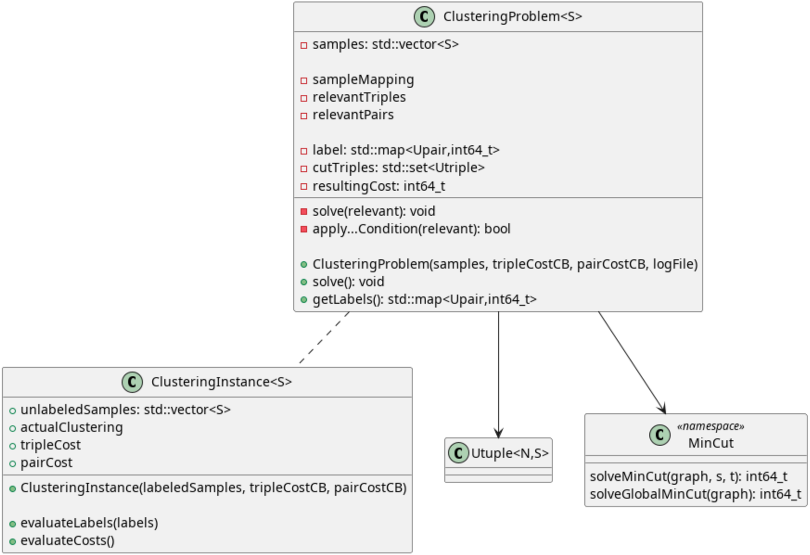
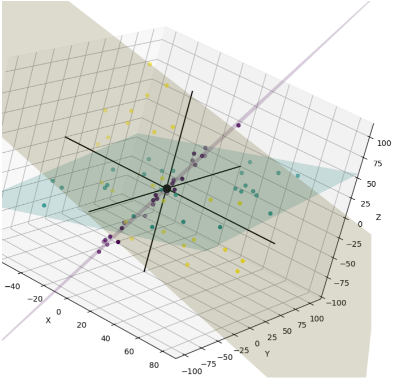
Samples in the pyramid with $c_{bcd} = 100$ are unjoinable!
Triple-CUT is applied to the triple *bcd*

Program Structure



Plane Generation:

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



Plane and Point Generation

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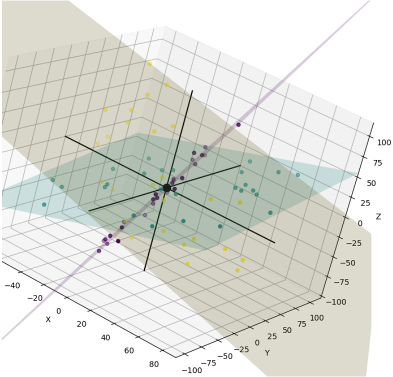

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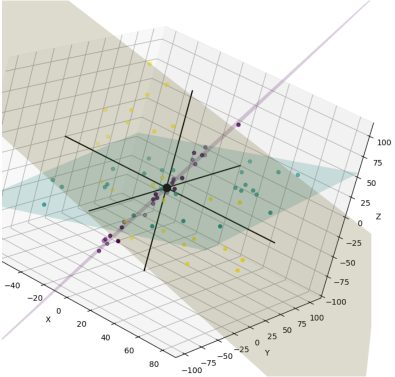

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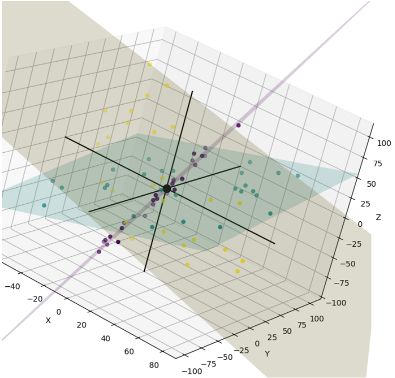

Point Generation on the plane $(\vec{n}, \vec{r}_1, \vec{r}_2)$, parameters (D, σ):

- 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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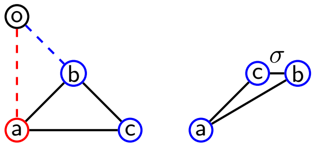

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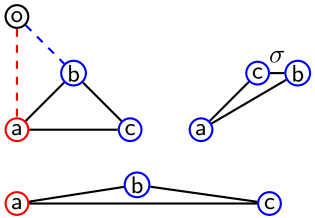

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(3) h_a, h_b, h_c: distances
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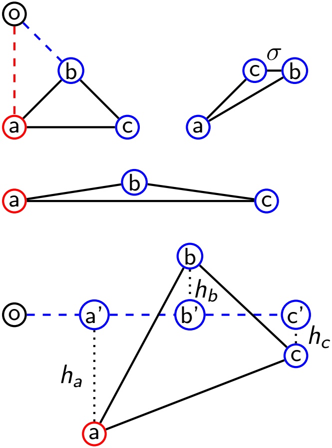
$h_a + h_b + h_c > 3\sigma + 10^{-6}$
$\rightarrow c_{abc} = \frac{(h_a+h_b+h_c)-(3\sigma+10^{-6})}{3D}$



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(4) h_o: distance from the origin to the triangle plane;
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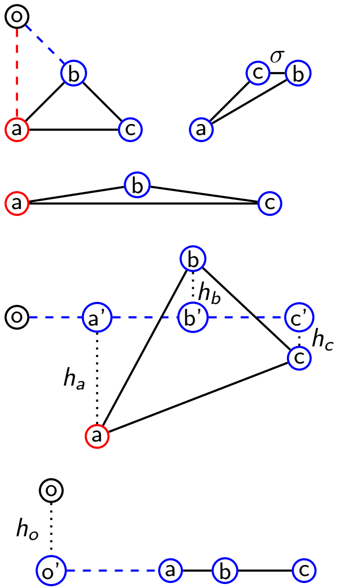
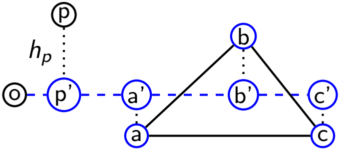


Cost Function (2)

(5) for all points p:
h_p: distance to the best fitted plane containing the origin;



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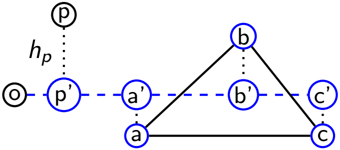

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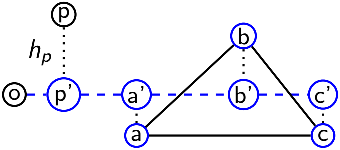

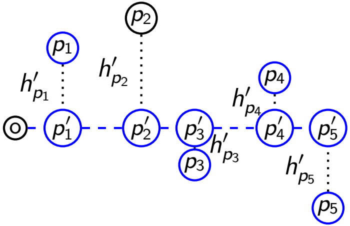

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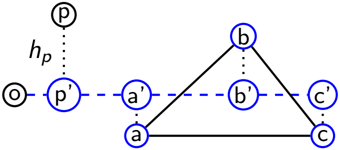

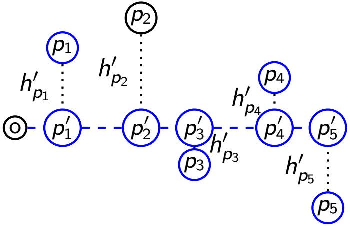

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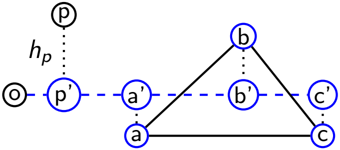

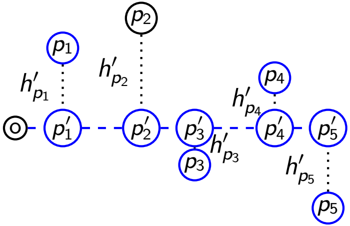

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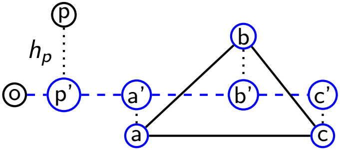
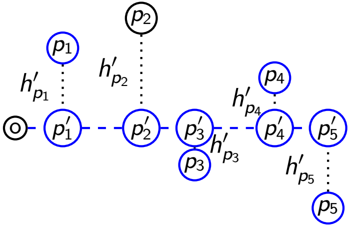
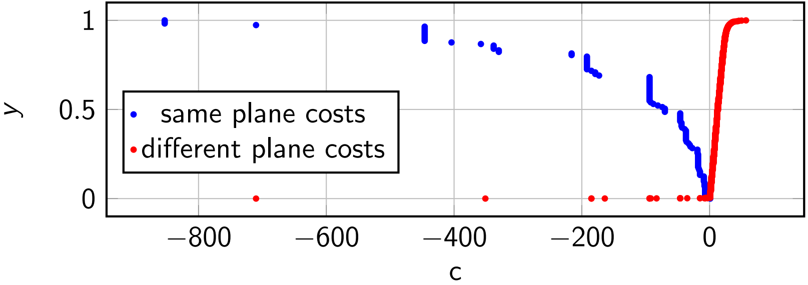




Cost Function Evaluation (3x15 points, $\sigma = 1$)



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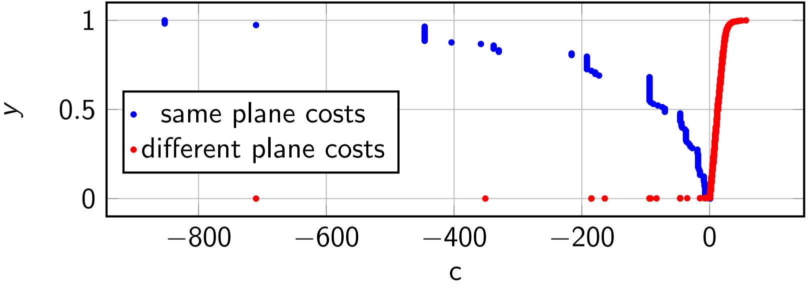

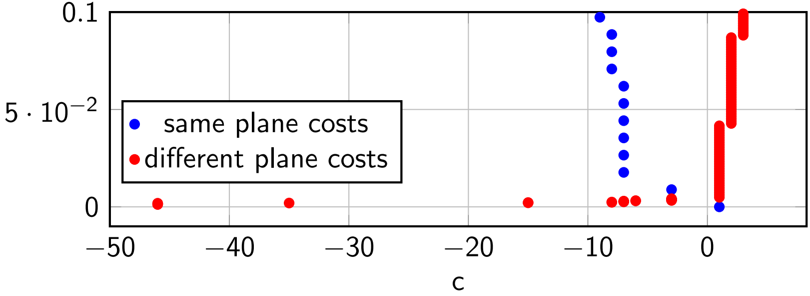

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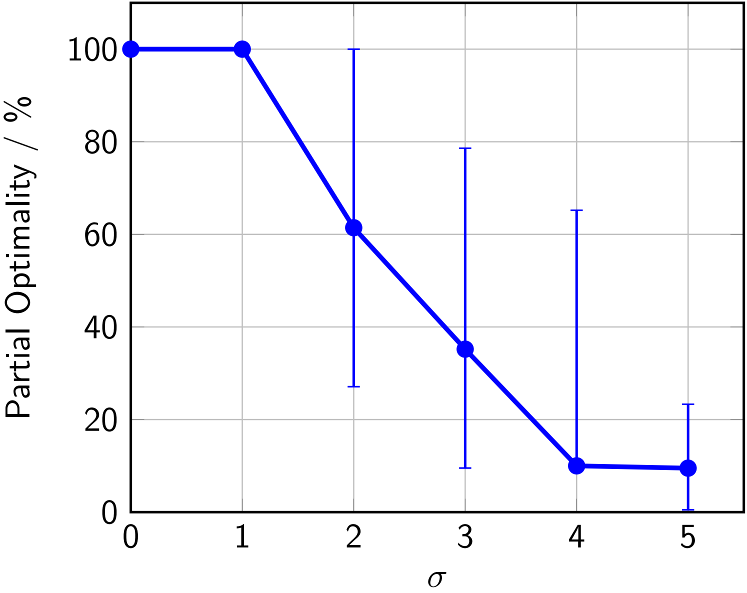
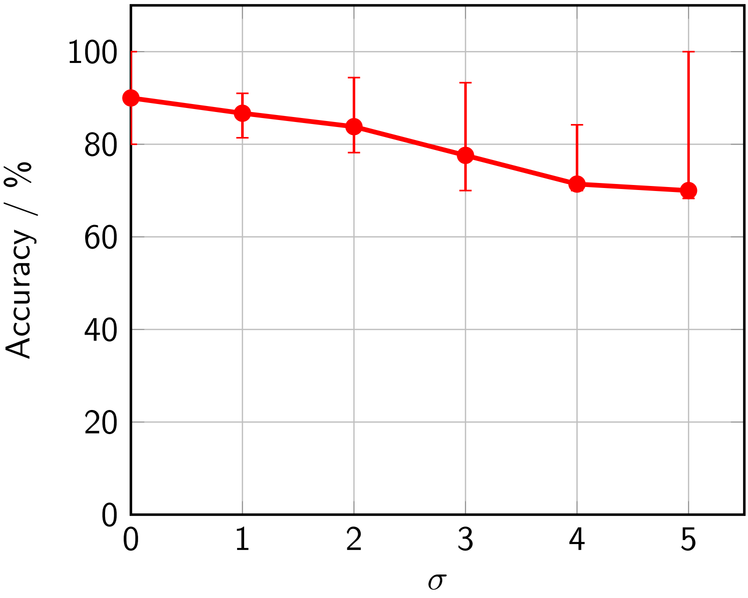
- Capture
  - 1.quartile (Q1)
  - median (Q2)
  - 3.quartile(Q3)
  - the worst computation time

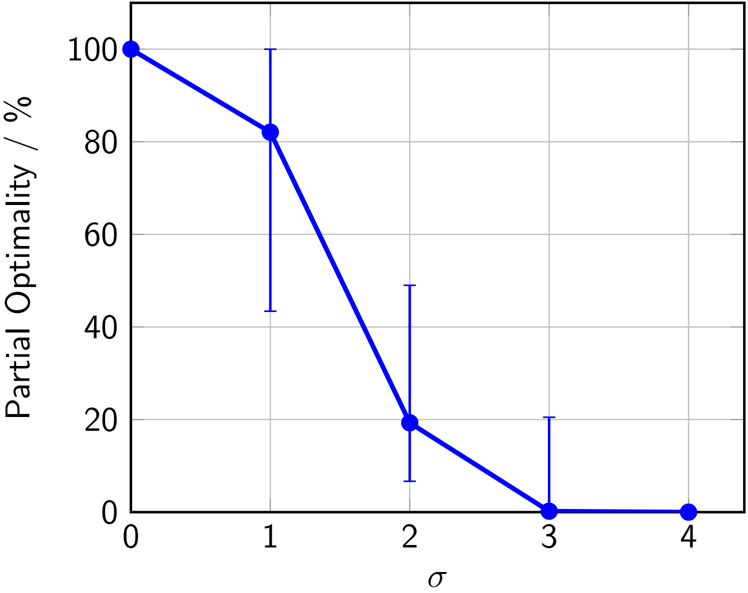
Partial Optimality (3x7 points)



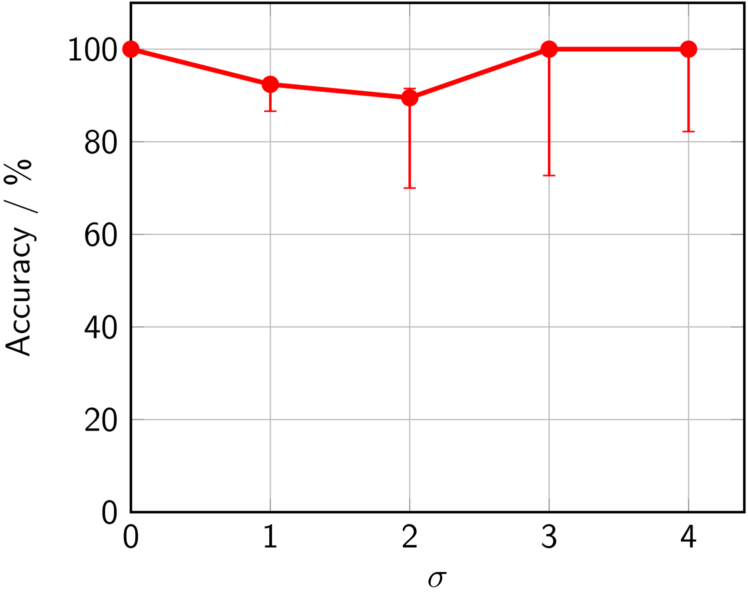
Accuracy (3x7 points)



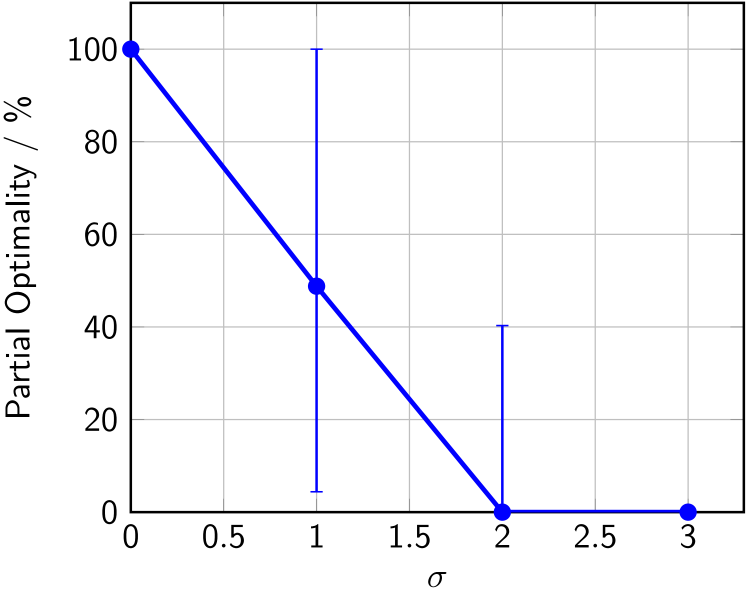
Partial Optimality (3x10 points)



Accuracy (3x10 points)



Partial Optimality (3x15 points)



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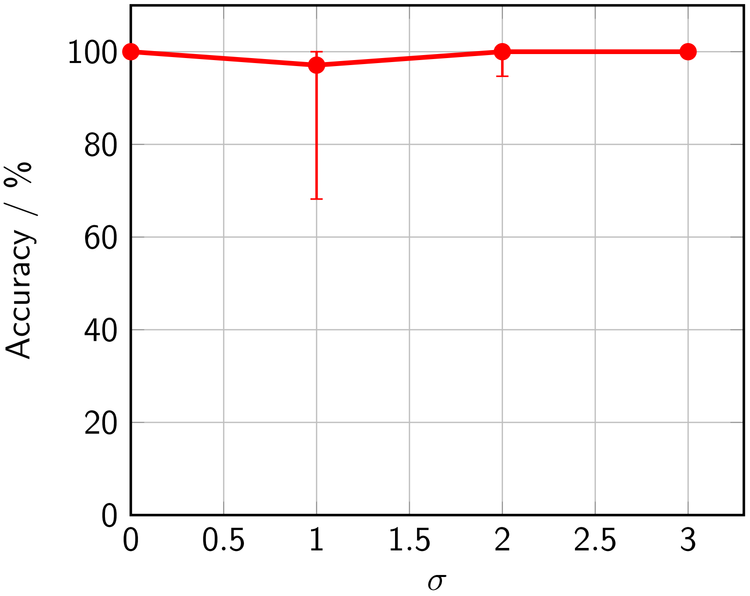

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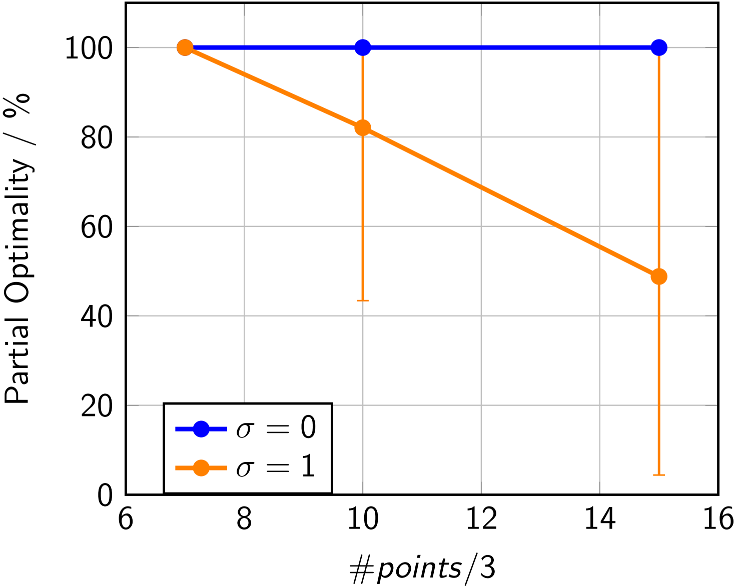

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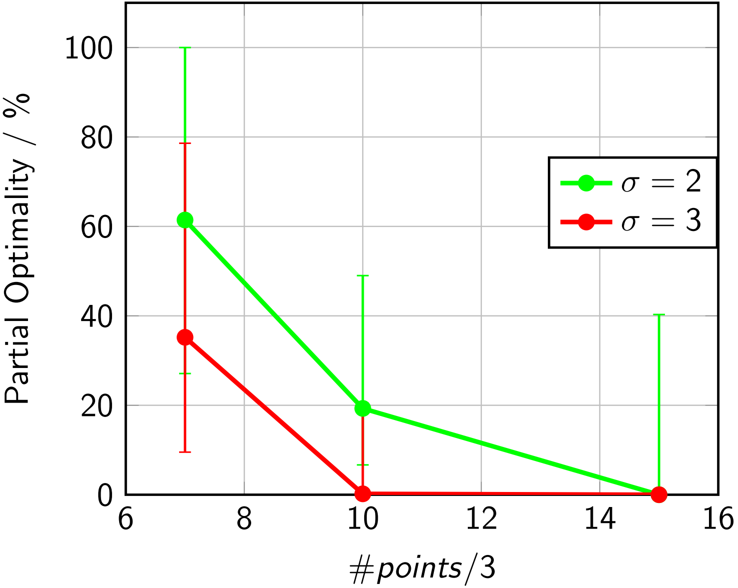
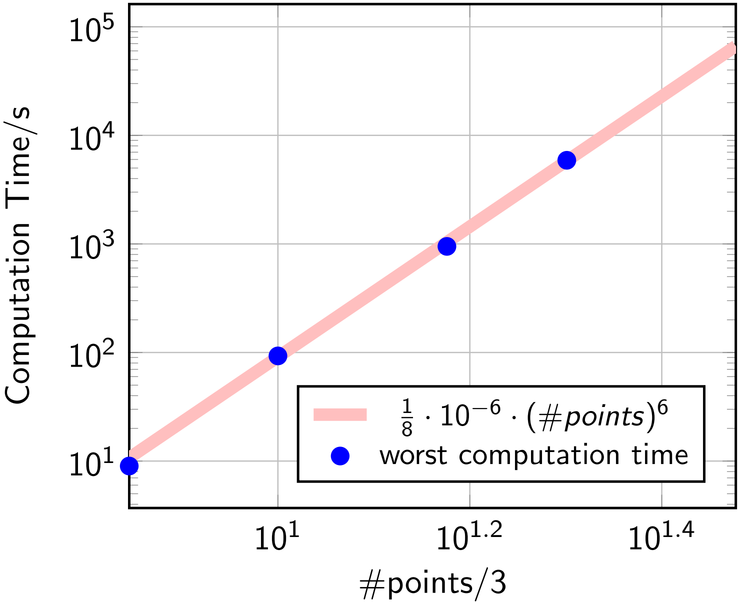


Computation Time (worst case)



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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

References

My program, scripts and presentation:

`https://github.com/Vovsanka/ResearchProjectML`

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