# COMBINATORIAL OPTIMIZATION PROBLEMS RELATED TO MACHINE LEARNING TECHNIQUES

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# Introduction

- Combinatorial optimization and machine learning appear to be extremely close fields of the modern computer science.
- Various areas in machine learning: PAC-learning, boosting, cluster analysis, feature and model selection, etc. are continuously presenting new challenges for designers of optimization methods due to the steadily increasing demands on accuracy, efficiency, space and time complexity and so on.

# CO and ML

- In many cases, learning problem can be successfully reduced to the appropriate combinatorial optimization problem: clique, max-cut, p-median, TSP, etc.
- To this end, all the results obtained for the latter problem (approximation algorithms, polynomial-time approximation schemas, approximation thresholds) can find their application in design precise and efficient learning algorithms for the former.
- In our paper (in proceedings), three examples of such a collaboration are considered.

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- In our paper (in proceedings), three examples of such a collaboration are considered.
- But, in this presentation, I would like to consider the case of the inverse collaboration when combinatorial optimization benefits from using of a ML technique

# Multiple TSP - overview

- For a given natural $k$, a problem of $k$ collaborating salesmen sharing the same set of cities (nodes of graph) to serve is studied.
- We call it Minimum Weight $k$-Size Cycle Cover Problem (Min-$k$-SCCP).
- Related problems
  - Min-1-SCCP is Traveling Salesman Problem (TSP)
  - **Vertex-Disjoint Cycle Cover Problem**
  - $k$-Peripatetic Salesmen Problem
  - Min-$L$-CCP
- Min-$k$-SCCP can be considered as a special case of Vehicle Routing Problem (VRP)

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# Multiple TSP — Motivation

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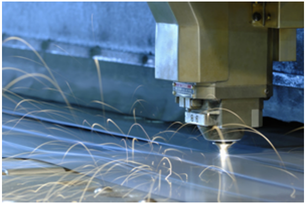
- high-precision metal shape cutting problem



# Multiple TSP — Results

1. Min-$k$-SCCP is strongly NP-hard and hardly approximable in the general case
2. Metric and Euclidean cases are intractable as well
3. 2-approximation algorithm for Metric Min-$k$-SCCP is proposed
4. Polynomial-time approximation scheme (PTAS) for Min-2-SCCP on the plane is constructed

# Definitions and Notation

Standard notation is used

- $\mathbb{R}$ — field of real numbers
- $\mathbb{N}$ — field of rational numbers
- $\mathbb{N}_m$ — integer segment $\{1, ..., m\}$,
- $\mathbb{N}_m^0$ — segment $\{0, ..., m\}$.
- $G = (V, E, w)$ is a simple complete weighted (di)graph with loops, edge-weight function $w : E \to \mathbb{R}$

# Minimum Weight $k$-Size Cycle Cover Problem (Min-$k$-SCCP)

**Input:** graph $G = (V, E, w)$.

**Find:** a minimum-cost collection $\mathcal{C} = C_1, ..., C_k$ of vertex-disjoint cycles such that $\bigcup_{i \in \mathbb{N}_k} V(C_i) = V$.

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$$\min \quad \sum_{i=1}^{k} W(C_i) \equiv \sum_{i=1}^{k} \sum_{e \in E(C_i)} w(e)$$

$$s.t.$$

$$C_1, \ldots, C_k \text{ are cycles in } G$$

$$C_i \cap C_j = \varnothing$$

$$V(C_1) \cup \ldots \cup V(C_k) = V$$

# Metric and Euclidean Min-$k$-SCCP

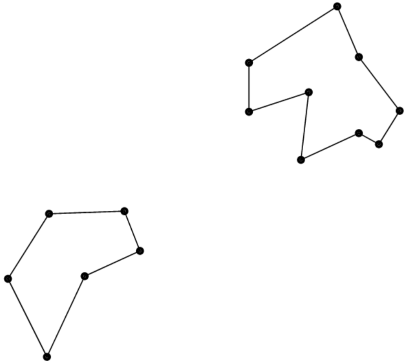
## Metric Min-$k$-SCCP

- $w_{ij} \geqslant 0$
- $w_{ii} = 0$
- $w_{ij} = w_{ji}$
- $w_{ij} + w_{jk} \geqslant w_{ik} \quad (\{i, j, k\})$

## Euclidean Min-$k$-SCCP

- For some $d > 1$, $V = \{v_1, \ldots, v_n\} \subset \mathbb{R}^d$
- $w_{ij} = \|v_i - v_j\|_2$

# Instance of Euclidean Min-2-SCCP



# Complexity

## Known facts

- (Karp, 1972) TSP is strongly NP-hard
- (Sahni and Gonzales, 1976) TSP can not be approximated within $O(2^n)$ (unless $P = NP$)
- (Papadimitriou, 1977) Euclidean TSP is NP-hard

# Complexity

**Theorem 1**

*For any* $k \geqslant 1$*, Min-k-SCCP is strongly NP-hard.*

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- Show that any optimal solution of Min-$k$-SCCP consists of cheapest Hamiltonian cycles for the initial TSP

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## Corollary

- Min-$k$-SCCP also can not be approximated within $O(2^n)$ (unless $P = NP$)
- Metric Min-$k$-SCCP and Euclidean Min-$k$-SCCP are NP-hard as well

# Minimum spanning forest

- $k$-forest is an acyclic graph with $k$ connected components
- For any $k$-forest $F$, weight (cost)

$$W(F) = \sum_{e \in E(F)} w(e)$$

- $k$-Minimum Spanning Forest ($k$-MSF) Problem

# Kruskal's algorithm for $k$-MSF

1. Start from the empty $n$-forest $F_0$.
2. For each $i \in \mathbb{N}_{n-k}$ add the edge

$$e_i = \arg\min\{w(e)\colon F_{i-1} \cup \{e\} \text{ remains acyclic}\}$$

   to the forest $F_{i-1}$.
3. Output $k$-forest $F^*$.

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**Theorem 2**

*$F^*$ is k-Minimum Spanning Forest.*

# 2-approximation algorithm for Metric Min-$k$-SCCP

Following to the scheme of well-known 2-approx. algorithm for Metric TSP.
Wlog. assume $k < n$.
**Algorithm:**

1. Build a k-MSF $F$
2. Take edges of $F$ twice
3. For any non-trivial connected component, find a Eulerian cycle
4. Transform them into Hamiltonian cycles
5. Output collection of these cycles adorned by some number of isolated vertices

# Correctness proof

## Assertion

Approximation ratio:

$$2(1 - 2/n) \leqslant \frac{APP}{OPT} \leqslant 2(1 - 1/n)$$

Running-time:

$$O(n^2 \log n).$$

## Proof sketch

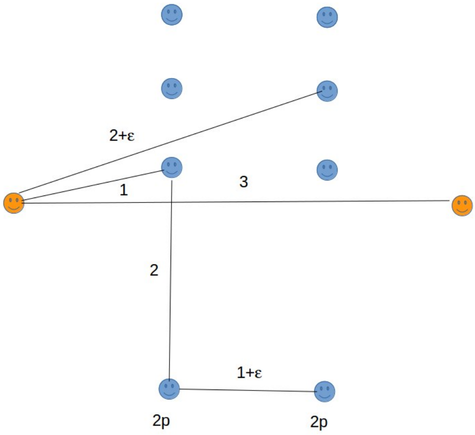
Consider optimal cycle cover $\mathcal{C}$ (with weight OPT).
Removing the most heavy edge from any non-empty cycle transform it into some spanning forest $F(\mathcal{C})$ with cost SF.
Then

$$MSF \leqslant SF \leqslant OPT(1 - 1/n),$$

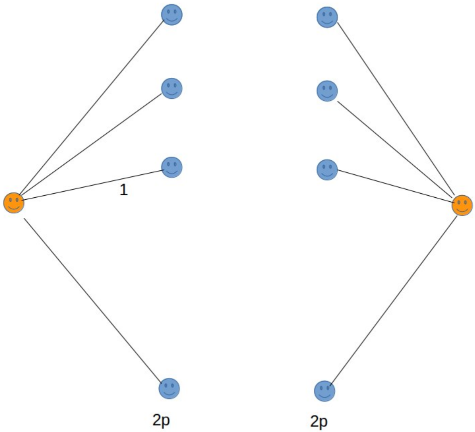
where

$$APP \leqslant 2 \cdot MSF \leqslant 2(1 - 1/n)OPT.$$

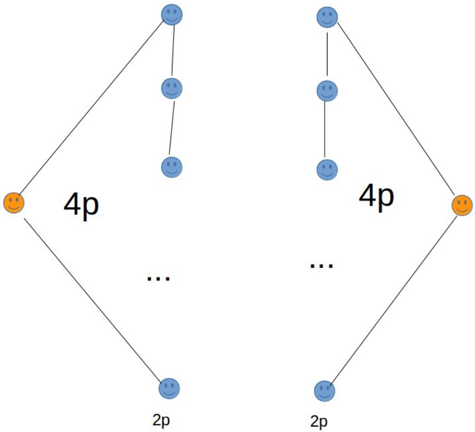
# Lower bound - instance



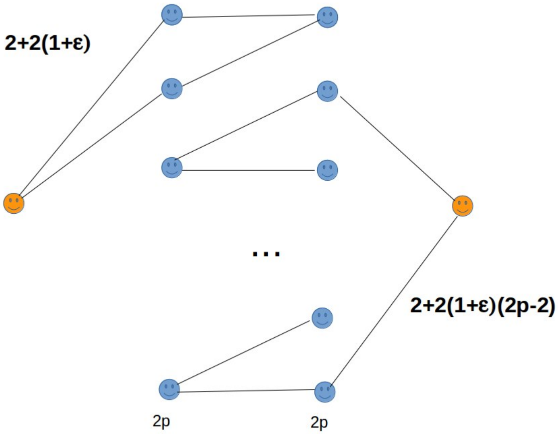
# Lower bound - 2-forest



# Lower bound - approximation



# Lower bound - better approximation



# Lower bound - discussion

- number of nodes $n = 4p + 2$
- $APP = 8p$
- $OPT \leq 4p + 2 + 2\varepsilon(2p - 1)$
- for approximation ratio $r$ we have

$$r \geq \sup_{\varepsilon \in (0,1)} \frac{8p}{4p + 2 + 2\varepsilon(2p - 1)} = \frac{4p}{2p + 1} = 2(1 - 2/n)$$

# PTAS for Euclidean Min-2-SCCP on the plane

**Definition**

For a combinatorial optimization problem, Polynomial-Time Approximation Scheme (PTAS) is a collection of algorithms such that for any fixed $c > 1$ there is an algorithm finding a $(1 + 1/c)$-approximate solution in a polynomial time depending on $c$.

# Instance preprocessing

For an arbitrary instance of Min-2-SCCP, there exists one of the following alternatives (each of them can be verified in polynomial time)

1. The instance in question can be decomposed into 2 independent TSP instances;
2. Inter-node distance can be overestimated using some function that depends on OPT linearly.

# Jung's inequality

Consider a set $S$ of diameter $D$ in $d$-dimensional Euclidean space, let $R$ be a radius of the smallest containing sphere.
Then

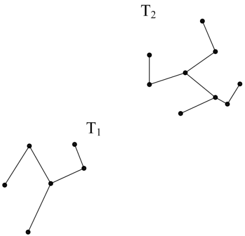
$$\frac{1}{2}D \leqslant R \leqslant \left(\frac{d}{2d+2}\right)^{\frac{1}{2}} D.$$

In particular, in the plane:

$$\frac{1}{2}D \leqslant R \leqslant \frac{\sqrt{3}}{3}D. \quad (1)$$

# Instance preprocessing - ctd.

- Construct 2-MSF consisting of trees $T_1$ and $T_2$.




- let $D_1$, $D_2$ be diameters of $T_1$ and $T_2$, and $R_1$, $R_2$ be radia of the smallest circles $B(T_1)$ and $B(T_2)$ containing the trees $T_1$ and $T_2$. Denote $D = \max\{D_1, D_2\}$ and $R = \max\{R_1, R_2\}$.

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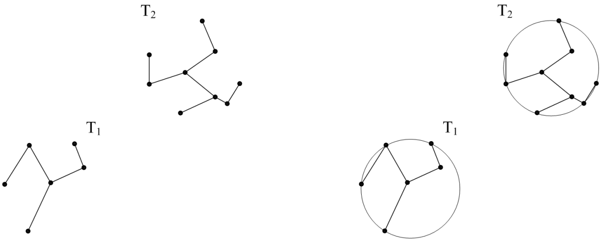


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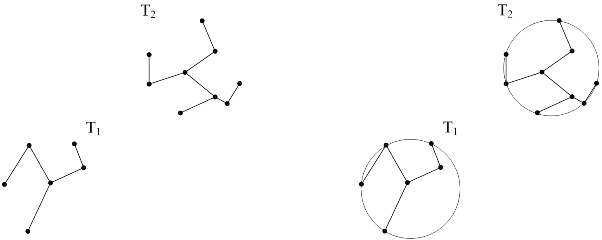


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# Problem decomposition

Define $\rho(T_1, T_2)$ as a distance between centers of circles $B(T_1)$ and $B(T_2)$.

**Assertion**

If $\rho(T_1, T_2) > 5R$ then the considered instance Min-2-SCCP can be decomposed into two TSP instances for $G(T_1)$ and $G(T_2)$.

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Suppose, on the contrary, that there is an optimal 2-SCC $\mathcal{C} = \{C_1, C_2\}$ such that $C_1 \cap T_1 \neq \varnothing$ and $C_1 \cap T_2 \neq \varnothing$.

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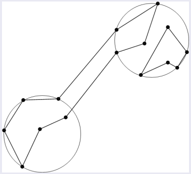

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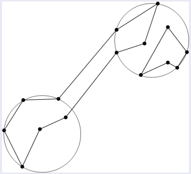
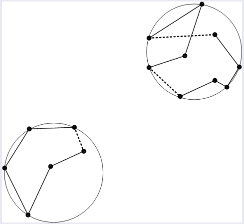


Then $C_1$ contains at least two edges, spanning $T_1$ and $T_2$

# Problem decomposition

## Proof (ctd.)

- By the condition, the weight of each of them is greater than $3R$
- Remove them and close the cycles inside $B(T_1)$ and $B(T_2)$



- Obtain the lighter 2-SCC

# Problem decomposition

**Statement**

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- In our case $D(G) \leqslant 7R$
- Due to Young's inequality and $D \leqslant MSF \leqslant OPT$ we have

$$R \leqslant \frac{\sqrt{3}}{3}D \leqslant \frac{\sqrt{3}}{3} \cdot OPT,$$

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In this case Min-2-SCCP instance can be enclosed into some axis-aligned square $\mathcal{S}$ of size $7/\sqrt{3} \cdot OPT$

# Rounding

**Definition**

Instance of Min-2-SCCP is called *rounded* if

- every vertex of the graph $G$ has integral coordinates $x_i, y_i \in \mathbb{N}^0_{O(n)}$
- for any edge $e$, $w(e) \geqslant 4$

**Lemma 3**

*PTAS for rounded Min-2-SCCP implies PTAS for Min-2-SCCP (in the general case)*

# Rounding: proof sketch

- partition the surrounding square by axis-alined lines with step of $L/(2nc)$
- move any node to nearest line-crossing point; inter-node distance change is bounded by $L/(nc)$; cycle cover weight change bound is $L/c$
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# Rounding: proof sketch - ctd.

- for weights $W$ and $W'$ of any corresponding cycle covers in the initial and the rounded instances

$$\frac{8nc}{L}\Big(W - \frac{L}{c}\Big) \leqslant W' \leqslant \frac{8nc}{L}\Big(W + \frac{L}{c}\Big)$$

- For optimum values $OPT$ and $OPT'$ and weights $W$ and $W'$ of the approximate solutions

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$$OPT \leqslant W \leqslant \Big(\frac{7\sqrt{3}}{3c^2} + \frac{17\sqrt{3}}{3c} + 1\Big) OPT.$$

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$$W-\frac{L}{c}\leqslant\Big(1+\frac{1}{c}\Big)\Big(OPT+\frac{L}{c}\Big)$$

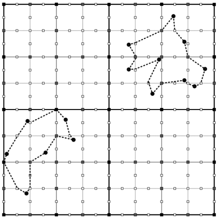
- And

$$OPT\leqslant W\leqslant\Big(\frac{7\sqrt{3}}{3c^2}+\frac{17\sqrt{3}}{3c}+1\Big)OPT.$$

# Main idea: construct PTAS for rounded instances

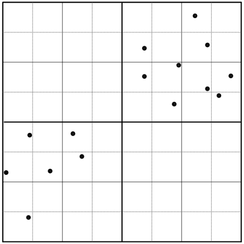
Randomized partitioning of the square $\mathcal{S}$ into smaller subsquares and subsequent search for minimum 2-SCC of special kind

1) every inter-node segment of its cycles is piece-wise linear and intersects all squares' borders at special points (*portals*) only;
2) portals number and locations together with maximum number of intersections (for each border) are defined in advance and depend on accuracy parameter $c$;



# Quad-trees for rounded Min-2-SCCP

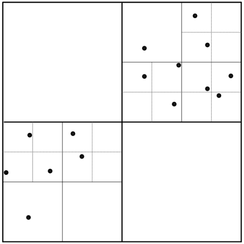
Set up a regular 1-step axis-aligned grid on the square $\mathcal{S}$ with side-length of $L = O(n)$.



We are using the concept of *quad-tree*

# Quad-trees for rounded Min-2-SCCP

Root is the square $\mathcal{S}$. For every square (including the root), make a partition of the square into 4 child subsquares. Repeat it until all child squares will contain no more than 1 node of the instance.



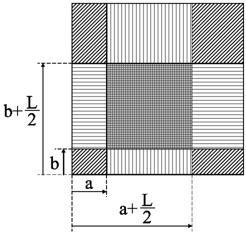
# Shifted Quad-tree

**Definition**

Suppose, $a, b \in \mathbb{N}_L^0$, we call the Quad-tree $T(a, b)$ *shifted Quad-tree*, if coordinates of its center is

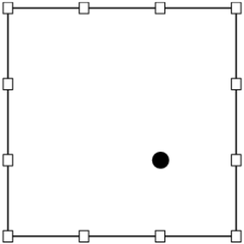
$$((L/2 + a) \mod L, (L/2 + b) \mod L).$$

Child squares of $T(a, b)$, as its center, is considered *modulo L*



# Definition

- Consider fixed values $m, r \in \mathbb{N}$.
- For any square $S$, assign regular partition of its border, including vertices of the square and consisting of $4(m+1)$ points.
- Such a partition is called *m-regular partition*, and all its elements — *portals*.



# Definitions

**$m$-regular portal set**

Union of $m$-regular partitions for all borders of not-a-leaf nodes of Quadro-tree $T(a, b)$ is called $m$-regular portal set. Denote it $P(a, b, m)$.

**$(m, r)$-approximation**

Suppose, $\pi$ is a simple cycle in the Min-2-SCCP instance graph $G$ (on the plane), $V(\pi)$ is its node-set. Closed piece-wise linear route $l(\pi)$ is called $(m, r)$-approximation (of the cycle $\pi$) if

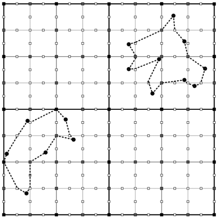
1) node-set of the route $l(\pi)$ is a some subset of $V(\pi) \cup P(a, b, m)$,
2) $\pi$ and $l(\pi)$ visit the nodes from $V(\pi)$ in the same order,
3) for any square (being a node of $T(a, b)$), $l(\pi)$ intersects its arbitrary edge no more than $r$ times, and exclusively in the points of $P(a, b, m)$.

# Once more definition

**$(k, m, r)$-cycle cover**

$k$-scc consisting of $(m, r)$-approximations is called $(k, m, r)$-cycle cover

Obviously, an arbitrary $(1, m, r)$-cycle cover contains the only $(m, r)$-approximation which is a Hamiltonian cycle.
Let us consider $(2, m, r)$-cycle covers. . .



# Structure Theorem for Euclidean Min-2-SCCP

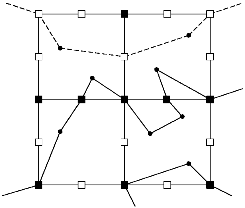
**Theorem 4**

- *Suppose* $c > 0$ *is fixed,*
- $L$ *is size of square* $\mathcal{S}$ *for a given instance of rounded 2-MHC.*
- *Suppose discrete stochastic variables* $a, b$ *are distributed uniformly on the set* $\mathbb{N}_L^0$.
- *Then for* $m = O(c \log L)$ *and* $r = O(c)$ *with probability at least* $\frac{1}{2}$ *there is* $(2, m, r)$*-cycle cover which weight is no more than* $(1 + \frac{1}{c})OPT$.

# Dynamic Programming

**$(2, m, r, S)$-segment**

Let some $(2, m, r)$-cycle cover $C$ and some node $S$ of the tree $T(a, b)$ be chosen. A family of partial routes $C \cap S$ is called $(2, m, r, S)$-segment (of the cover $C$).



# Bellman equation

**Task $(S, R_1, R_2, \kappa)$**

Input.

- Node $S$ of the tree $T(a, b)$.
- Cortege $R_i : \mathbb{N}_{q_i} \to (P(a, b, m) \cap \partial S)^2$ defines a sequence of the start-finish pairs of portals $(s^i_j, t^i_j)$ which are crossing-points of $\partial S$ by $(m, r)$-approximation $l_i$.
- Number $\kappa$ is equal to the number of cycles of the building $(2, m, r)$-cycle cover, intersecting the interior of $S$.

Output minimum-cost $(2, m, r, S)$-segment.

Denote by $W(S, R_1, R_2, \kappa)$ value of the task $(S, R_1, R_2, \kappa)$.

$$W(S, R_1, R_2, \kappa) = \min_{\tau} \sum_{i=I}^{IV} W(S^i, R^i_1(\tau), R^i_2(\tau), \kappa^i(\tau)),$$

# Derandomization

Denote by $APP(a,b)$ a weight of the approximate solution constructed by DP for the tree $T(a,b)$.

$$P\left(APP(a,b) \leqslant (1+\frac{1}{c})OPT\right) \geqslant 1/2,$$

Hence, there is a pair $(a^*,b^*) \in \mathbb{N}_L^0$, for which the equation

$$OPT \leqslant APP(a^*,b^*) \leqslant (1+1/c)OPT$$

is valid.

**Theorem 5**

*Euclidean Min-2-SCCP has a Polynomial-Time Approximation Scheme with complexity bound $O(n^3(\log n)^{O(c)})$.*

# Conclusion and Open Problems

- The proposed PTAS seems to be easily extendable onto Min-$k$-SCCP in $d$-dimensional Euclidean space
- Due to well-known PCP theorem there is no PTAS for Metric Min-$k$-SCCP. But, what about approximation threshold value for this problem?

*Thank you for your attention!*