Partially Optimal Cubic Subspace Clustering

Research Project Machine Learning

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Problem Statement (1)

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

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

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

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

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

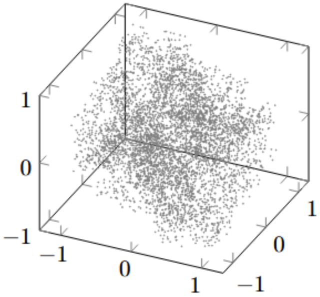
$$\begin{cases} \mathrm{y}_{ab} = 1 & \text{join } a, b \\ \mathrm{y}_{ab} = 0 & \text{cut } a, b \\ \mathrm{y}_{ab} = ? & \text{unknown} \end{cases}$$

in such way that there still exists an optimal solution.

Problem Statement (2)

Subspace Instances of the Cubic Clique Partition Problem

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



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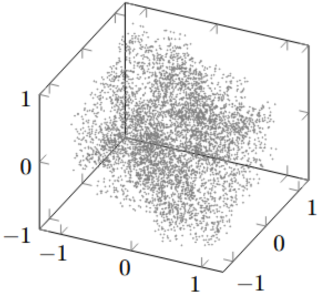

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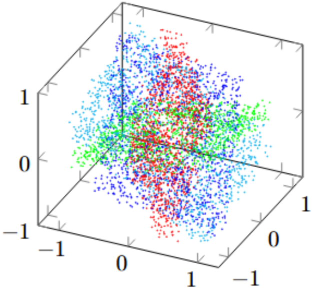

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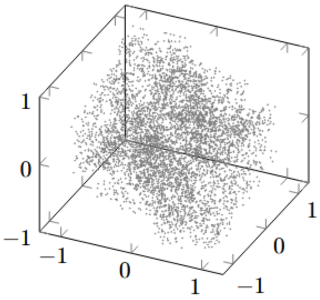

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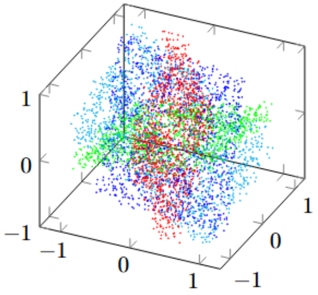

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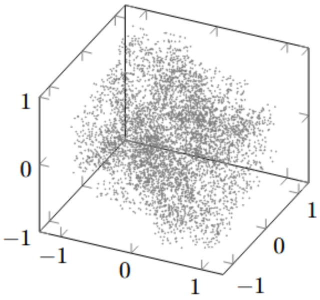
Optimal labeling y^*: original planes
Cost function c? (no concrete plane information given)



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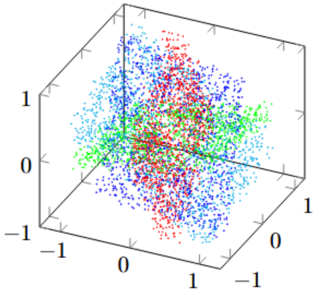

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Research Goals and Contributions

Related Work:

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   $\rightarrow$ point generation, appropriate cost function c
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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 (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)

Partial Optimality for Cubic Clique Partition Problem

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Apply partial optimality connditions $\rightarrow$ solve subproblems

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Partial Optimality Algorithm:

Input: clustering y without fixed labels

while condition applied **do**

  apply subproblem-CUT-condition exhaustively

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end while

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Output: partially optimal clustering y with some fixed labels

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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;

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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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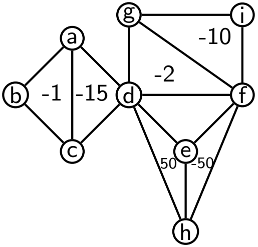

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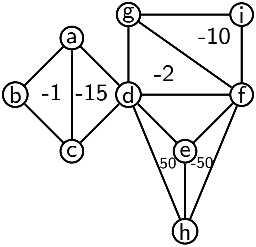

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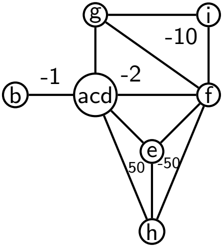

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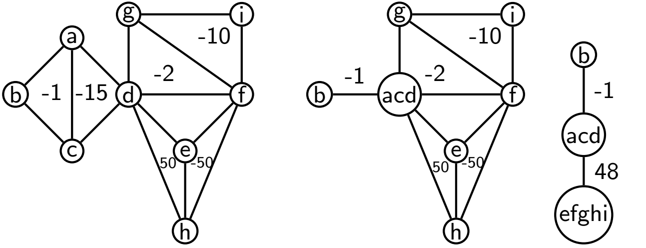

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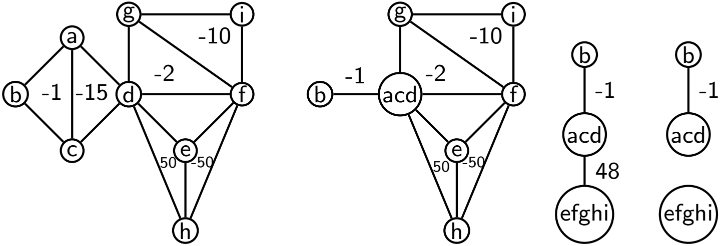

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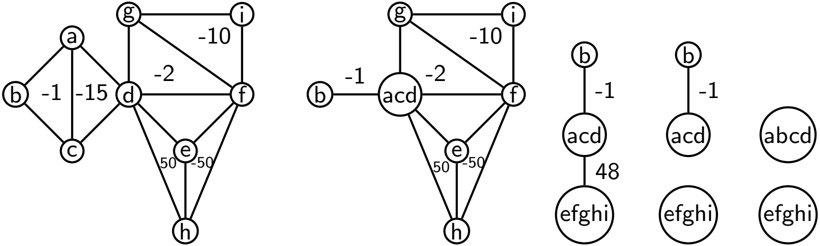

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Other JOIN-conditions

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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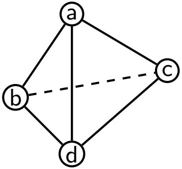

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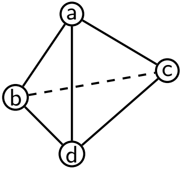

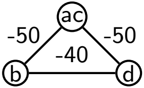

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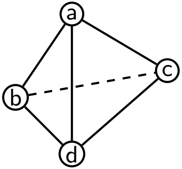

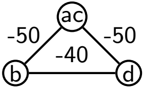

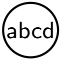

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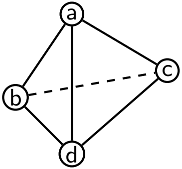

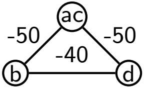

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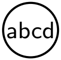

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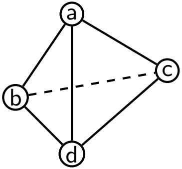

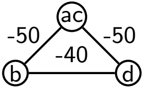

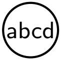

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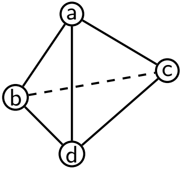
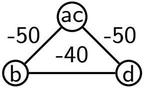
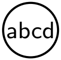
Pyramid Instance and CUT-conditions

$c_{\{b,c,d\}} = 10$
$c_{\{a,b,c\}} = c_{\{a,b,d\}} = c_{\{a,c,d\}} = -50$







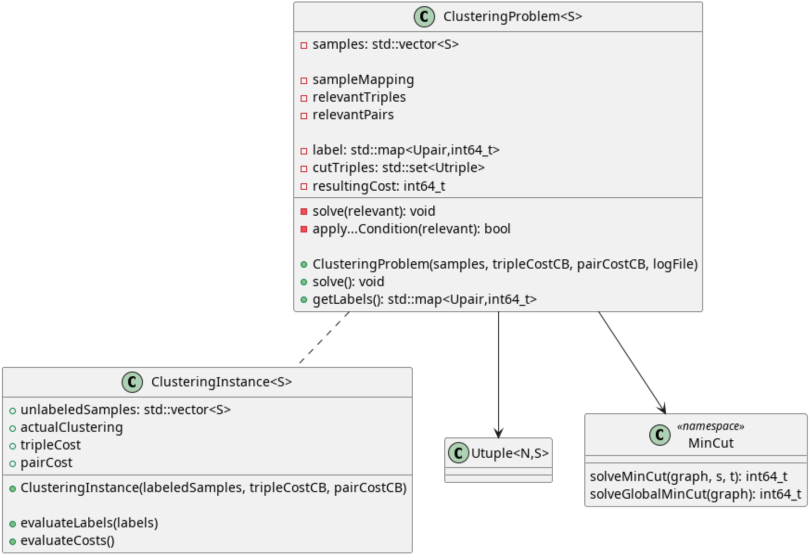
Pair-JOIN-2 Subset-JOIN $c_{\emptyset} = -140$

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)

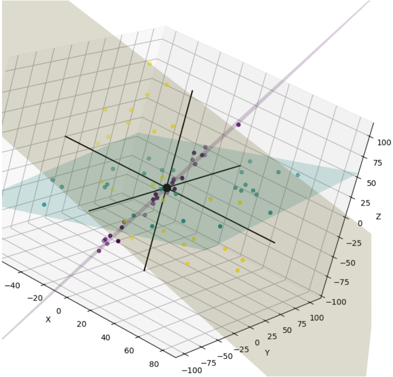
Samples in the pyramid with $c_{\{b,c,d\}} = 100$ are unjoinable!
Triple-CUT is applied to the triple *bcd*

Program Structure



Plane Generation:

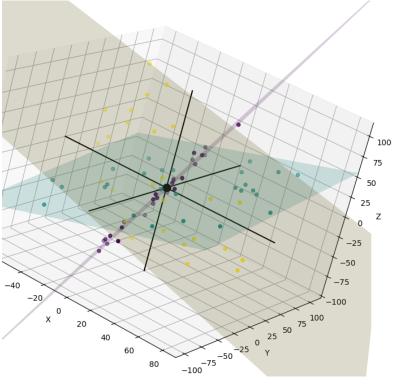
- generate 3 planes
  as distinct normal vectors
  $\vec{n}_1, \vec{n}_2, \vec{n}_3$ (normalized)



Plane and Point Generation

Plane Generation:

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



Plane Generation:

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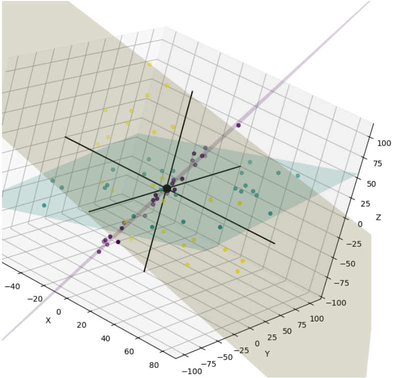
- compute the $\vec{r}_{i,2}$ (normalized) orthogonal to $\vec{n}_i$ and $\vec{r}_{i,1}$



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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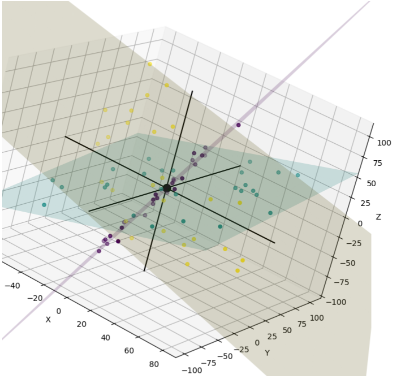


Point Generation on the plane $(\vec{n}, \vec{r}_1, \vec{r}_2)$, parameters (D, σ):

- 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 $\rightarrow c_{abc} = 2^{|SAME|-4} rew$

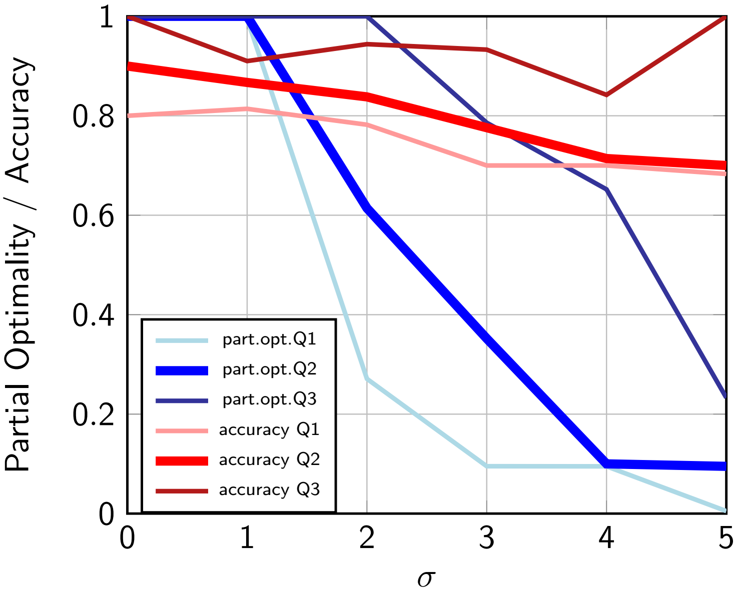
Experiments

My laptop characteristics, Random cubic subspace instances with different seeds max point component size 100 (noise are the percents then) no noise 0, small noise 1, significant noise 3, large noise 5, (Table: instance size + noise + instance count)

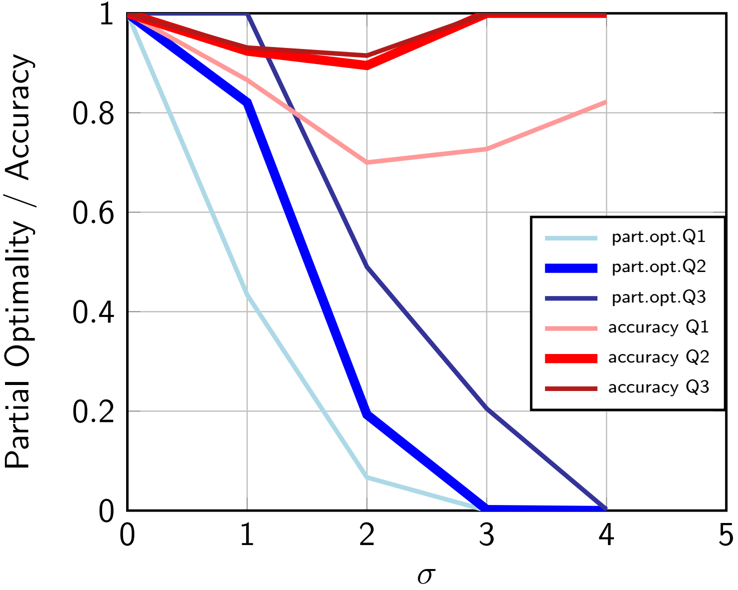
Cost Function Evaluation

blue and red dots, conflicts and and their effect (picture of the typical cost function evaluation)

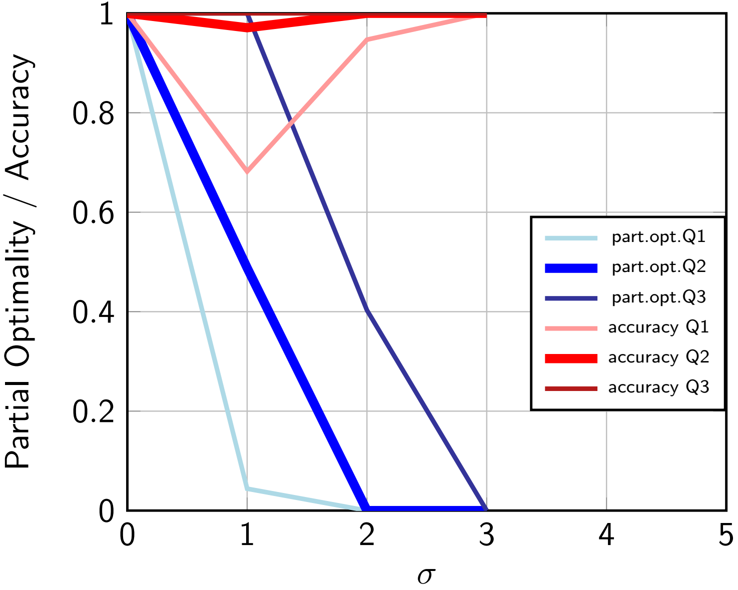
3x7 Partial Optimality / Accuracy



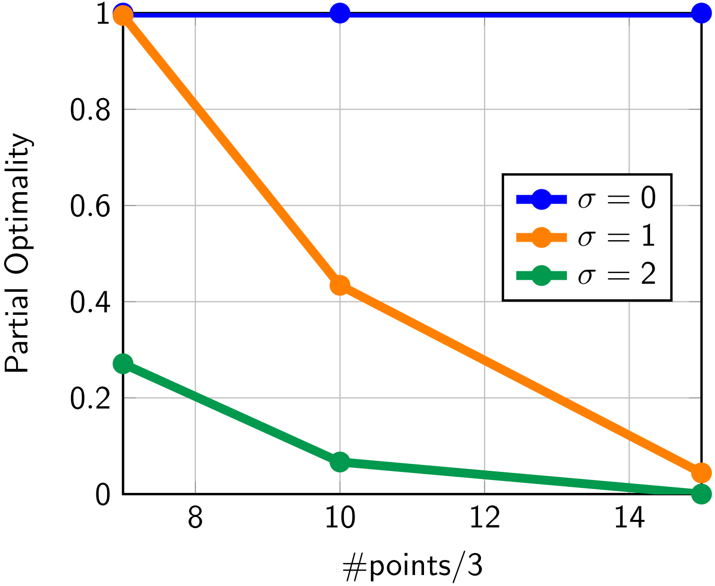
3x10 Partial Optimality / Accuracy



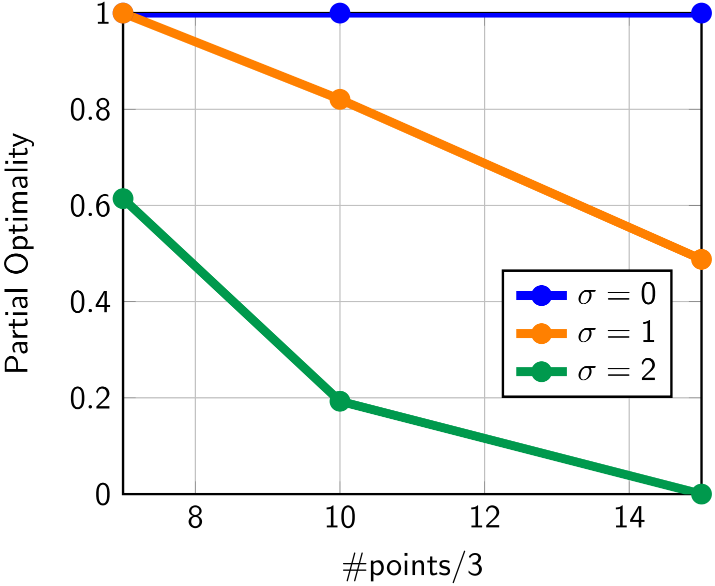
3x15 Partial Optimality / Accuracy



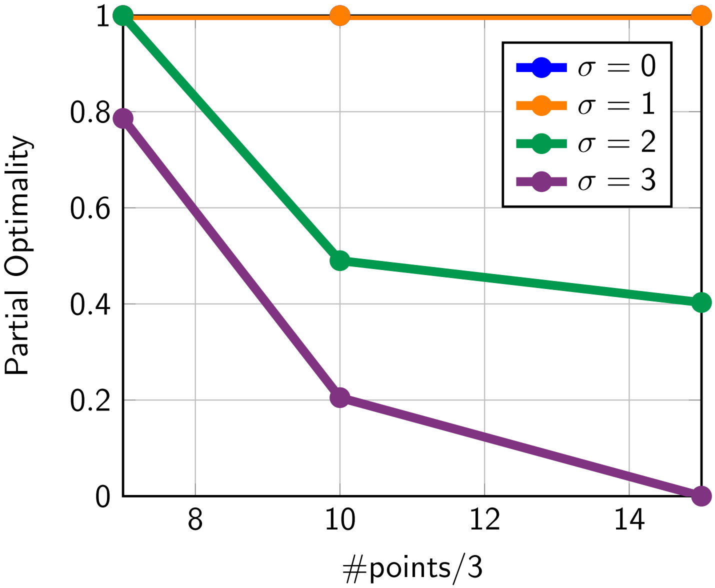
Partial Optimality (Q1)



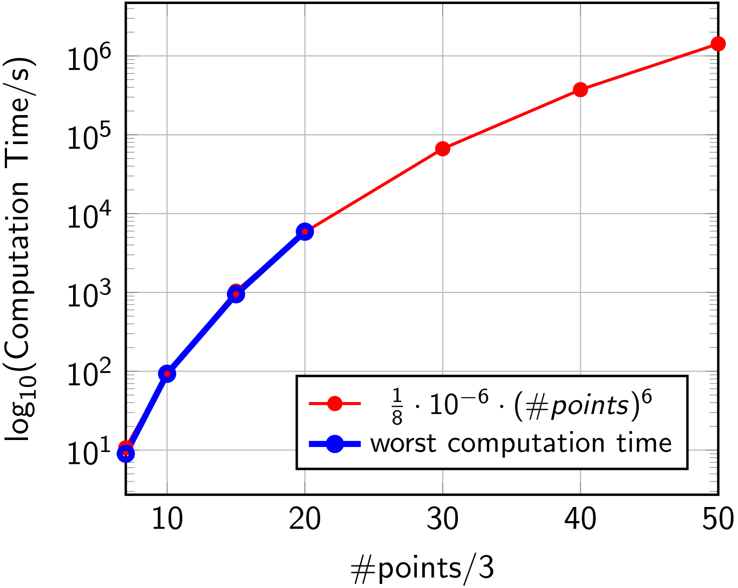
Partial Optimality (Q2)



Partial Optimality (Q3)



Computation Time (worst case)



Conclusion

TODO: summarize the research results Partial optimality reimplementation, Dedicated Cost Function, Efficiency and Accuracy (shown by the experiments)

Future Work :

References

TODO: summarize the research results Partial optimality reimplementation, Dedicated Cost Function, Efficiency and Accuracy (shown by the experiments)
Future Work :