Partially Optimal Cubic Subspace Clustering

Research Project Machine Learning

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Technische Universität Dresden

21.07.2025

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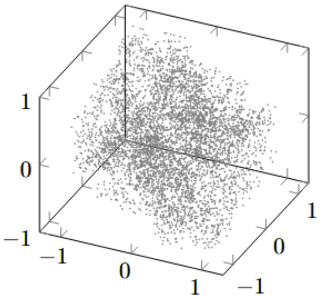
Find a **partially optimal solution**, i.e. fix some labels y_{ab} for distinct $a, b \in S$

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

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

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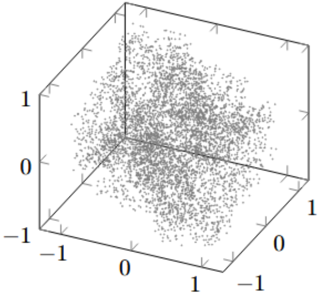
Samples S: points $S \subset \mathbb{R}^3$
Point generation: 3 distinct planes containing the origin, noise σ



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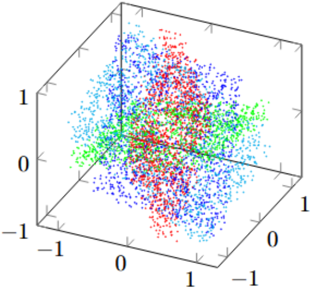

(b) Optimal labeling y^*

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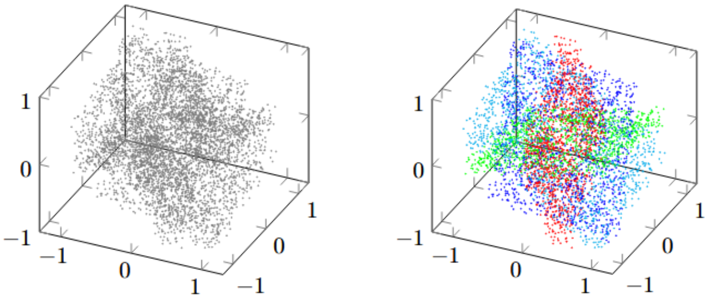

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Subspace Instances of the Cubic Clique Partition Problem

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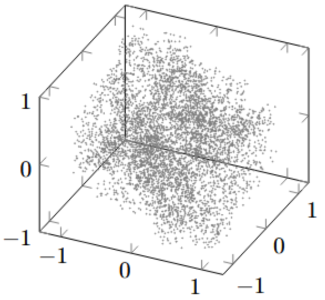
Point generation: 3 distinct planes containing the origin, noise σ
Optimal labeling y^*: original planes
Cost function c? (no concrete plane information given)



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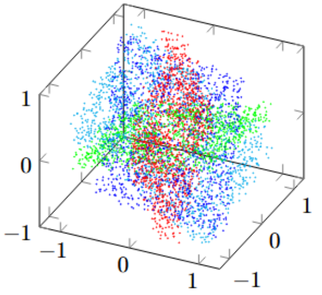

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Research Goals and Contributions

Related Work:

TODO: $1 + 2$ (citation at the end!)

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Tasks and Solutions:

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   → point generation, appropriate cost function c
   (high accuracy, significant noise tolerance)

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   $\rightarrow$ implementation in C++ (with some adjustments)
2. Construct subspace instances of increasing difficulty
   $\rightarrow$ point generation, appropriate cost function c
   (high accuracy, significant noise tolerance)
3. Apply algorithm to the subspace instances, assess partial optimality, accuracy and computation time
   $\rightarrow$ experiments and evaluation (prove the quality of c)

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Apply partial optimality connditions → solve subproblems

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

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Output: partially optimal labeling y with some fixed labels

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Reduction to subproblems:

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2. JOIN-Conditions: fix JOIN 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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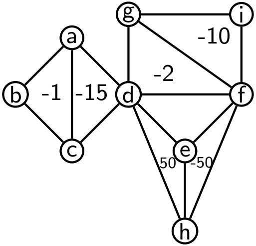

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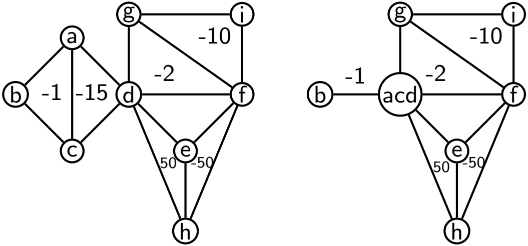

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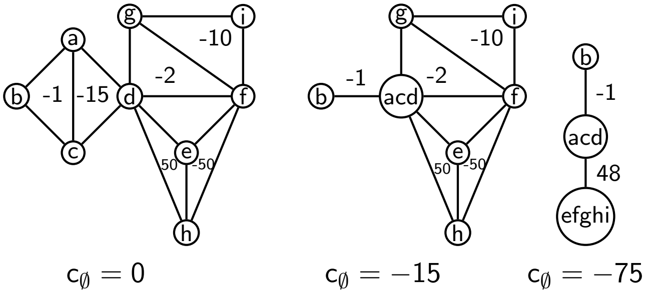

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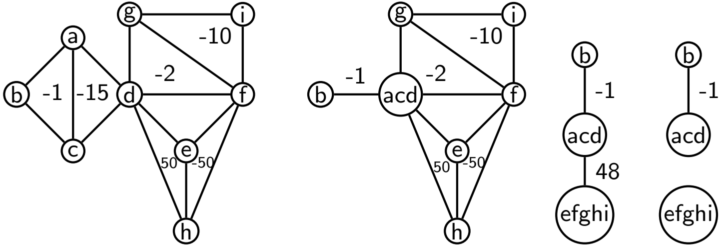

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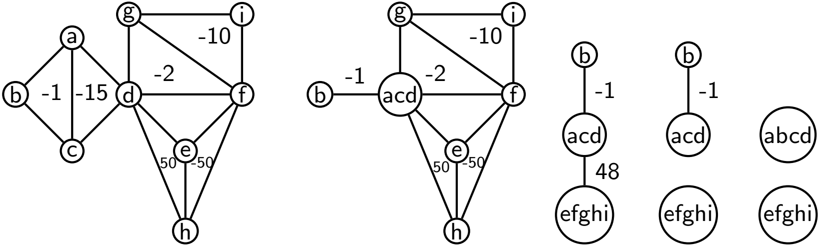

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Other JOIN-conditions

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

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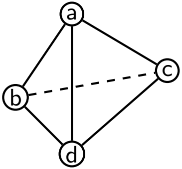
$c_{abc} = c_{abd} = c_{acd} = -50$



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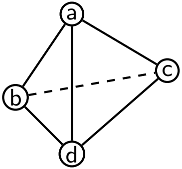

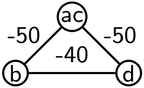

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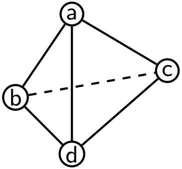

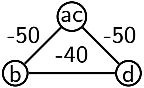

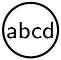

Pair-JOIN-2 Subset-JOIN $c_{\emptyset} = -140$

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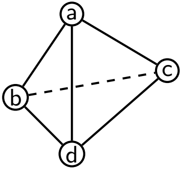

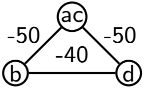

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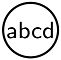

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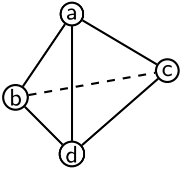

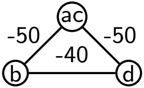

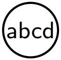

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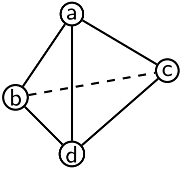

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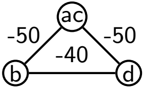
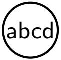


Subset-JOIN



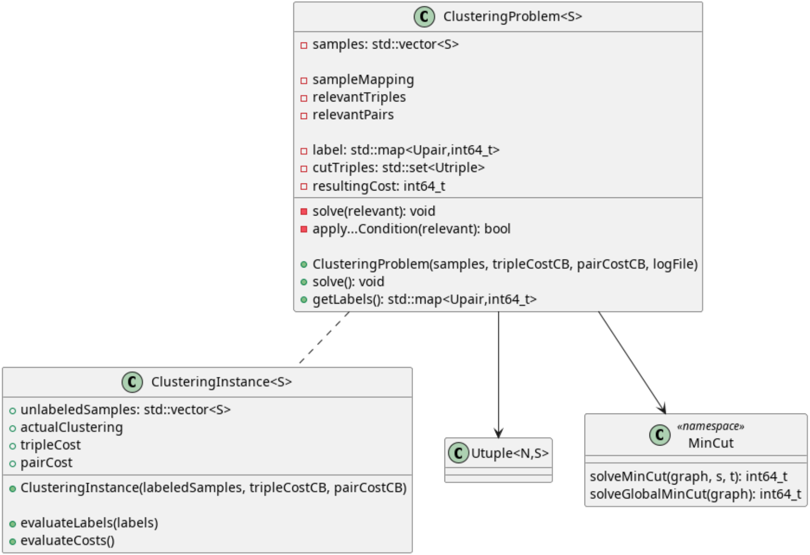
$c_{\emptyset} = -140$

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

Triple-CUT: cut samples i, j, k if the condition holds (similar to Pair-CUT) ($\approx$ i-jk min-cut)

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

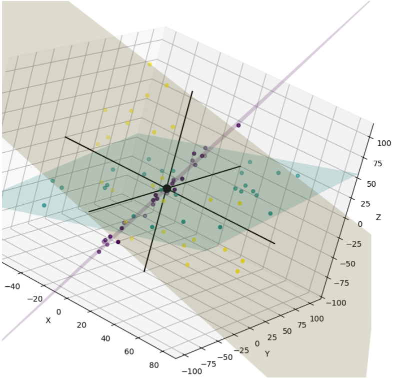
Program Structure



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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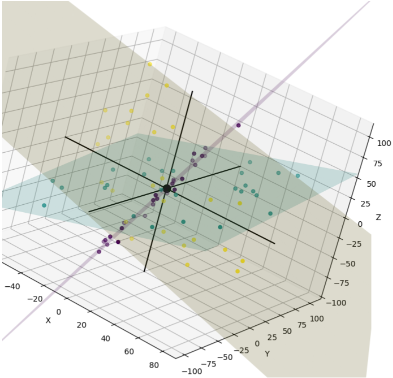
  orthogonal to $\vec{n}_i$
  $(i \in \{1, 2, 3\})$



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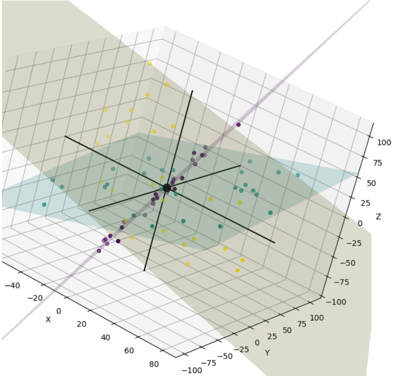

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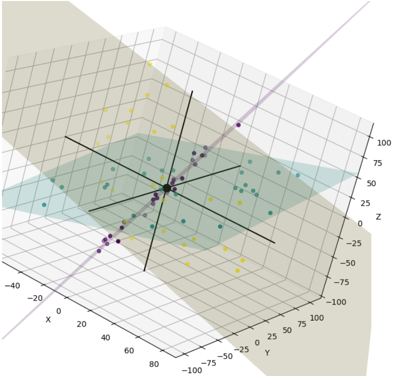

Point Generation on the plane $(\vec{n}, \vec{r}_1, \vec{r}_2)$, parameters (D, σ):

- 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

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

1. Smallest side $s < D/2 \rightarrow c_{abc} = 0$
2. Largest angle $\alpha > 150^\circ \rightarrow c_{abc} = 0$
3. ha, hb, hc: distances to the best fitting plane
   $ha + hb + hc > 3\sigma + 10^{-6}$
   $\rightarrow c_{abc} = \frac{(ha+hb+hc)-(3\sigma+10^{-6})}{3D}$
4. ho: distance from the origin to the triangle plane
   $ho > \frac{10\sigma}{\#points} + 10^{-6} \rightarrow c_{abc} = 0$
5. for all points p: hp: distance to the best fitting plane
   choose p if $hp < \sigma + 10^{-6}$ and $|\vec{p}| > 0.3D$
   hp': distance to the best fitting plane of all chosen points
   $\delta_p = \frac{hp'-(\sigma+10^{-6})}{D}$, $SAME = \{p\colon \delta_p < 0\}$, $rew = \sum_{p \in SAME} \delta_p$,
   $|SAME| \leq 3 \rightarrow c_{abc} = 0$
   else $\rightarrow c_{abc} = 2^{|SAME|-4} rew$

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

Blue:
same
plane

Red:
different
planes

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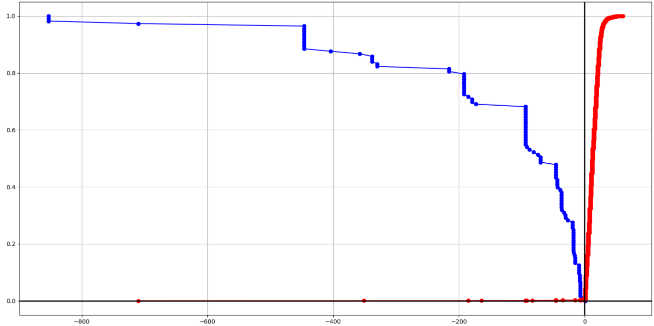

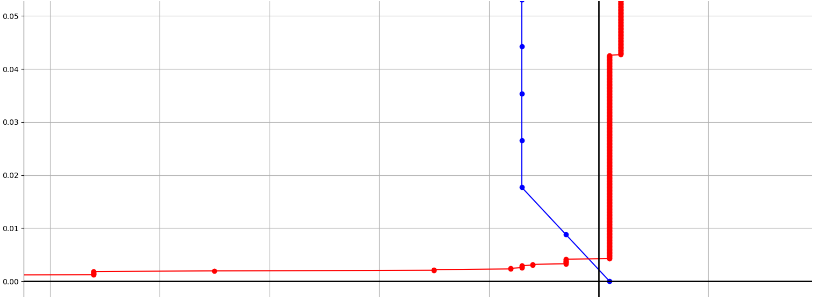

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  - partial optimality (%)
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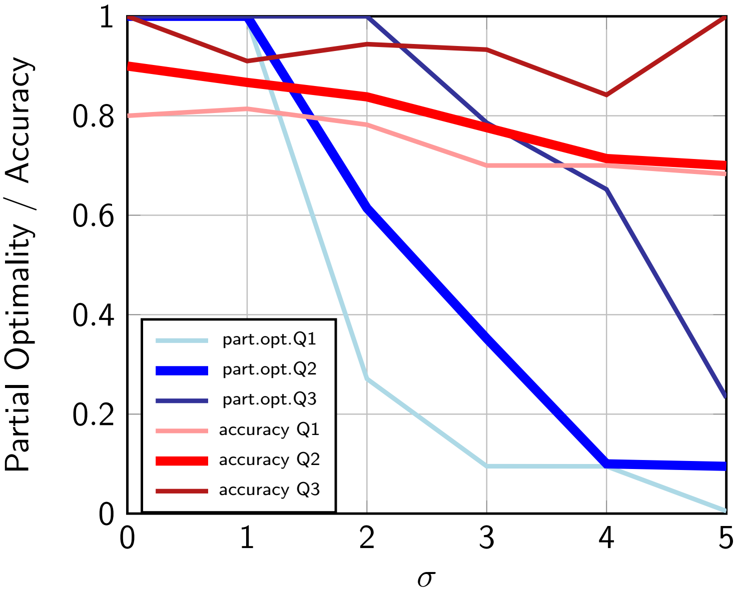
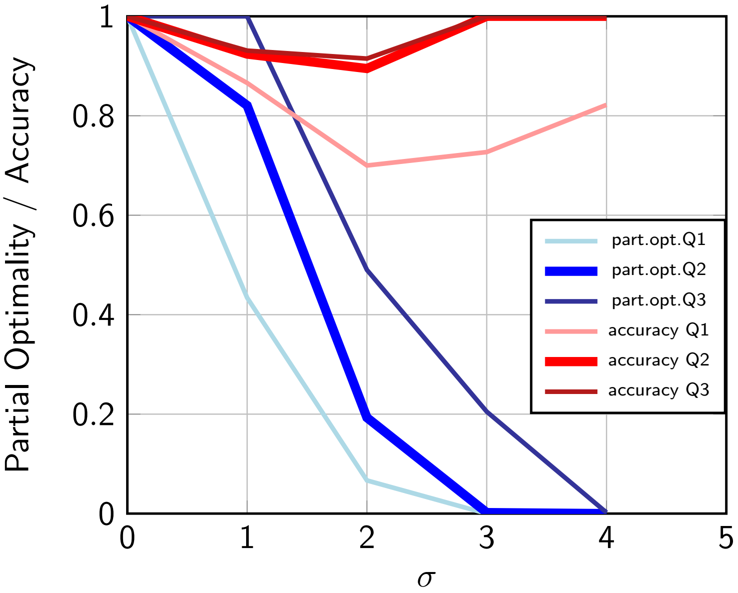
- Capture
  - 1.quartile (Q1)
  - median (Q2)
  - 3.quartile(Q3)
  - the worst computation time

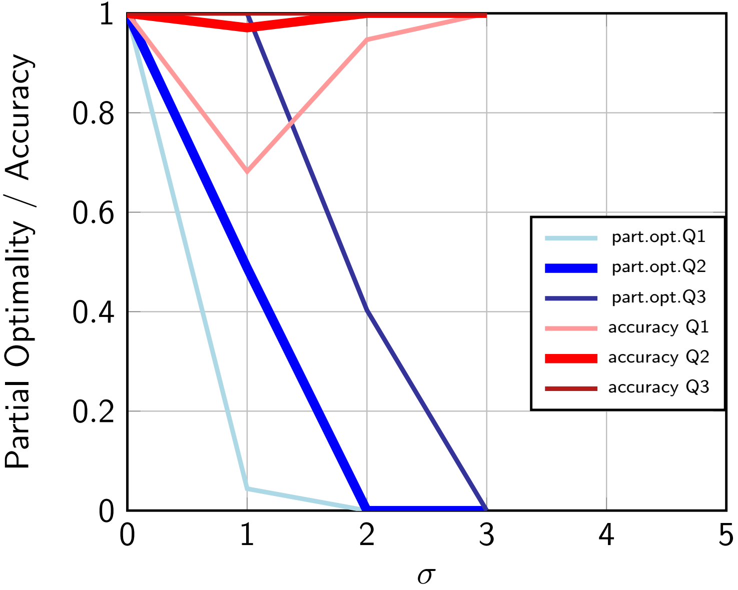
Partial Optimality / Accuracy (3x7 points)



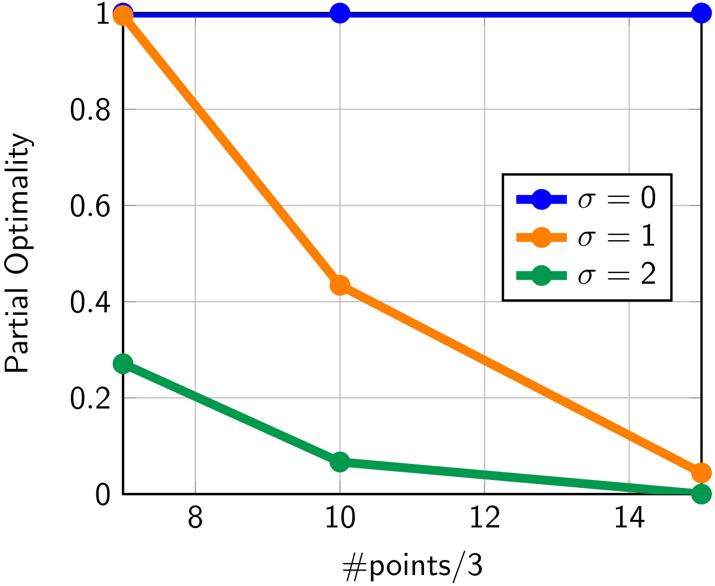
Partial Optimality / Accuracy (3x10 points)



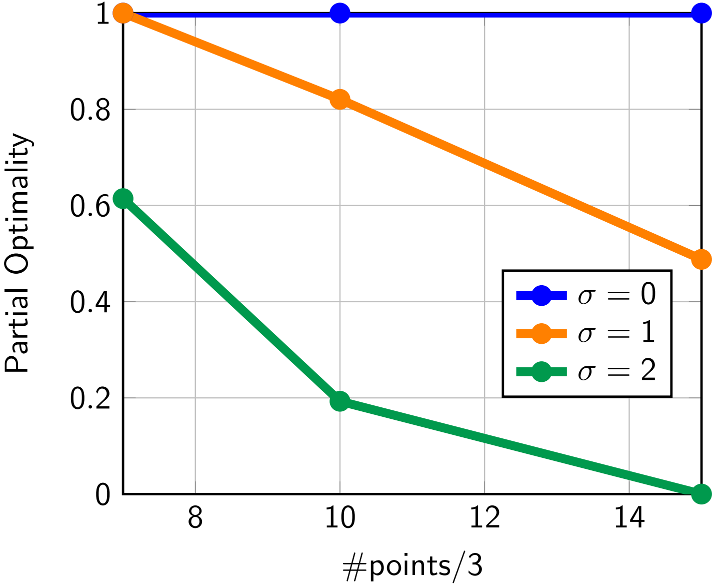
Partial Optimality / Accuracy (3x15 points)



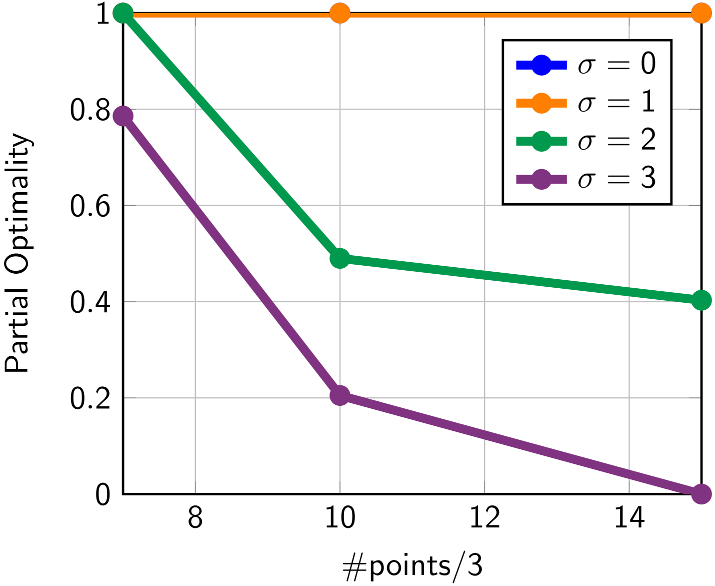
Partial Optimality (Q1)



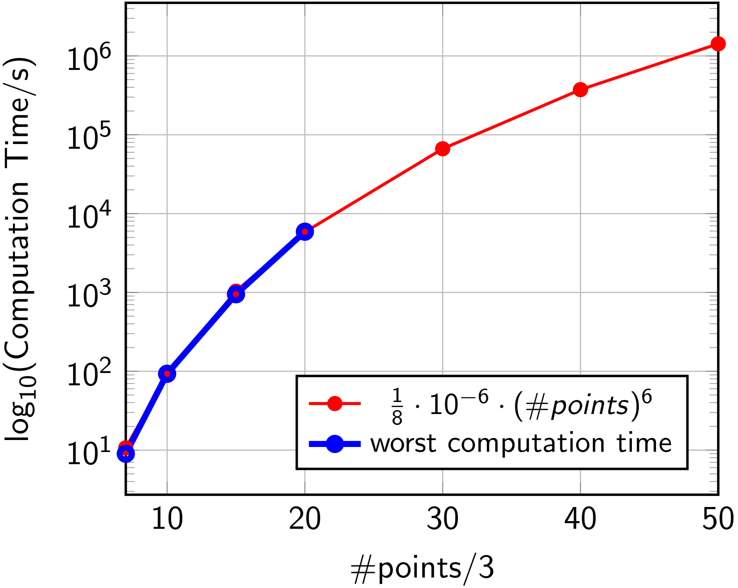
Partial Optimality (Q2)



Partial Optimality (Q3)



Computation Time (worst case)



Conclusion

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   - arbitrary sample type
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   - pair labeling and triple cuts
   - reasonable adjustments of the partial optimality conditions
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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`

TODO: citation