From theory to practice in k-OPT heuristic for Travelling Salesman Problem

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(joint work with Marek Cygan, Arkadiusz Socała and Kamil Żyła)

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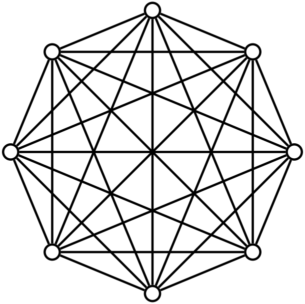
Traveling Salesman Problem (TSP)

Input

complete undirected graph $G = (V, E)$ and
a weight function $w : E \to \mathbb{N}$.

Problem

Find a tour (Hamiltonian cycle) of minimum weight.



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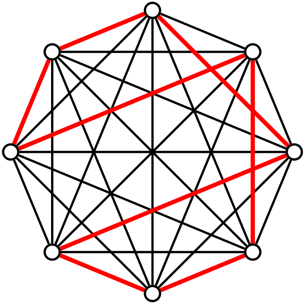
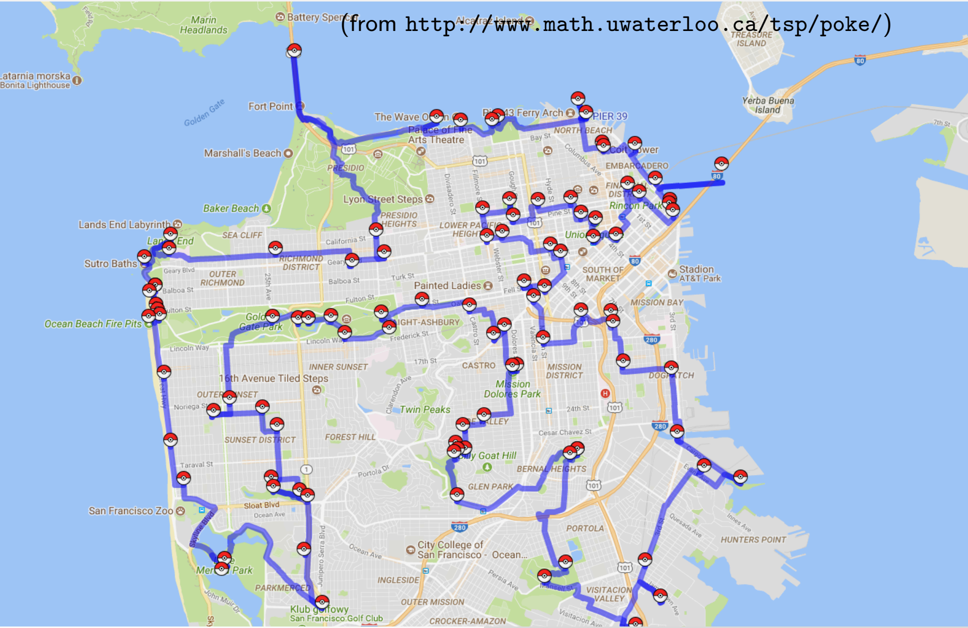


The shortest tour catching all San Francisco pokemons

(from http://www.math.uwaterloo.ca/tsp/poke/)

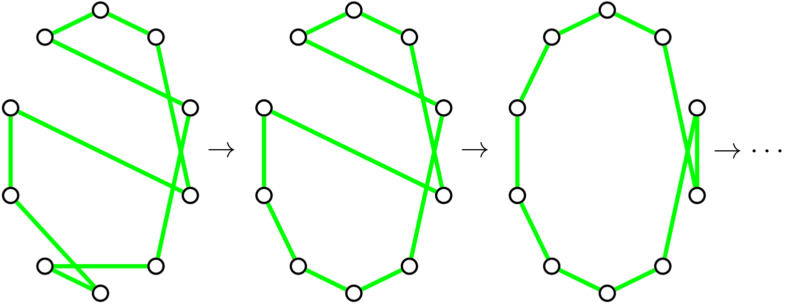


Solving TSP

- Problem is NP-hard
- Best exact algorithm in time $2^n n^{O(1)}$.
- No approximation possible in general (unless P=NP)
- Some nice approximation algorithm under additional assumptions
  - w is a metric: 1.5-approximation (Christofides 1976)
  - Euclidean metric: a PTAS (Arora 1996)
  - Graphic metric: 1.4-approximation (Sebo, Vygen, 2012)
- In practice: people use heuristics.

k-OPT local search heuristic

1. $H_0 :=$ arbitrary Hamiltonian cycle.
2. As long as possible, get a **better** cycle H_i by means of the k-**move** operation.

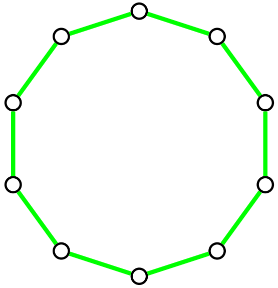


k-move

For a tour H, a k-**move** is defined by a pair (E^-, E^+) such that

- $|E^-| = |E^+| = k$ and
- $H' = H \setminus E^- \cup E^+$ is a Hamiltonian cycle.

Example for $k = 3$:



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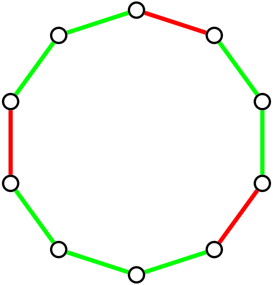

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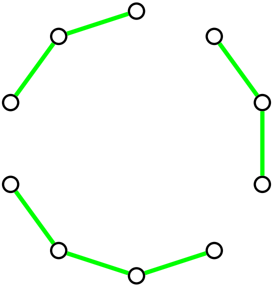

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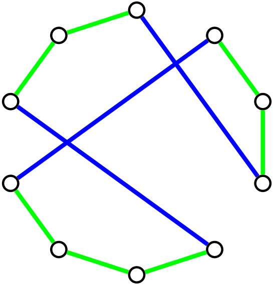

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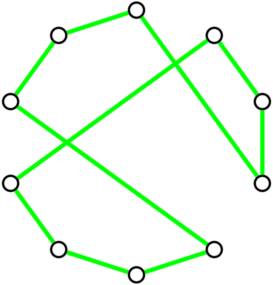

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k-OPT heuristic

Practice

An implementation of a variant, called Lin-Kernighan heuristic solves 80K-vertex instances optimally (Hellsgaun '09).

Theory

Interesting results (lower, upper bounds) on

- quality of local optima (e.g. Chandra et al, SICOMP'99),
- number of steps needed to find local optimum (e.g., Johnson et al, JCSS'88),
- smoothed analysis of 2-opt (e.g. Künnemann and B. Manthey, ICALP'15).

Today's question

How fast can we perform a **single step**,

i.e.,

How fast can we find an improving k-move?

Today's question

k-OPT OPTIMIZATION

INPUT: symmetric function $w : V^2 \to \mathbb{N}$, a Hamiltonian cycle H

OUTPUT: a k-move that maximizes improvement over H.

k-OPT DETECTION

OUTPUT: Is there a k-move improving over H?

Upper bounds

- $O(n^k)$ exhaustive search,

Lower bounds

- $W[1]$-hard [Marx '08]
- no $n^{o(k/\log k)}$ algorithm under ETH [Guo et al. '13]
- no $o(n^2)$ algorithm for $k = 2$ (folklore),

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Upper bounds

- $O(n^k)$ exhaustive search,
- $O(n^{\lfloor 2k/3 \rfloor + 1})$ time, $O(n)$ additional space [de Berg, Buchin, Jansen, Woeginger '16]

Lower bounds

- $W[1]$-hard [Marx '08]
- no $n^{o(k/\log k)}$ algorithm under ETH [Guo et al. '13]
- no $o(n^2)$ algorithm for $k = 2$ (folklore),
- if $o(n^{2.99})$ algorithm for $k = 3$, then APSP in time $o(n^{2.99})$ [de Berg et al].

Part I: Theory

(joint work with Marek Cygan and Arkadiusz Socała)

Our results

Theorem

For every fixed integer k, k-OPT OPTIMIZATION can be solved in time $O(n^{(1/4+\epsilon_k)k})$ and space $O(n^{(1/8+\epsilon_k)k})$, where $\lim_{k\to\infty} \epsilon_k = 0$.

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Values of ϵ_k (computed by a program)

k	3	4	5	6	7	8
de Berg et al.	$O(n^3)$	$O(n^3)$	$O(n^4)$	$O(n^5)$	$O(n^5)$	$O(n^6)$
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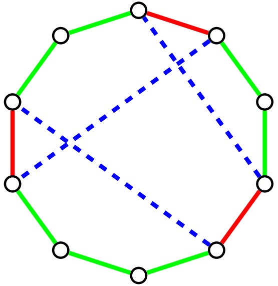
Theorem

If there is $\epsilon > 0$ such that 4-OPT DETECTION admits an algorithm in time $O(n^{3-\epsilon} \cdot \text{polylog}(M))$, then there is $\delta > 0$ such that ALL PAIRS SHORTEST PATHS admits an algorithm in time $O(n^{3-\delta} \cdot \text{polylog}(M))$, assuming integer weights from $\{-M, \dots, M\}$.

An equivalent representation of k-move

(The most intuitive) representation of k-move

A pair (E^-, E^+), where $E^- \subseteq H, E^+ \subseteq E(G)$



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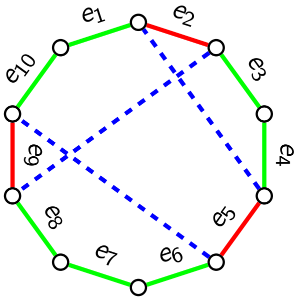

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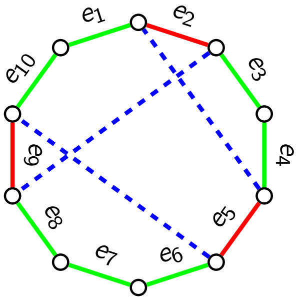

$f(1) = 2$
$f(2) = 5$
$f(3) = 9$

A more useful representation: a pair $(f, \quad)$

- an embedding $f : \{1, \ldots, k\} \to \{1, \ldots, n\}$

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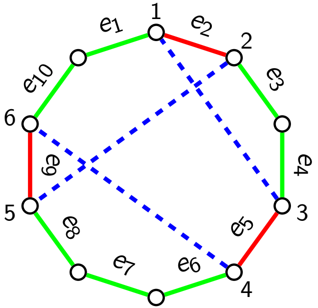

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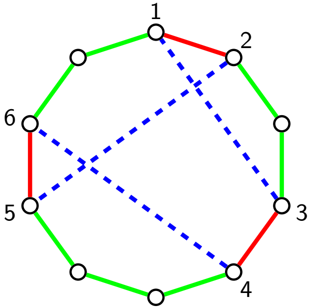
$M = \{13, 25, 46\}$

A more useful representation: a pair (f, M)

- an embedding $f : \{1, \ldots, k\} \to \{1, \ldots, n\}$
- connection pattern: a perfect matching M on $\{1, .., 2k\}$

de Berg et al.'s idea



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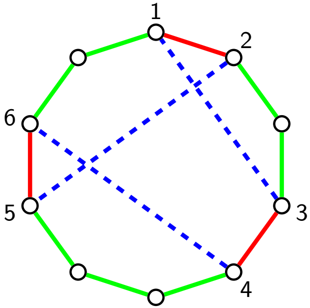
Observation 1

Now we can specify a connection pattern M **before** specifying an embedding f.

Observation 2

There are only $O((2k)!)$ connection patterns, i.e., $O(1)$ for fixed k.

de Berg et al.'s idea



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Idea

- For each of the $O((2k)!)$ connection patterns M, find the embedding f_M which maximizes weight improvement.
- Fixing M allows for exploiting the structure of the solution.

From now on, assume M is fixed.

Key notion: the dependence graph D_M

$$V(D_M) = [k].$$

Vertex i corresponds to the i-th deleted edge from the Hamiltonian cycle $e_1 e_2 \cdots e_n$.

$$E(D_M) = O \cup I_M,$$

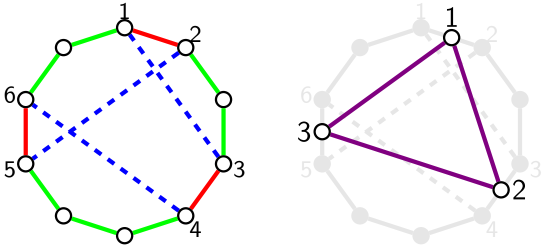
where

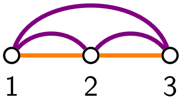
$$O = \{12, 23, \ldots, (k-1)k\}$$

- Edge $j(j+1) \in O$ represents the property $f(j) < f(j+1)$.
- I_M is defined by M. Edge $ij \in I_M$ means that the cost of embedding i-the edge depends on $f(j)$.

$E(D_M) = O \cup I_M$

- $O = \{12, 23, \ldots, (k-1)k\}$
- Get I_M from M by identifying $2i-1$ with $2i$ for $i \in [k]$:
  $I_M = \{ij \ : \ i'j' \in M, i' \in \{2i-1, 2i\}, j' \in \{2j-1, 2j\}\}$





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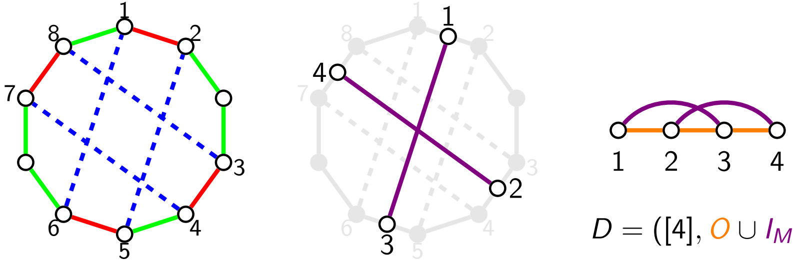
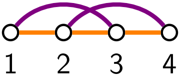


$D = ([4], O \cup I_M)$

The algorithm of de Berg, Buchin, Jansen and Woeginger



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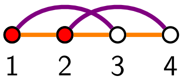

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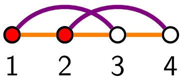

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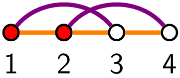


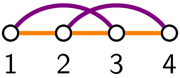
$$D = ([4], O \cup I_M)$$

1. Find a minimum vertex cover A of I_M
2. Embed A in all $n^{|A|}$ ways
3. Dependence graph of the rest D' has only some edges of O. D' is a collection of **paths** so we can find optimal embedding in $O(nk)$ time using dynamic programming.

We have $|A| \leq \lfloor 2/3k \rfloor$ (worst case: I_M is a collection of 3-cycles).

Hence, time is $O(n^{\lfloor 2/3k \rfloor + 1} k)$ for every connection pattern.

Another possible algorithm



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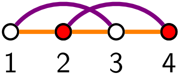

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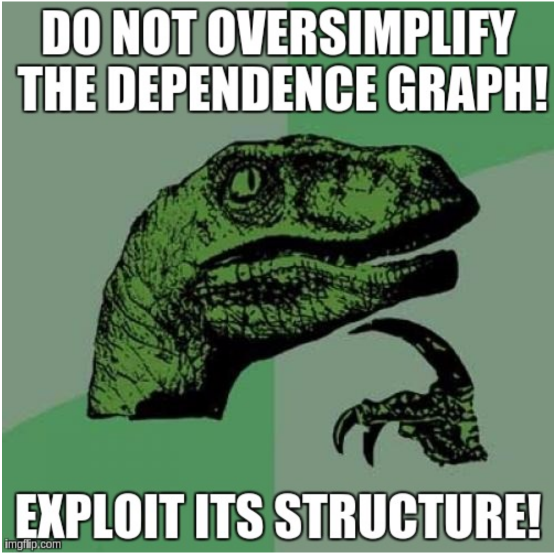
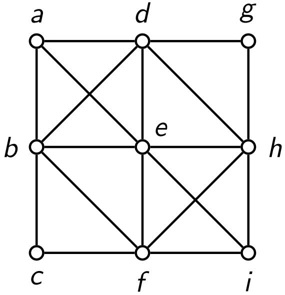
2. Dependence graph of the rest D' has only some edges of I_M.
   D' is a collection of **cycles and paths** so we can find optimal embedding in $O(n^3)$ time using dynamic programming.

Hence, time is $O(n^{\lfloor k/2 \rfloor + 3})$ for every connection pattern.

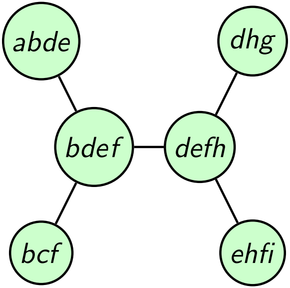

DO NOT OVERSIMPLIFY THE DEPENDENCE GRAPH!
EXPLOIT ITS STRUCTURE!
imgflip.com

Tree decompositions and treewidth

Graph $G = (V, E)$



Tree decomposition of G



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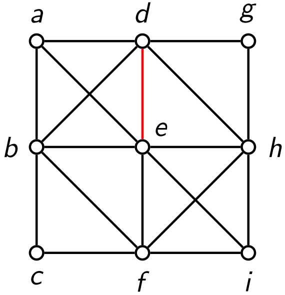

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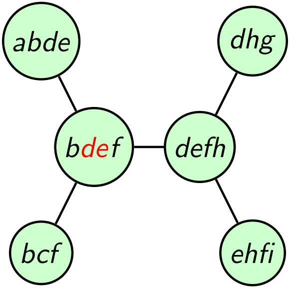

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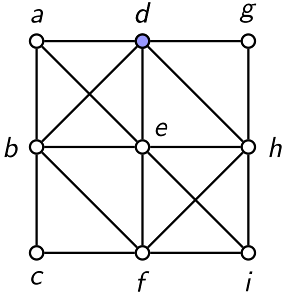

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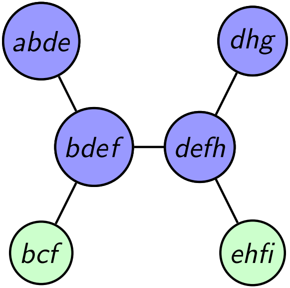

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- For every edge $uv \in E$ some bag contains u and v
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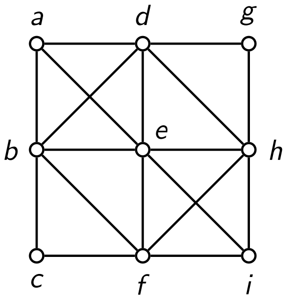

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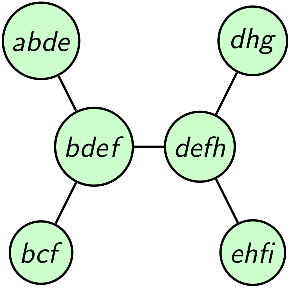

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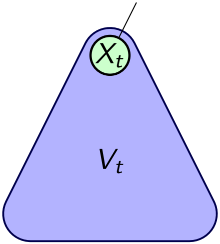
Width of the decomposition: maximum bag size -1 (here: 3).

Treewidth of G: minimum width of a decomposition of G .

Dynamic programming

For every node t of a tree decomposition of the graph D_M:

- X_t = the bag at t,
- V_t = union of all bags in the subtree rooted at t.

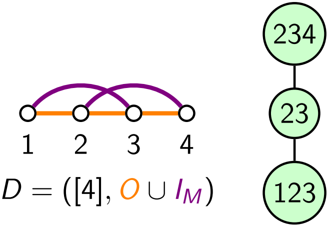


For every node t and partial embedding $f : X_t \to [n]$, compute

$$T_t[f] = \max_{\substack{g: V_t \to [n] \\ g|_{X_t} = f}} \text{gain}_M(g).$$

in the bottom-up fashion.

Dynamic programming: example



$$T_{123}[f] = w(e_{f(1)}) + w(e_{f(2)}) + w(e_{f(3)}) - w(E^+_{f,M})$$

$$T_{23}[f] = \max_{\substack{g:\{1,2,3\}\to[n] \\ g|_{\{2,3\}=f}}} T_{123}[g].$$

$$T_{234}[f] = T_{23}[f|_{\{2,3\}}] + w(e_{f(4)}) - w(E^+_{f,M} \setminus E^+_{f|_{\{2,3\}},M})$$

The $O(n^{(1/3+\epsilon_k)k})$-time algorithm

Theorem

Given a connection pattern M, the best k-move (f, M) can be found in time $n^{\mathrm{tw}(D_M)+1}k^2 + 2^k$.

Theorem (Fomin et al. 2009)

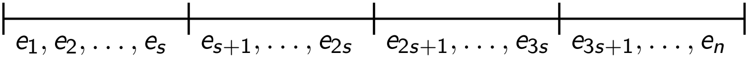
Treewidth a k-vertex graph of maximum degree 4 is bounded by $(\frac{1}{3} + \epsilon_k)k$, where $\lim_{k\to\infty} \epsilon_k = 0$.

Corollary

For every fixed integer k, k-OPT OPTIMIZATION can be solved in time $O(n^{(1/3+\epsilon_k)k})$, where $\lim_{k\to\infty} \epsilon_k = 0$.

One more idea: bucketing

Divide the n edges of the Hamiltonian cycle into $n^{1/4}$ buckets of size $s = n^{3/4}$.



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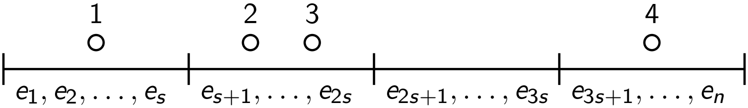

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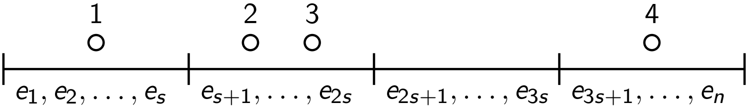

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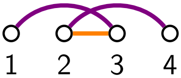

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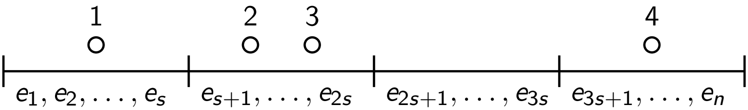

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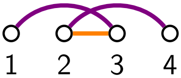

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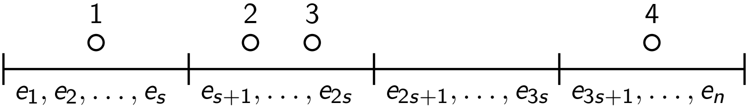

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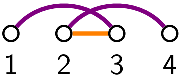

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- Dynamic programming works faster, in time $O(n^{\frac{3}{4}(\mathrm{tw}(D_{M,b})+1)})$
- Price: many bucket assignments to consider.

The $O(n^{(1/4+\epsilon_k)k})$-time algorithm

Plugging in the bucketing idea gives our main result (calculations skipped).

Theorem

For every fixed integer k, k-OPT OPTIMIZATION can be solved in time $O(n^{(1/4+\epsilon_k)k})$, where $\lim_{k\to\infty} \epsilon_k = 0$.

Part II: Practice

(joint work with Marek Cygan and Kamil Żyła)

A new heuristic based on theory

(k, t)-OPT heuristic

For every connection pattern M, find the best k-move, restricted only to the k-moves with dependence graph D_M of treewidth at most t.

Some statistics

tw	$k = 2$	3	4	5	6	7	8	9
1	1	0	1	0	1	0	1	0
2		1	4	11	37	106	334	1004
3			1	11	90	645	4423	29234
4				0	2	71	1444	22303
5					0	0	0	11

Some thoughts

Possible goals

- (minor:) show an improvement over 2-OPT, 3-OPT,
- (major:) add as an element of a state-of-the-art solver, check if it helps.

Some ideas

- A question to address: How one should control k, t (bound on treewidth) and n (length of a fragment of the tour) during the whole local search process? (Increase parameters when stuck?)
- Make sure space usage is relatively low (embed some edges by brute-force? use bucketing?)