Taxonomization of combinatorial optimization problems

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Dream: Optimal Optimization

Given a problem, tell me the best algorithm for it!!!

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Given an instance of a problem, tell me the best algorithm for it

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Taxonomize problems and instances

Taxonomize algorithms

Outline of the presentation

Taxonomization

- The most common taxonomy: P vs NP-complete
- More advanced: parameterized complexity

Challenges

- Problems have disparate definitions: distances, flows, etc..
- There are infinite number of functions

Infinite number of functions

The space of permutations

- Most heuristic algorithms do not use $f(x)$ but its ranking
- These algorithms behave the same in two functions f and g such that for all x and y if $f(x) > (<) f(y)$ then $g(x) > (<) g(y)$

Taxonomization

Any function can be seen as a permutation of the solutions

$f(\mathbf{x})$	$\mathbf{x}$
0	$(1, 0, 1)$
1	$(1, 0, 0)$
2	$(0, 1, 1)$
7	$(1, 1, 0)$
13	$(0, 0, 1)$
22	$(1, 1, 1)$
40	$(0, 1, 0)$
100	$(0, 0, 0)$

$g(\mathbf{x})$	$\mathbf{x}$
15	$(1, 0, 1)$
25	$(1, 0, 0)$
53	$(0, 1, 1)$
69	$(1, 1, 0)$
93	$(0, 0, 1)$
122	$(1, 1, 1)$
140	$(0, 1, 0)$
200	$(0, 0, 0)$

Taxonomization

Any function can be seen as a permutation of the solutions

$f(\mathbf{x})$	$\mathbf{x}$	ranking
0	$(1,0,1)$	1
1	$(1,0,0)$	2
2	$(0,1,1)$	3
7	$(1,1,0)$	4
13	$(0,0,1)$	5
22	$(1,1,1)$	6
40	$(0,1,0)$	7
100	$(0,0,0)$	8

$g(\mathbf{x})$	$\mathbf{x}$	ranking
15	$(1,0,1)$	1
25	$(1,0,0)$	2
53	$(0,1,1)$	3
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The space of permutations

- Any injective function $f : \Omega \rightarrow \mathcal{R}$ can be considered as a permutation of the numbers $\{1, 2, \ldots, m\}$ with $|\Omega| = m$

- Expansion of a combinatorial optimization problem $\mathcal{P}$:

$$E_m(\mathcal{P}) \subset \Sigma_m$$

Interesting questions

- Given a problem $\mathcal{P}$, what is the set of rankings that it can generate, $E_m(\mathcal{P})$?

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Interesting questions

- Given a problem $\mathcal{P}$, what is the set of rankings that it can generate, $E_m(\mathcal{P})$?
- Given two problems $\mathcal{P}$ and $\mathcal{Q}$, which is set of permutations that can be generated by both problems? i.e. $E_m(\mathcal{P}) \cap E_m(\mathcal{Q})$
- Some rankings could be efficiently solved for some algorithms. Therefore knowing the rankings that can be produced by a problem could give us an idea of the goodness of an algorithm for that particular problem

Even more interesting questions?

- Is there a problem (with a closed form expression for the objective function) able to generate all the possible permutations depending on a polynomial number of parameters?

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- Is there a problem (with a closed form expression for the objective function) able to generate all the possible permutations depending on a polynomial number of parameters?
- Given two problems $\mathcal{P}$ and $\mathcal{Q}$, assume that $\mathcal{P}$ is defined using a number of parameters r and $\mathcal{Q}$ with r' such that $r > r'$. Let's also assume that $|E_m(\mathcal{P})| < |E_m(\mathcal{Q})|$. Is it possible to reparameterized $\mathcal{P}$ with a lower number of parameters?

Example: Linear ordering problem

Definition

Given a matrix $B = [b_{ij}]_{n \times n}$ of numbers, find a simultaneous permutation σ of the rows and columns of B, such that the sum of the elements above the main diagonal is maximized:

$$\sigma^* = \arg\max_{\sigma} f(\sigma) = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} b_{\sigma_i \sigma_j}$$

Equivalently, the sum of the elements below the main diagonal is minimized

Example: Linear ordering problem

	1	2	3	4	5
1	0	16	11	15	7
2	21	0	14	15	9
3	26	23	0	26	12
4	22	22	11	0	13
5	30	28	25	24	0

$\sigma = (1,2,3,4,5)$
$f(\sigma) = 138$

	2	3	1	4	5
2	0	14	21	15	9
3	23	0	26	26	12
1	16	11	0	15	7
4	22	11	22	0	13
5	28	25	30	24	0

$\sigma' = (2,3,1,4,5)$
$f(\sigma') = 158$

	5	3	4	2	1
5	0	25	24	28	30
3	12	0	26	23	26
4	13	11	0	22	22
2	9	14	15	0	21
1	7	11	15	16	0

$\sigma^* = (5,3,4,2,1)$
$f(\sigma^*) = 247$

Example: Linear ordering problem

	5	3	4	2	1
5	0	25	24	28	30
3	12	0	26	23	26
4	13	11	0	22	22
2	9	14	15	0	21
1	7	11	15	16	0

$$\sigma^* = (5, 3, 4, 2, 1)$$
$$f(\sigma^*) = 247$$

- If $\sigma^* = (5, 3, 4, 2, 1)$ is the optimum then Reverse$(\sigma^*) = (1, 2, 4, 3, 5)$ is the worst
- If σ is the k-th best, then Reverse(σ) si the k-th worst

Example: Linear ordering problem

	5	3	4	2	1
5	0	25	24	28	30
3	12	0	26	23	26
4	13	11	0	22	22
2	9	14	15	0	21
1	7	11	15	16	0

$\sigma^* = (5, 3, 4, 2, 1)$
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(1 2 3)
(2 1 3)
(2 3 1)
(1 3 2)
(3 1 2)
(3 2 1)

Example: Linear ordering problem

Conclusions

- The linear ordering problem can only create functions that are symmetric with respect to the operation *Reverse*
- It is possible to bound the number of possible functions (permutations) it can generate:

$$|E_{n!}(LOP)| \leq 2^{n/2} \frac{n}{2}!$$

- When n increases:

$$\lim_{n \to \infty} \frac{|E_{n!}(LOP)|}{|\Sigma_{n!}|} \leq \lim_{n \to \infty} \frac{2^{n/2} \frac{n}{2}!}{(n!)!} = 0$$

Example: Asymmetric TSP

Non-reverse cyclic ranking

- The ATSP generates a partial ranking of solutions
- Each solution has at least $n-1$ solutions with the same objective function value
- Example (n=4):

(1 2 3 4)	(4 1 2 3)	(3 4 1 2)	(2 3 4 1)
(4 1 3 2)	(2 4 1 3)	(3 2 4 1)	(1 3 2 4)
...	...	...	...

LOP ∩ ASTP

LOP

$$A = \begin{pmatrix} 0 & 4 & 1{,}5 & 0{,}5 \\ 1 & 0 & 9{,}5 & 0 \\ 2 & 4 & 0 & 8{,}5 \\ 3 & 2{,}5 & 3{,}5 & 0 \end{pmatrix}$$

ATSP

$$D = \begin{pmatrix} 0 & 1{,}7 & 7{,}1 & 8{,}5 \\ 8 & 0 & 1{,}6 & 7 \\ 6 & 9 & 0 & 1{,}5 \\ 1 & 2 & 8 & 0 \end{pmatrix}$$

$$|E_{n!}(LOP) \cap E_{n!}(ATSP)| \leq 2^{(n-1)!/2} \cdot \left(\frac{(n-1)!}{2}\right)!$$

L. Hernando, A. Mediburu and J.A. Lozano. *Characterising the Rankings Produced by Combinatorial Optimisation Problems and Finding their Intersections*. GECCO 2019.

Example: quadratic assignment problem

Quadratic Assignment Problem

Given two matrices of distances and flows $D = [d_{ij}]$ and $F = [f_{kl}]$ respectively calculate the permutation that maximises:

$$f(\sigma) = \sum_{i=1}^{n} \sum_{j=1}^{n} f_{ij} d_{\sigma(i)\sigma(j)}$$

Problems

- We could not find any regularity in the functions ranking
- For $n = 3$ all the permutations are obtained
- For $n = 4$, the space of functions $(4!)!$ is too big

Solution: Fourier Transform of the Symmetric Group???

Outline of the presentation

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Representation of a group

They are the equivalent to the sin/cos in the real line

A representation of a group Σ_n is a map $\rho : \Sigma_n \longrightarrow R^{d_\rho \times d_\rho}$ such that $\forall \sigma_1, \sigma_2 \in \Sigma_n, \rho(\sigma_1 \sigma_2) = \rho(\sigma_1) \cdot \rho(\sigma_2)$

$$\rho(\sigma) = \begin{bmatrix} \rho_{11}(\sigma) & \rho_{12}(\sigma) & \cdots & \rho_{1d_\rho}(\sigma) \\ \rho_{21}(\sigma) & \rho_{22}(\sigma) & \cdots & \rho_{2d_\rho}(\sigma) \\ \vdots & \vdots & \ddots & \vdots \\ \rho_{d_\rho 1}(\sigma) & \rho_{d_\rho 2}(\sigma) & \cdots & \rho_{d_\rho d_\rho}(\sigma) \end{bmatrix}$$

Examples of representations

Trivial representation

$$\rho_{(n)} : \Sigma_n \longrightarrow R^{1\times 1} \quad \text{such that} \quad \rho_{(n)}(\sigma) = 1$$

First-order permutation representation

map σ to its permutation matrix: $[\tau_{(n-1,1)}(\sigma)]_{ij} = 1\{\sigma(j) = i\}$

$$\tau_{(2,1)}(\varepsilon) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad \tau_{(2,1)}(1,2) = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad \tau_{(2,1)}(2,3) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

New representations

Equivalence

Given an invertible matrix C we can define a new representation departing from ρ_1:

$$\rho_2(\sigma) = C^{-1} \cdot \rho_1(\sigma) \cdot C$$

Direct Sum

$$\rho_1 \oplus \rho_2(\sigma) \triangleq \left[\begin{array}{c|c} \rho_1(\sigma) & 0 \\ \hline 0 & \rho_2(\sigma) \end{array}\right]$$

Irreducible Representations

The Fourier Transform

Given a function $f : \Sigma_n \longrightarrow \mathbb{R}$ and ρ a representation. The Fourier transform of f at ρ is:

$$\hat{f}_\rho = \sum_\sigma f(\sigma)\rho(\sigma)$$

The collection of Fourier Transforms at all irreducible representations of Σ_n form the Fourier Transform of f

Fourier Inversion Theorem

$$f(\sigma) = \frac{1}{|G|} \sum_\lambda d_{\rho_\lambda} Tr\left[\hat{f}^T_{\rho_\lambda} \cdot \rho_\lambda(\sigma)\right]$$

where λ indexes over the collection of irreducibles of Σ_n

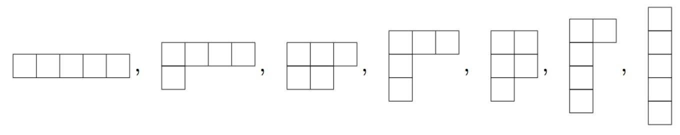
Irreducible representations

Partitions of n

Tuples of numbers that sum to n:

$$(5),\ (4,1),\ (3,2),\ (3,1,1),\ (2,2,1),\ (2,1,1,1),\ (1,1,1,1,1)$$

Ferrers diagrams:



Irreducible representations are indexed by the partitions of n.

Fourier transform of LOP

Theorem

If $f : \Sigma_n \longrightarrow \mathbb{R}$ is the objective function of a Linear Ordering Problem and $\lambda \vdash n$ is a partition, then the Fourier coefficients of f have the following properties:

1. $\hat{f}_\lambda = 0$ if $\lambda \neq (n), (n-1, 1), (n-2, 1, 1)$
2. $\hat{f}_\lambda$ has at most rank one for $\lambda = (n-1, 1), (n-2, 1, 1)$. Having rank one is equivalent to the fact that the matrix columns are proportional. For the mentioned partitions and a fixed dimension n, the proportions among the columns of $\hat{f}_\lambda$ are the same for all the instances.

Conjecture

The opposite is also true

Fourier transform of the asymetric TSP

Theorem

If $f : \Sigma_n \longrightarrow \mathbb{R}$ is the objective function of a Traveling Salesman Problem and $\lambda \vdash n$ is a partition, then the Fourier coefficients of f have the following properties:

1. $\hat{f}_\lambda = 0$ if $\lambda \neq (n), (n-2, 2), (n-2, 1, 1)$
2. $\hat{f}_\lambda$ has at most rank one for $\lambda = (n-2, 2), (n-2, 1, 1)$. In addition, for the mentioned partitions and a fixed dimension n, the proportions among the columns of $\hat{f}_\lambda$ are the same for all the instances.

Conjecture

The opposite is also true

Consequences

Reparameterization

- LOP: $n(n-1) \rightarrow 1 + (n-1) + \frac{(n-1)(n-2)}{2}$
- ATSP: $n(n-1) \rightarrow 1 + \frac{n(n-3)}{2} + \frac{(n-1)(n-2)}{2}$

Final remarks

- Many open questions, low number of answers
  - Which rankings/functions can be generated with some non-zero Fourier coefficients?
  - QAP: for $n = 4$ not all rankings can be generated
- We have settle up the first step in the process of taxonomization of combinatorial optimization problems

Collaboration

- Anne Elorza (UPV/EHU), Leticia Hernando (UPV/EHU)
- Josu Ceberio (UPV/EHU), Alex Mediburu (UPV/EHU)
- Roberto Santana (UPV/EHU)

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