Robust Discrete Optimization Under Ellipsoidal Uncertainty

Chifaa Dahik

Jean-Marc Nicod, Landy Rabehasaina and Zeina Al Masry

Université de Bourgogne Franche-Comté

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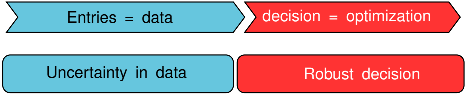
Need for robustness

Context



Entries = data

decision = optimization

Uncertainty in data

Robust decision

Need for robustness

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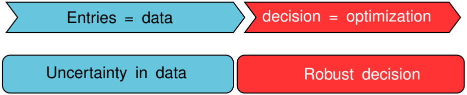

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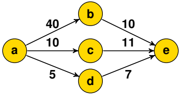
Situation example



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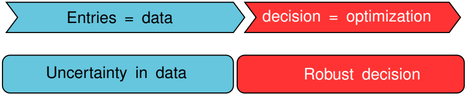

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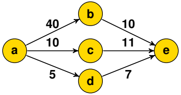
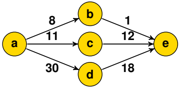


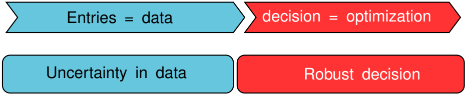
Scenario 1



Scenario 2

Need for robustness

Context



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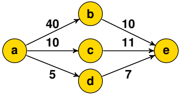

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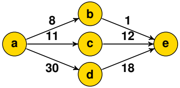

Scenario 2

	Scenario 1	Scenario 2	Worst Scenario
a → b → e	50 min	9 min	50 min
a → c → e	21 min	23 min	23 min
a → d → e	12 min	48 min	48 min

Need for robustness

Resulting facts

⇨ Uncertainty exists

Need for robustness

Resulting facts

- Uncertainty exists
- Considering it is important

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- It makes problems harder

Need for robustness

Resulting facts

- Uncertainty exists
- Considering it is important
- It makes problems harder
- Optimal solutions are not valid

Uncertainty definition

Definition, cause, available information

➡ Uncertainty= *epistemic situation with unknown or imperfect information*

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Uncertainty definition

Definition, cause, available information

- Uncertainty= *epistemic situation with unknown or imperfect information*
- It can be caused by future events, physical measurements that are already made, or the unknown
- Available information or assumptions can exist: probability distribution, belonging to a set, information from the past, etc.
- Uncertainty in an optimization problem:

$$\min_{x \in X_d} f(x, d),$$

X_d: feasible set under the realization d.

Chosen model of uncertainty

- Different approaches exist
- The choice of the approach is made for many reasons: how close to representing the reality, how easy the problem is to solve

Chosen model of uncertainty

Different definitions of worst case based approaches

Absolute robust decision

Chosen model of uncertainty

Different definitions of worst case based approaches

Absolute robust decision

[Kouvelis *et al.* 2004, Buchheim and Kurtz 2018]

$$\min_{x \in X_d} f(x, d)$$

$$z_A = \min_{x \in \cap_{d \in U} X_d} \max_{d \in U} f(x, d)$$

U is an uncertainty set
Best in worst case, with cost=objective

Chosen model of uncertainty

Different definitions of worst case based approaches

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Robust deviation decision

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[Kouvelis *et al.* 2004, Buchheim and Kurtz 2018]

$$\min_{x \in X_d} f(x, d)$$

$$z_D = \min_{x \in \cap_{d \in U} X_d} \max_{d \in U} \left(f(x, d) - f(x_d^*, d) \right)$$

Best in worst case, with cost=deviation from optimal

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Relative robust decision

Chosen model of uncertainty

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[Kouvelis *et al.* 2004, Buchheim and Kurtz 2018]

$$\min_{x \in X_d} f(x, d),$$

$$z_R = \min_{x \in \cap_{d \in U} X_d} \max_{d \in U} \frac{f(x, d) - f(x_d^*, d)}{f(x_d^*, d)}$$

Best in worst case, with cost=relative deviation from optimal

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Why absolute robust decision?

- Avoid to compute optimal solutions of all scenarios

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Relative robust decision

Uncertainty sets

Discrete set

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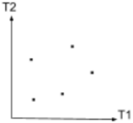

[Li *et al.* 2011]

$U = \{c_1, \ldots, c_n\}$

- Good model
- Combinatorial

$\Longrightarrow$ explosion

Chosen model of uncertainty

Different definitions of worst case based approaches

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Discrete set

Interval set

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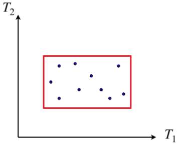
[Li *et al.* 2011]
$U = \Pi_{i=1}^{m}[a_i, b_i]$



- Do not consider correlation
- Easy

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Ellipsoidal set

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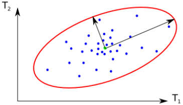
[Li *et al.* 2011]

Confidence region for multinormal distribution

$U = \{c \in \mathbb{R}^m; (c-\mu)^T \Sigma^{-1} (c-\mu) \leq \Omega^2\}$

- Consider correlation
- Hard



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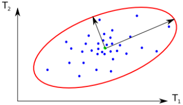

Why ellipsoidal uncertainty?

- Consider correlations
- Avoid the pessimism of general robust min-max optimization

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Chosen problem to solve

General problems:

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Consider binary linear problems with uncertainty in cost

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Examples: Shortest path problem, k-median clustering problem, etc.

Complexity and existing methods

The absolute robust counterpart of binary linear problems under ellipsoidal uncertainty gives

$$\min_{x\in X}\max_{c\in U} c^T x \quad \rightarrow \min_{x\in X} \mu^T x + \sqrt{x^T\Sigma x} = \min_{x\in X} g(x) \qquad (1)$$

[Ilyina 2017] ($\mu^T x + \Omega\sqrt{x^T\Sigma x} \rightarrow \mu^T x + \sqrt{x^T\Sigma x}$: replace Σ by $\Omega^2\Sigma$)

Problem (1) is a binary non-linear problem $\implies$ NP-hard

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Exact methods

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Methods to solve Problem (1)

Exact methods

- Writing (1) as a Binary Second Order Cone Program permits us to use existing exact solvers based on Branch-and-Bound methods (e.g., CPLEX)
- Research work about exact methods are proposed :
- [Ilyina *et al* 2017]
- [Buchheim *et al.* 2017]: A Frank-Wolfe based Branch-and-bound algorithm

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Methods to solve Problem (1)

Exact methods

Heuristic approaches

There is no proposition of a heuristic approach

Exact methods are not scalable

$\implies$ Proposition of a heuristics with the idea of adapting Frank-Wolfe, this time for a heuristics

Outline

1. Context and positioning

2. A Frank-Wolfe based heuristic approach applied on the robust shortest path problem

3. Another Frank-Wolfe based heuristic approach applied on the robust k-median clustering problem

4. Conclusions and perspectives

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Postitioning

Recall the positioning

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Since, the work is based on Frank-Wolfe, recall first the classical Frank-Wolfe algorithm

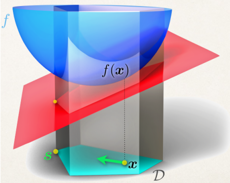
The classical Frank-Wolfe algorithm

f convex, continuously differentiable defined on a compact convex D.
Consider convex optimization problems of the form

$$\min_{x \in D} f(x)$$

Frank-Wolfe algorithm

```
Let $x^{(0)} \in D$
**for** $k = 0$ to $K$ **do**
    compute $s^{(k)} := \underset{s \in D}{\operatorname{argmin}} \nabla f(x^{(k)})^T s$
    update $x^{(k+1)} := (1 - \gamma^{(k)})x^{(k)} + \gamma^{(k)} s^{(k)}$
**end for**
```



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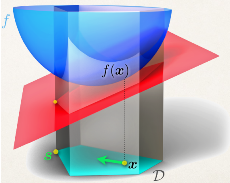

[Jaggi 2013]

$$s^{(k)} = \operatorname*{argmin}_{s \in D} [f(x^{(k)}) + \nabla f(x^{(k)})^T (s - x^{(k)})] = \operatorname*{argmin}_{s \in D} \nabla f(x^{(k)})^T s$$

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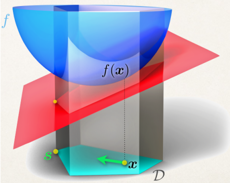

[Jaggi 2013]

Step-size

- $\gamma^{(k)} = \frac{2}{k+2}$
- $\gamma^{(k)} = \operatorname{argmin}_{\alpha \in [0,1]} f\big((1 - \alpha) x^{(k)} + \alpha s^{(k)}\big)$ (line search step)

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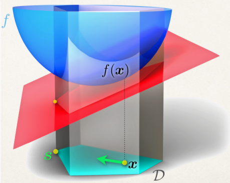

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Limits: Assumptions of Frank-Wolfe are not valid in our case

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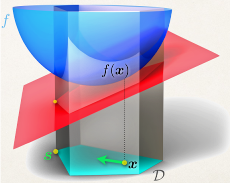

[Jaggi 2013]

- Limits: Assumptions of Frank-Wolfe are not valid in our case
- Need for an adapted algorithm

The proposed approach

The idea behind

➡ Use classical Frank-Wolfe to solve

$$\min_{x \in \textcolor{red}{\mathrm{Conv}(X)}} \mu^T x + \sqrt{x^T \Sigma x}$$

$X = \{x \in \{0,1\}^m ; Ax = b\}$
$\mathrm{Conv}(X) = \{x \in [0,1]^m ; Ax = b\}$

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➡ The solution is not feasible

➡ The gradient is not well defined in zero

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Before proceeding, some assumptions are needed

The proposed approach

First some assumptions

Three assumptions are necessary to our approach

(A1) For any real-valued vector a, there exists an efficient algorithm to solve $\min_{x \in X} a^T x$

(A2) For any real-valued vector a, there exists a solution for $\min_{x \in \mathrm{Conv(X)}} a^T x$ that belongs to X

(A3) $0_{\mathbb{R}^m}$ does not belong to X

Recall X, Conv(X)

$$X = \{x \in \{0,1\}^m ; Ax = b\}$$

$$\mathrm{Conv}(X) = \{x \in [0,1]^m ; Ax = b\}$$

The proposed approach

First some assumptions

Three assumptions are necessary to our approach

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$$\mathrm{Conv}(X) = \{x \in [0,1]^m ; Ax = b\}$$

Thanks to **(A3)**, for all $x \in X$, the gradient of g is well defined

$$\nabla g(x) = \mu + \frac{\Sigma x}{\sqrt{x^T \Sigma x}}$$

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➡ Consider the best intermediate solution, that is feasible thanks to the assumptions.

The proposed approach

DFW: a Frank-Wolfe based algorithm to solve (2)

```
$x^{(0)}$ a random feasible solution, $\varepsilon > 0$ close to zero, $K$ a maximum number of iterations.
$k \leftarrow 1$
stop $\leftarrow$ false
**while** $k \leq K$ and $\neg$stop **do**
    **if** $g(x^{(k-1)}) - g(x^{(k)}) < \varepsilon$: **then**
        stop $\leftarrow$ true
    **else**
        $s^{(k)} \in \underset{y \in \mathrm{Conv}(X)}{\mathrm{argmin}} \nabla g(x^{(k)})^T y$, with $s^{(k)} \in X$
        $\gamma^{(k)} \leftarrow \underset{\alpha \in [0,1]}{\mathrm{argmin}}\, g(x^{(k)} + \alpha(s^{(k)} - x^{(k)}))$
        $x^{(k+1)} \leftarrow (1 - \gamma^{(k)})x^{(k)} + \gamma^{(k)} s^{(k)}$
    **end if**
    $k++$
**end while**
return $\underset{s \in \{s^{(1)}, \ldots, s^{(k-1)}\}}{\mathrm{argmin}} g(s)$
```

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    $k++$
**end while**
return $\underset{s \in \{s^{(1)}, \ldots, s^{(k-1)}\}}{\mathrm{argmin}} \; g(s)$
```

- $s^{(k)}$ minimum linear approximation
- $s^{(k)} \in X$ thanks to Assumption **(A2)**

The proposed approach

DFW: a Frank-Wolfe based algorithm to solve (2)

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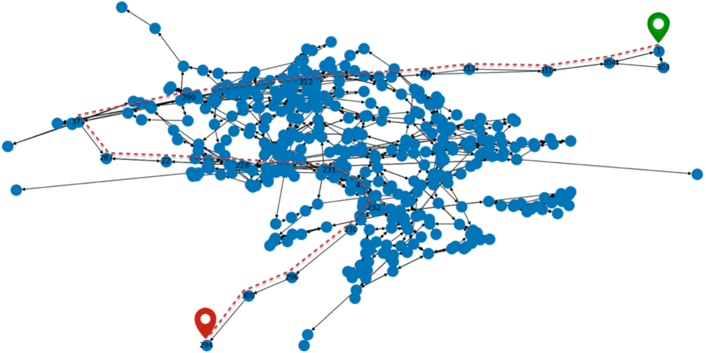
- We look at $s^{(k)}$: return the best one of all the iterations

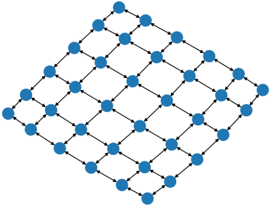
Numerical setup



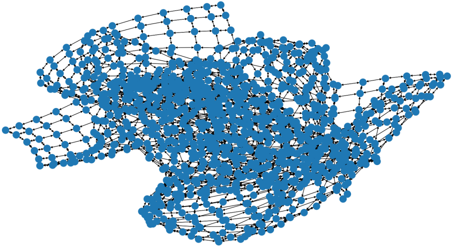
Berlin Mitte-Center graph with 398 nodes and 871 edges with an illustration of a path from node 1 to node 294

Numerical setup

Undirected grid graph $L \times L$, source node: 1, destination node L^2



Grid graph 6 × 6 with 36 nodes and 60 edges



Grid graph 34 × 34 with 1156 nodes and 2244 edges

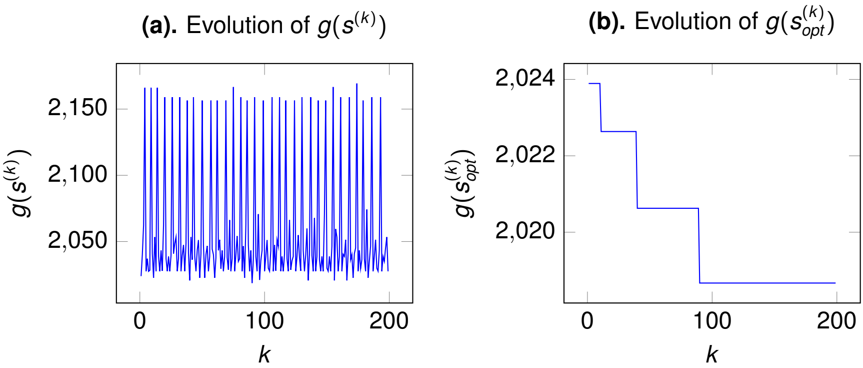
Numerical setup

Setup

- The robust shortest path problem from node 1 to node L^2
- $\Omega = 1$, (μ, Σ, x_0) random

Numerical results: behavior of the algorithm for $L = 34$

Denote, at each iteration k, the best solution so far as $s_{opt}^{(k)} = \text{argmin}_{s^{(l)} \in \{s^{(1)},\ldots,s^{(k)}\}} g(s^{(l)})$



Numerical results

Results

- Change size of the graph

Numerical results

Results

- Change size of the graph
- Compare with the solutions provided by `CPLEX`

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  200 iterations of DFW takes half an hour

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  200 iterations of DFW takes half an hour

  Same solution as best integer of `CPLEX`

Outline

1. Context and positioning

2. A Frank-Wolfe based heuristic approach applied on the robust shortest path problem

3. Another Frank-Wolfe based heuristic approach applied on the robust $\mathtt{k}$-median clustering problem

4. Conclusions and perspectives

The $\mathtt{k}$-median clustering problem

Choose $\mathtt{k}$ clusters to minimize the sum of the distances between the points and their cluster centers

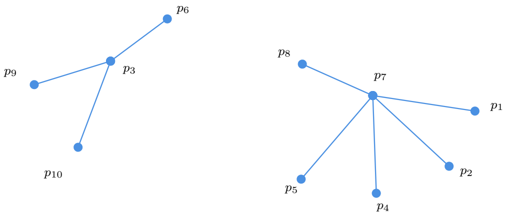
$$\min_{z \in \mathbb{R}^{n \times n}} \sum_{i=1}^{n} \sum_{j=1}^{n} d(p_i, p_j) z_{ij}$$

$$\text{s.t.} \quad \sum_{i=1}^{n} z_{ij} = 1 \quad \forall j \in \{1, \dots, n\}$$

$$z_{ij} \leq y_i \quad \forall i, j \in \{1, \dots, n\}^2$$

$$\sum_{i=1}^{n} y_i = \mathtt{k}$$

$$z_{ij}, y_i \in \{0, 1\}$$



Simple example of a two cluster solution of a $\mathtt{k}$-median problem for $n = 10$ points

The $\mathtt{k}$-median clustering problem

Choose $\mathtt{k}$ clusters to minimize the sum of the distances between the points and their cluster centers

$$
\begin{aligned}
\min_{z \in \mathbb{R}^{n \times n}} \sum_{i=1}^{n} \sum_{j=1}^{n} d(p_i, p_j) z_{ij} & \\
\text{s.t. } \sum_{i=1}^{n} z_{ij} = 1 \quad \forall j \in \{1, \ldots, n\} & \\
z_{ij} \leq y_i \quad \forall i, j \in \{1, \ldots, n\}^2 & \\
\sum_{i=1}^{n} y_i = \mathtt{k} & \\
{\color{red} z_{ij}, y_i \in \{0, 1\}} &
\end{aligned}
$$

In a matrix representation,

$z_{ii} = y_i$, $i \in \{1, \ldots, n\}$

$y_i = 1 \implies p_i$ center

$z_{ij} = 1 \implies p_j$ associated to center p_i

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z_{ij} \leq y_i \quad \forall i, j \in \{1, \dots, n\}^2 \\
\sum_{i=1}^{n} y_i = \mathtt{k} \\
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\end{aligned}$$

Constraint **(C1)**:

Sum of each column $= 1$

Every point is associated to one and only cluster center

The k-median clustering problem

Choose k clusters to minimize the sum of the distances between the points and their cluster centers

$$\min_{z \in \mathbb{R}^{n \times n}} \sum_{i=1}^{n} \sum_{j=1}^{n} d(p_i, p_j) z_{ij}$$

$$\text{s.t.} \sum_{i=1}^{n} z_{ij} = 1 \quad \forall j \in \{1, \dots, n\}$$

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$$\sum_{i=1}^{n} y_i = \mathrm{k}$$

$$z_{ij}, y_i \in \{0, 1\}$$

Constraint **(C2)**:

Non-diagonal $\leq$ diagonal

If associate point to point

$\implies$ the second is a center

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Constraint **(C3)**:

Trace $= \mathtt{k}$

Exactly $\mathtt{k}$ centers

Presence of uncertainty

➡ If the distances are uncertain in the $\mathtt{k}$-median clustering problem

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- If the distances are uncertain in the $\mathtt{k}$-median clustering problem
- Need for a robust solution

Presence of uncertainty

- If the distances are uncertain in the k-median clustering problem
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- The k-median clustering problem can be written as

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& \min d^T z \\
\text{s.t. } & \Sigma_{i=1}^{n} z_{n(i-1)+j} = 1 \quad \forall j \in \{1, \dots, n\} \\
& z_{n(i-1)+j} \leq z_{n(i-1)+i} \quad \forall i, j \in \{1, \dots, n\}^2 \\
& \Sigma_{i=1}^{n} z_{n(i-1)+i} = \mathtt{k} \\
& z \in \{0, 1\}^{n^2}
\end{aligned}
\tag{3}
$$

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- If the distances are uncertain in the $\mathtt{k}$-median clustering problem
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- A flattening step
- A proof for equivalence of the definition of uncertainty between the two writings

Robust decision under ellipsoidal uncertainty

➡ The absolute robust $\mathtt{k}$-median clustering problem under ellipsoidal uncertainty is

$$\min_{z\in X} \mu^T z + \sqrt{z^T \Sigma z} \tag{4}$$

with

$$\begin{aligned} X = \Big\{ z \in \{0,1\}^{n^2} \text{ s.t.} \\ \Sigma_{i=1}^{n} z_{n(i-1)+j} = 1 \quad \forall j \in \{1,\dots,n\}, \\ z_{n(i-1)+j} \leq z_{n(i-1)+i} \forall i,j \in \{1,\dots,n\}^2, \\ \Sigma_{i=1}^{n} z_{n(i-1)+i} = \mathtt{k} \Big\} \end{aligned}$$

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  $\Longrightarrow$ cannot apply DFW

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We propose another Frank-Wolfe based algorithm for the robust $\mathtt{k}$-median clustering

The proposed approach

The idea behind

➡ Use classical Frank-Wolfe to solve

$$\min_{x \in \text{Conv}(X)} \mu^T x + \sqrt{x^T \Sigma x}$$

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Conv(X): Constraints **(C1)**, **(C2)**, **(C3)** satisfied, variables not binary

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⇨ Consider the feasible round of the mean of all the intermediate solutions.

The proposed approach

MFW: a Frank-Wolfe based algorithm to solve Problem (4)

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$\mathring{K}$ a maximum number of iterations.
$\mathring{k} \leftarrow 1$
stop $\leftarrow$ false
**while** $\mathring{k} \leq \mathring{K}$ and $\neg$stop **do**
    **if** $g(x^{(\mathring{k}-1)}) - g(x^{(\mathring{k})}) < \varepsilon$: **then**
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return a feasible round of $\mu_{\mathring{k}-1} = \frac{\sum_{i=1}^{\mathring{k}-1} s^{(i)}}{\mathring{k} - 1}$
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- $x^{(k)}$ converges in $\mathrm{Conv}(X)$
- We look at $s^{(k)}$: return the feasible round of the mean of all the iterations

A feasible rounding algorithm: example of a 2-median clustering with 10 points

$$\begin{bmatrix}
0.53 & 0 & 0.53 & 0 & 0 & 0 & 0 & 0.05 & 0 & 0.53 \\
0 & 0.14 & 0.14 & 0.14 & 0.02 & 0 & 0.14 & 0.14 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0.39 & 0 & 0.38 & 0.38 & 0.38 & 0 & 0 & 0.32 & 0.25 \\
0 & 0 & 0 & 0.09 & 0.09 & 0.09 & 0.09 & 0 & 0 & 0.09 \\
0 & 0 & 0 & 0.04 & 0.04 & 0.04 & 0 & 0 & 0.04 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0.47 & 0.47 & 0.01 & 0 & 0.46 & 0.14 & 0.43 & 0.47 & 0.3 & 0.13 \\
0 & 0 & 0.32 & 0.34 & 0 & 0.34 & 0.34 & 0.34 & 0.34 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}$$

A feasible rounding algorithm: example of a 2-median clustering with 10 points

$$
\begin{bmatrix}
{\color{blue}0.53} & 0 & 0.53 & 0 & 0 & 0 & 0 & 0.05 & 0 & 0.53 \\
0 & 0.14 & 0.14 & 0.14 & 0.02 & 0 & 0.14 & 0.14 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0.39 & 0 & 0.38 & 0.38 & 0.38 & 0 & 0 & 0.32 & 0.25 \\
0 & 0 & 0 & 0.09 & 0.09 & 0.09 & 0.09 & 0 & 0 & 0.09 \\
0 & 0 & 0 & 0.04 & 0.04 & 0.04 & 0 & 0 & 0.04 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0.47 & 0.47 & 0.01 & 0 & 0.46 & 0.14 & 0.43 & {\color{blue}0.47} & 0.3 & 0.13 \\
0 & 0 & 0.32 & 0.34 & 0 & 0.34 & 0.34 & 0.34 & 0.34 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\rightarrow
\begin{bmatrix}
{\color{blue}1} & & & & & & & 0 & & \\
0 & 0 & & & & & & 0 & & \\
0 & & 0 & & & & & 0 & & \\
0 & & & 0 & & & & 0 & & \\
0 & & & & 0 & & & 0 & & \\
0 & & & & & 0 & & 0 & & \\
0 & & & & & & 0 & 0 & & \\
0 & & & & & & & {\color{blue}1} & & \\
0 & & & & & & & 0 & 0 & \\
0 & & & & & & & 0 & & 0
\end{bmatrix}
$$

Sort the diagonal elements, and choose the 2 biggest elements

A feasible rounding algorithm: example of a 2-median clustering with 10 points

$$\begin{bmatrix} 0.53 & 0 & 0.53 & 0 & 0 & 0 & 0 & 0.05 & 0 & 0.53 \\ 0 & 0.14 & 0.14 & 0.14 & 0.02 & 0 & 0.14 & 0.14 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.39 & 0 & 0.38 & 0.38 & 0.38 & 0 & 0 & 0.32 & 0.25 \\ 0 & 0 & 0 & 0.09 & 0.09 & 0.09 & 0.09 & 0 & 0 & 0.09 \\ 0 & 0 & 0 & 0.04 & 0.04 & 0.04 & 0 & 0 & 0.04 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.47 & 0.47 & 0.01 & 0 & 0.46 & 0.14 & 0.43 & 0.47 & 0.3 & 0.13 \\ 0 & 0 & 0.32 & 0.34 & 0 & 0.34 & 0.34 & 0.34 & 0.34 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \rightarrow \begin{bmatrix} 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & & & & & & 0 & & \\ 0 & & 0 & & & & & 0 & & \\ 0 & & & 0 & & & & 0 & & \\ 0 & & & & 0 & & & 0 & & \\ 0 & & & & & 0 & & 0 & & \\ 0 & & & & & & 0 & 0 & & \\ 0 & 1 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 0 \\ 0 & & & & & & & 0 & 0 & \\ 0 & & & & & & & 0 & & 0 \end{bmatrix}$$

Sort the diagonal elements, and choose the 2 biggest elements

In reduced matrix, sort each column

A feasible rounding algorithm: example of a 2-median clustering with 10 points

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Then the rest equals zero, and the rounding is done!

Numerical setup

Setup

- We changed the number of points *n* for the $\mathtt{k}$-median problem for $\mathtt{k} = 2$
- We compared with the solutions provided by `CPLEX`
- $\Omega = 1$, and for every *n*, 80 different (μ, Σ, x_0)

Numerical results of MFW Algorithm

$$E_r = \frac{g(\hat{x}) - p^*}{p^*} \qquad \#\{E_r = 0\}$$

n	Time(s) of CPLEX	Time(s) MFW	$\#\{E_r = 0\}$	$\overline{E_r}$
5	0.1644	5.0149	55 %	0.0555
6	0.5424	7.8	71.25 %	0.0513
7	0.8296	12.9796	48.75 %	0.0486
8	0.9948	6.9707	67.5 %	0.0186
9	1.9202	9.6168	63.75 %	0.0246
10	2.1028	16.6282	58.75 %	0.0432
11	2.1607	14.1045	70 %	0.0447
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➡ The relative error is in average small (0.0186 to 0.0862)

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➡ The relative error equals zero in up to 70% of the cases

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CPLEX is faster but the difference in time between MFW Algorithm and CPLEX is not very big (around $1/5$ in average)

Outline

1. Context and positioning

2. A Frank-Wolfe based heuristic approach applied on the robust shortest path problem

3. Another Frank-Wolfe based heuristic approach applied on the robust `k`-median clustering problem

4. Conclusions and perspectives

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- Numerical results show that the heuristic approach gives the optimal solution
- An extension on the robust $\mathtt{k}$-median clustering has been studied
- A heuristic algorithm based on Frank-Wolfe has been proposed, with a feasible rounding algorithm
- Results show that this algorithm gives the optimal solution in most of the cases, and that it gives close-to-optimal solutions when they are not optimal

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- Improve MFW Algorithm (e.g., by improving the rounding technique)
- Test MFW with different uncertainty configurations of the clusters

Thank you for your attention