Taxonomization of Combinatorial Optimization Problems in Fourier Space

Anne Elorza

Advisors: Leticia Hernando and Jose A. Lozano

Research area

Research area

- Optimization
- Permutation-based combinatorial optimization problems (COPs)

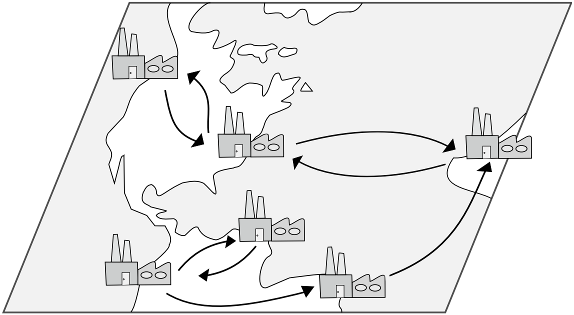
Permutation-based COPs

- Quadratic assignment problem (QAP)
- Linear ordernig problem (LOP)
- Traveling salesman problem (TSP)

Quadratic Assignment Problem

Interpretation

A set of n facilities have to be assigned to n locations with the goal of minimizing the cost, which is a function of the flows and distances.



Source: https://www.localsolver.com/docs/last/exampletour/qap.html

Quadratic Assignment Problem

Interpretation

A set of n facilities have to be assigned to n locations with the goal of minimizing the cost, which is a function of the flows and distances.

Mathematical definition

Given a distance matrix $A = [a_{ij}]$ and a flow matrix $A' = [a'_{ij}]$, minimize the following objective function:

$$f(\sigma) = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{\sigma(i)\sigma(j)} a'_{ij}.$$

Linear Ordering Problem

Interpretation

Given a matrix A, maximize the sum of the elements above the main diagonal when the rows and columns of A are jointly reordered.

Mathematical definition

Given a matrix $A = [a_{ij}]$, maximize the following objective function:

$$f(\sigma) = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} a_{\sigma(i)\sigma(j)}.$$

Linear Ordering Problem: example

	1	2	3
1	0	2	4
2	7	0	3
3	5	1	0

$f(\sigma) = 9$

	1	3	2
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3	5	0	1
2	7	3	0

$f(\sigma) = 7$

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3	1	5	0

$f(\sigma) = 14$

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$f(\sigma) = 15$

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$f(\sigma) = 8$

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$f(\sigma) = 13$

Linear Ordering Problem

Mathematical definition

Given a matrix $A = [a_{ij}]$, maximize the following objective function:

$$f(\sigma) = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} a_{\sigma(i)\sigma(j)}.$$

Particular case of the QAP

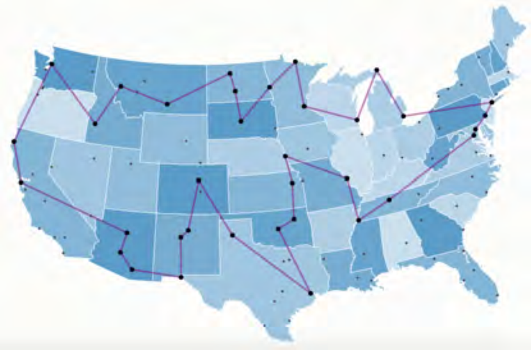
The LOP is a particular case of the QAP if

$$a'_{ij} = \begin{cases} 1 & \text{if } i < j \\ 0 & \text{otherwise} \end{cases}$$

Traveling Salesman Problem

Interpretation

Given *n* cities and the distances between them, find the shortest tour that passes exactly once through all of the cities.



Source: https://blog.essaycorp.com/travelling-salesman-problem/

Traveling Salesman Problem

Interpretation

Given n cities and the distances between them, find the shortest tour that passes exactly once through all of the cities.

Mathematical definition

Given a distance matrix $A = [a_{ij}]$, minimize the following objective function:

$$f(\sigma) = a_{\sigma(n)\sigma(1)} + \sum_{i=1}^{n-1} a_{\sigma(i)\sigma(i+1)}.$$

Traveling Salesman Problem

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Given a distance matrix $A = [a_{ij}]$, minimize the following objective function:

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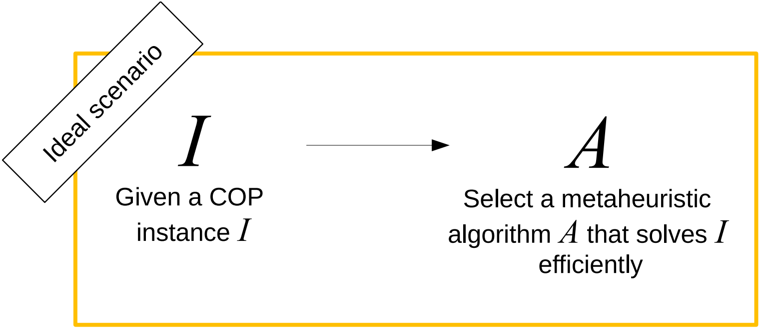
Particular case of the QAP

The TSP is a particular case of the QAP if

$$a'_{ij} = \begin{cases} 1 & \text{if } j = i+1 \text{ or } (i = n \text{ and } j = 1) \\ 0 & \text{otherwise} \end{cases}$$

Ideal scenario

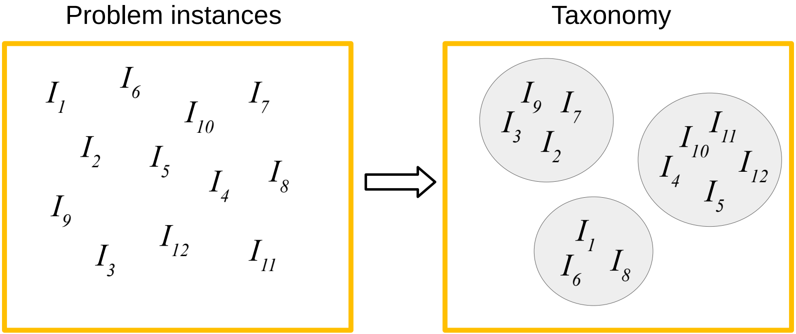
The behaviour of metaheuristic algorithms varies from problem to problem and even from instance to instance



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

Taxonomy

Final objective



Instances that can be solved efficiently by the same algorithms are grouped together

Initial questions and motivation

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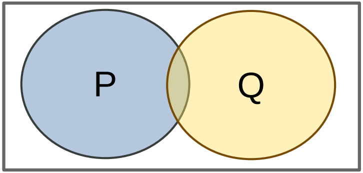
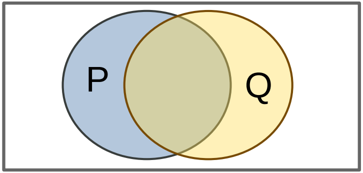
- Example:
  intersection between problems (in terms of objective functions).





Initial questions and motivation

- Is there a tool for comparing instances coming from different problems easily?
- We would like to look for properties that affect the beahaviour of algorithms and that are shared by instances of different problems.
- Example: intersection between problems (in terms of objective functions).
- Is there a framework that puts instances of different problems in the same terms?

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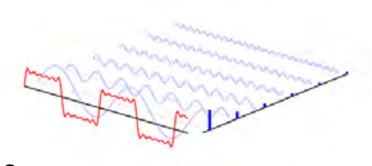
- Is there a framework that puts instances of different problems in the same terms?

SOLUTION: USE THE FOURIER TRANSFORM

Classic Fourier transform

Fourier coefficients

$$\begin{cases} a_0 = \frac{1}{L}\int_{-L}^{L} f(x)dx \\ a_n = \frac{1}{L}\int_{-L}^{L} f(x)\cos\left(\frac{n\pi x}{L}\right)dx \\ b_n = \frac{1}{L}\int_{-L}^{L} f(x)\sin\left(\frac{n\pi x}{L}\right)dx \end{cases}$$



Source: https://pgfplots.net/fourier-transform/

Decomposition of f

$$f(x) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n \cos\left(\frac{n\pi x}{L}\right) + \sum_{n=1}^{\infty} b_n \sin\left(\frac{n\pi x}{L}\right)$$

Fourier transform over the symmetric group

Base functions

Irreducible representations of the symmetric group.

- Matrix-valued functions.
- The number of irreducible representations of Σ_n is the number of partitions of n.

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Partition of n

A partition of a number n is a tuple that sums to n.

Example ($n = 5$)

Partitions of 5:

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

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Irreducible representations of Σ_5:

$$\rho_{(5)}, \rho_{(4,1)}, \rho_{(3,2)}, \rho_{(3,1,1)}, \rho_{(2,2,1)}, \rho_{(2,1,1,1)}, \rho_{(1,1,1,1,1)}.$$

Fourier transform over the symmetric group

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Example: $\rho_{(n)}$

$\rho_{(n)} : \Sigma_n \longrightarrow \mathbb{R}^{1\times 1}$ is the constant function $\rho_{(n)}(\sigma) = (1)$.

Fourier transform over the symmetric group

Base functions

Irreducible representations of the symmetric group.

- Matrix-valued functions.
- The number of irreducible representations of Σ_n is the number of partitions of n.

Example: $\rho_{(2,1)}$

$$\rho_{(2,1)}(1,2,3) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad \rho_{(2,1)}(1,3,2) = \begin{bmatrix} 1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{bmatrix}$$

$$\rho_{(2,1)}(2,1,3) = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \qquad \rho_{(2,1)}(2,3,1) = \begin{bmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{bmatrix}$$

$$\rho_{(2,1)}(3,1,2) = \begin{bmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{bmatrix} \qquad \rho_{(2,1)}(3,2,1) = \begin{bmatrix} 1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{bmatrix}$$

Fourier transform over the symmetric group

Fourier coefficients

Given a function $f : \Sigma_n \longrightarrow \mathbb{R}$, the Fourier coefficient associated with partition λ is:

$$\hat{f}_\lambda = \sum_\sigma f(\sigma) \cdot \rho_\lambda(\sigma).$$

The collection of all Fourier coefficients is the Fourier transform of f.

Fourier transform over the symmetric group

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Fourier inversion theorem

$$f(\sigma) = \frac{1}{|\Sigma_n|} \sum_\lambda d_{\rho_\lambda} Tr[\hat{f}_\lambda \cdot \rho_\lambda(\sigma)]$$

Fourier transform over the symmetric group

Interpretation

Coefficient $\hat{f}_{(n)}$

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

Directly related to the mean value of f.

Other coefficients

If $f = p$ (probability),

- $\hat{p}_{(n-1,1)}$ captures information about first order marginals: $p(\sigma : \sigma(i) = j)$.
- $\hat{p}_{\lambda}$ $(\lambda \neq (n), (n-1,1))$ captures information about higher order marginals.

Characterization of the LOP

Example

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Fitness function:

$$f(1,2,3) = 9$$
$$f(1,3,2) = 7$$
$$f(2,1,3) = 14$$
$$f(2,3,1) = 15$$
$$f(3,1,2) = 8$$
$$f(3,2,1) = 13$$

Fourier transform (alternative representation of f):

$$\hat{f}_{(3)} \approx (66) \qquad \hat{f}_{(2,1)} \approx \begin{pmatrix} -6.5 & -11.3 \\ 0.9 & 1.5 \end{pmatrix} \qquad \hat{f}_{(1,1,1)} \approx (-2).$$

Characterization of the LOP

Structure for low dimensions

Structure of the example

$\hat{f}_{(3)}$ and $\hat{f}_{(1,1,1)}$ are arbitrary, while

$$\hat{f}_{(2,1)} \approx \begin{pmatrix} -6.5 & -11.3 \\ 0.9 & 1.5 \end{pmatrix} \approx \begin{pmatrix} -6.5 & \sqrt{3} \cdot (-6.5) \\ 0.9 & \sqrt{3} \cdot 0.5 \end{pmatrix}.$$

Structure when $n = 3$

$\hat{f}_{(3)}$ and $\hat{f}_{(1,1,1)}$ are arbitrary, while

$$\hat{f}_{(2,1)} = \begin{bmatrix} | & | \\ \mathbf{x} & \sqrt{3}\mathbf{x} \\ | & | \end{bmatrix}$$

Characterization of the LOP

Structure for low dimensions

Structure when $n = 4$

- $\hat{f}_{(4)}$ is arbitrary
- $\hat{f}_{(3,1)}$ and $\hat{f}_{(2,1,1)}$ are rank-1:

$$\hat{f}_{(3,1)} = \begin{bmatrix} | & | & | \\ \mathbf{x} & \sqrt{3}\mathbf{x} & \sqrt{6}\mathbf{x} \\ | & | & | \end{bmatrix} \qquad \hat{f}_{(2,1,1)} = \begin{bmatrix} | & | & | \\ \sqrt{2}\mathbf{y} & \mathbf{y} & \sqrt{3}\mathbf{y} \\ | & | & | \end{bmatrix}$$

- $\hat{f}_{(2,2)}, \hat{f}_{(1,1,1,1)} = 0$

Characterization of the LOP

Theorem

Theorem

If $f : \Sigma_n \longrightarrow \mathbb{R}$ is the objective function of an LOP instance, then its FT has 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.*
3. *For* $\lambda = (n-1, 1), (n-2, 1, 1)$ *and a fixed dimension* n*, the proportions among the columns of* $\hat{f}_\lambda$ *are the same for all the instances.*

Characterization of the LOP

Reciprocal implication

Theorem

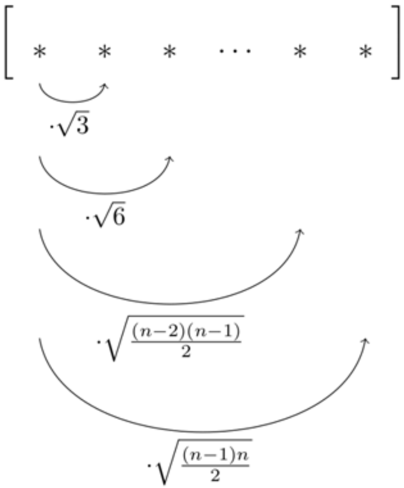
If f is an LOP function with non-null $(n-1,1)$ and $(n-2,1,1)$ Fourier coefficients, and a function g satisfies the conditions mentioned in the previous theorem, that is,

1. $\hat{g}_\lambda = 0$, *for* $\lambda \neq (n), (n-1,1), (n-2,1,1)$.
2. $\hat{g}_{(n-1,1)}$ *is 0 or rank-one with the same column proportions as* $\hat{f}_{(n-1,1)}$.
3. $\hat{g}_{(n-2,1,1)}$ *is 0 or rank-one with the same column proportions as* $\hat{f}_{(n-2,1,1)}$.

Then, g is the objective function of an LOP instance.

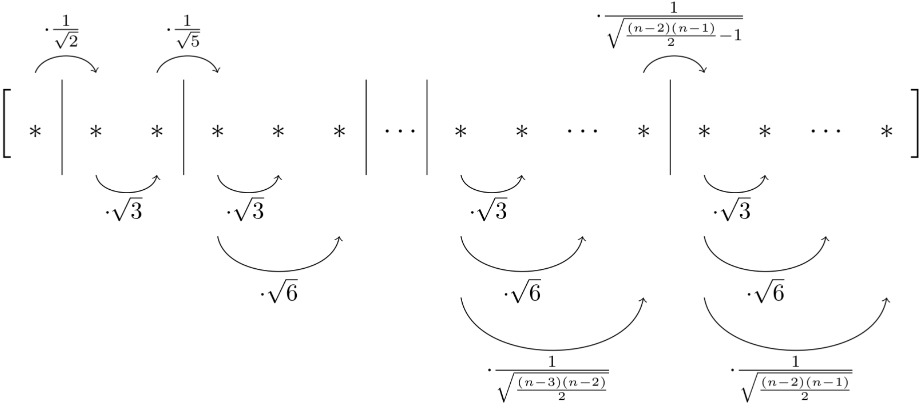
Characterization of the LOP

Proportions of coefficient $(n-1,1)$



Characterization of the LOP

Proportions of coefficient $(n-2,1,1)$



Characterization of the TSP

Structure for low dimensions

Structure when $n = 4$

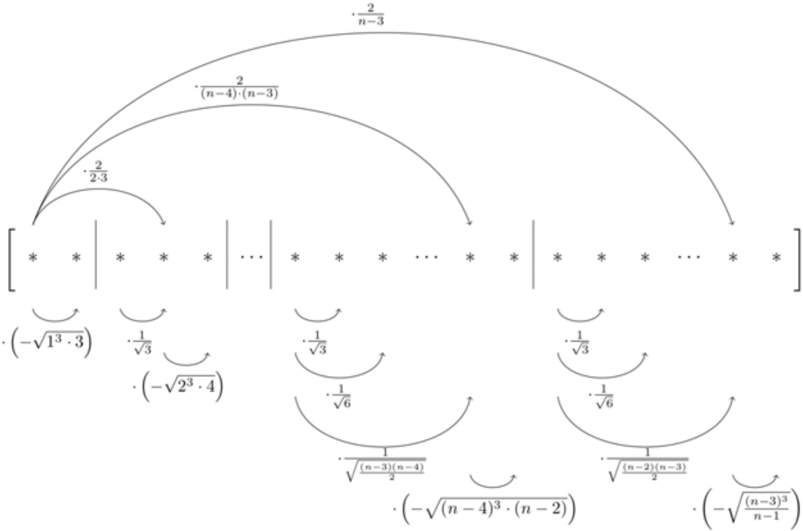
- $\hat{f}_{(4)}$ is arbitrary.
- $\hat{f}_{(2,2)}$ and $\hat{f}_{(2,1,1)}$ are rank-1:

$$\hat{f}_{(2,2)} = \begin{bmatrix} | & | \\ \mathbf{x} & -\frac{1}{\sqrt{3}}\mathbf{x} \\ | & | \end{bmatrix} \qquad \hat{f}_{(2,1,1)} = \begin{bmatrix} | & | & | \\ \mathbf{y} & \sqrt{\frac{1}{2}}\mathbf{y} & \sqrt{\frac{3}{2}}\mathbf{y} \\ | & | & | \end{bmatrix}$$

- $\hat{f}_{(3,1)}, \hat{f}_{(1,1,1,1)} = 0$.
- If the TSP is symmetric, $\hat{f}_{(2,1,1)} = 0$.

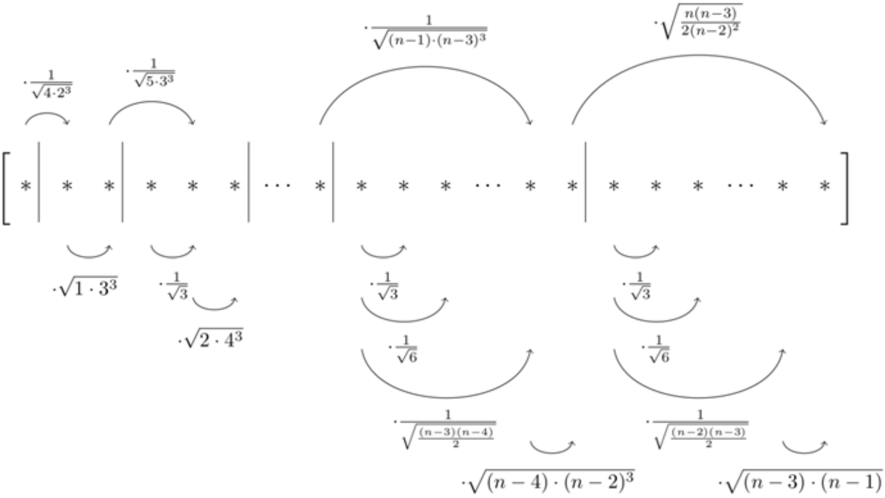
Characterization of the TSP

Proportions of coefficient $(n-2,2)$



Characterization of the TSP

Proportions of coefficient $(n-2,1,1)$



Characterization of the QAP

Theorem

If $f : \Sigma_n \longrightarrow \mathbb{R}$ is the objective function of a QAP instance, then its FT has the following properties:

1. $\hat{f}_\lambda = 0$, *if* $\lambda \neq (n), (n-1,1), (n-2,2), (n-2,1,1)$.
2. $\hat{f}_\lambda$ *has at most rank one for* $\lambda = (n-2,2), (n-2,1,1)$.
3. $\hat{f}_\lambda$ *has at most rank two for* $\lambda = (n-1,1)$.

- The reciprocal is also true (proved).

Characterizations: summary

Non-zero Fourier coefficients when $n = 5$:

COPs	Fourier coefficients						
	(5)	(4, 1)	(3,2)	(3,1,1)	(2,2,1)	(2,1,1,1)	(1,1,1,1,1)
LOP	✓	✓		✓			
STSP	✓		✓				
TSP	✓		✓	✓			
QAP	✓	✓	✓	✓			

- As n grows, the number of Fourier coefficients grows, but these problems still have at most 4 non-zero coefficients.

Consequences of the characterizations

Intrinsic dimensions of the problems

Number of parameters needed to define the different problems:

COP	Usual representation	Fourier representation
LOP	$n^2 - n$	$\frac{n^2-n}{2} + 1$
TSP	$n(n-1)$	$(n-1)(n-2)$
STSP	$\frac{n(n-1)}{2}$	$\frac{(n-1)(n-2)}{2}$
QAP	$2(n^2 - n)$	$2(n^2 - n) - 7$

Consequences of the characterizations

Intersections between problems

Consider a COP as a set of objective functions, then:

- The intersection between the LOP and the symmetric TSP is the set of constant functions.

COPs	Fourier coefficients						
	(n)	$(n$-1, 1)	$(n$-2,2)	$(n$-2,1,1)	$(n$-2,2,1)	…	(1,1,...,1)
LOP	✓	✓		✓			
STSP	✓		✓				

Consequences of the characterizations

Intersections between problems

Consider a COP as a set of objective functions, then:

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- The intersection between the LOP and the TSP is the set of constant functions.

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LOP	✓	✓		✓			
TSP	✓		✓	✓			

Consequences of the characterizations

Intersections between problems

Consider a COP as a set of objective functions, then:

- The intersection between the LOP and the symmetric TSP is the set of constant functions.
- The intersection between the LOP and the TSP is the set of constant functions.
- The intersection between the LOP/(symmetric)TSP and the QAP is the LOP/(symmetric)TSP.

Breaking down the LOP

Consider the problem composed by those objective functions with a given coefficient equal to 0.

What happens if coefficient $(n-2,1,1)$ is 0?

- The problem is P (proved)
- We implemented a polynomial algorithm

What happens if coefficient $(n-1,1)$ is 0?

The problem is NP-hard (proved)

Conclusion

Many interesting open questions:

- Which is the minimal Fourier representation for a problem to be NP-hard?

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- Other problems?

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- Relation between the Fourier decomposition and elementary lanscape decomposition?
- Other problems?
- Taxonomy

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