Where the Really Hard Quadratic Assignment Problems Are: the QAP-SAT instances

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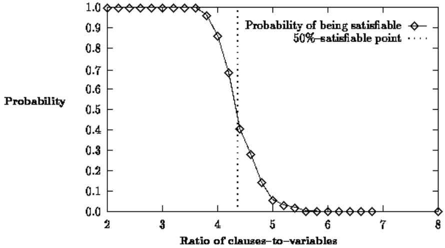
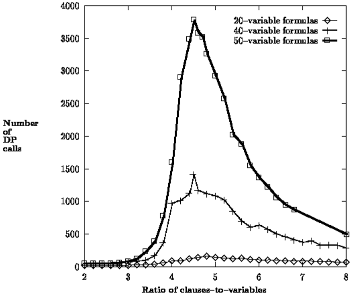
EvoCOP conference,
April, 5, 2024

Phase transition, and solvers : SAT problems

"Where the Really Hard Problems Are", Cheeseman *et al.*, IJCAI-91

Mitchell, Selman & Levesque, AAAI-92





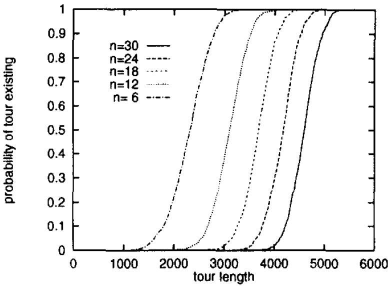
Phase transition in decision problems :

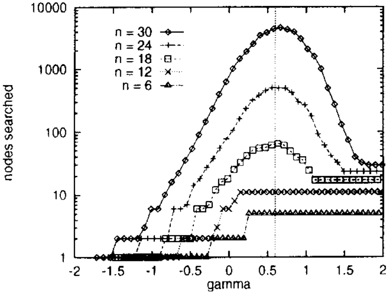
- Satisfiability drops quickly around a phase parameter transition
- Link to optimization difficulty

For rnd. SAT, ratio clause-to-variable. For 3-SAT, $\alpha = m/n \approx 4.3$

Phase transition : TSP problem

TSP phase transition, Gent & Walsh, AI, 1996





Phase transition in optimization problems : $\Pr(\exists \sigma : f_{TSP}(\sigma) \leq \ell)$

- Satisfiability drops quickly around a phase parameter transition
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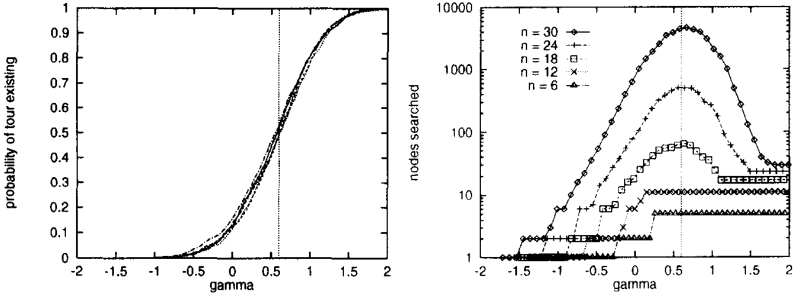
For random TSP, n cities in area A, $\gamma = (\frac{\ell}{\sqrt{nA}} - 0.78)n^{1/1.5}$

Phase transition : TSP problem

TSP phase transition, Gent & Walsh, AI, 1996



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Objectives of this work

Quadratic Assignement Problem (QAP)

- Well-known problem in evolutionary computation
- Very challenging problem

Goals

- Show a phase transition in "pure" QAP
  First phase transition to our best knowledge
- Benchmark of easy/difficult instances
- Propose a design principle to better understand difficulty in QAP

Definition : QAP [Koopmans, 1957]

Assignment problem (minimization), quadratic costs :

$$\forall \sigma \in \mathcal{S}_n,\ \ Q_{A,B}(\sigma) = \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} B_{\sigma_i \sigma_j} = \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} B_{ij}^{\sigma}$$

$\mathcal{S}_n$: Search space, symmetric group of dim. n (permutations)
A, and B matrices $n \times n$,
A_{ij} "flow" (cost) between objects i, and j,
B_{ij} "distance" (cost) between positions i, and j

Here, $A_{ij} \geq 0$, and $B_{ij} \geq 0$
B not necessary distance matrix, not necessary symmetric,
but $B_{ii} = 0$, and $A_{ii} = 0$.

QAP benchmark instances

- Many applications in real-world [3]
- Many benchmark instances :
  to understand difficulty, and design better algorithm

QAPLib [1]

Collection of real-world small size, artificial larger ones

- Taillard instances (*Taia*, and *Taib*)
- *Taie* and *Dre* instances : difficult for metaheuristics [5]
- Stützle *et al.* instances : flow dominance and sparsity [12]

Problems difficulty in QAP

Matrices features

Flow dominance [14] : imbalance in matrices ("variance" in matrix)
Sparsity [11] : number of zero-entries as a proportion of the n^2

Fitness landscape features

Correlation length, fitness-distance correlation [9]
Information metrics estimate with random walks [10]
Autocorrelation and plateaus size $\sim$ number of similar values [13]
Local Optima Network [4]

Fourier features

B&Bound which operates in the Fourier space [8]
Elementary landscape decomposition [2] Fourier decomposition [6]

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Surprisingly, features are tuned for each matrix independently

From SAT to QAP-SAT

Phase transition in rnd. SAT/MAX-SAT

$f(x) = \sum_{i=1}^{m} c_i(x_{i_1}, x_{i_2}, x_{i_3})$: sum of clauses *i.e.* low dim. problems

One clause is satisfied when $c(x_{i_1}, x_{i_2}, x_{i_3}) = 1$, the upper bound

When the num. of clauses increases, transition to unsatisfiability

Difficulties with QAP

- QAP space is **not** a vector space. Bi-linear property :

$$\begin{aligned} Q_{A+A',B+B'} &= Q_{A,B} + Q_{A,B'} + Q_{A',B} + Q_{A',B'} \\ \text{but,} \quad Q_{A+A',B} &= Q_{A,B} + Q_{A',B} \end{aligned}$$

- Sub-spaces of $\mathcal{S}_n$:

  Subspaces are **not** isomorphic to $\mathcal{S}_3$, given by (i_1, i_2, i_3),
  but, depend on other values/objects $\{1, \ldots, n\}$

Design components : A-clauses and B-clauses

A-clause and B-clause of size $k > 0$

A-clause : $\exists V_A \subset [n]$ of size k s. t. : $\forall i \in [n]\ A_{ii} = 0$, $\forall (i,j) \in V_A^2,\ i \neq j,\ A_{ij} > 0$, and $\forall (i,j) \notin V_A^2,\ A_{ij} = 0$.

B-clause : $\exists V_B \subset [n]$ of size k s. t. : $\forall i \in [n]\ B_{ii} = 0$, $\forall (i,j) \in V_B^2,\ i \neq j,\ B_{ij} = 1$, and $\forall (i,j) \notin V_B^2,\ B_{ij} = \textsc{m}$.

$V_A = \{2, 3, 5\}$

$$A_3 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 2 \\ 0 & 2 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 1 & 0 & 0 \end{bmatrix} \qquad A^{(3)} = \begin{bmatrix} 0 & 1 & 2 \\ 2 & 0 & 1 \\ 3 & 1 & 0 \end{bmatrix}$$

$V_B = \{1, 2, 5\}$

$$B_3 = \begin{bmatrix} 0 & 1 & \textsc{m} & \textsc{m} & 1 \\ 1 & 0 & \textsc{m} & \textsc{m} & 1 \\ \textsc{m} & \textsc{m} & 0 & \textsc{m} & \textsc{m} \\ \textsc{m} & \textsc{m} & \textsc{m} & 0 & \textsc{m} \\ 1 & 1 & \textsc{m} & \textsc{m} & 0 \end{bmatrix} \qquad B^{(3)} = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}$$

Design components : aggregation of clauses

A is composed of m A-clauses when :

$A = A_1 + \ldots + A_m$ with $A_1, \ldots, A_m$ A-clauses

nota : $Q_{A_i,B}$ is a clause

B is composed of m_1 B-clauses when :

$B = B_1 \odot \ldots \odot B_{m_1} \odot C$ with $B_1, \ldots, B_{m_1}$ B-clauses,

$C_{ij} > 1$, $C_{ii} = 0$. $\odot$ minimum element by element

$$A = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 2 \\ 0 & 2 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 1 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 2 \\ 0 & 0 & 2 & 0 & 1 \\ 0 & 0 & 3 & 1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 2 \\ 0 & 2 & 0 & 1 & 3 \\ 0 & 0 & 2 & 0 & 1 \\ 0 & 3 & 4 & 1 & 0 \end{bmatrix}$$

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$$B = \begin{bmatrix} 0 & 1 & M & M & 1 \\ 1 & 0 & M & M & 1 \\ M & M & 0 & M & M \\ M & M & M & 0 & M \\ 1 & 1 & M & M & 0 \end{bmatrix} \odot \begin{bmatrix} 0 & 1 & 1 & M & M \\ 1 & 0 & 1 & M & M \\ 1 & 1 & 0 & M & M \\ M & M & M & 0 & M \\ M & M & M & M & 0 \end{bmatrix} \odot C = \begin{bmatrix} 0 & 1 & 1 & 2 & 1 \\ 1 & 0 & 1 & 2 & 1 \\ 1 & 1 & 0 & 3 & 2 \\ 3 & 2 & 2 & 0 & 5 \\ 1 & 1 & 2 & 4 & 0 \end{bmatrix}$$

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QAP-SAT

$Q_{A,B}$ is a *QAP-SAT* with m A-clauses and m_1 B-clauses when :

A is composed of m A-clauses, and

B is composed of m_1 B-clauses

Satisfiability

Lower bound of single clauses (A-clause, B-clause) :

$$Q_{A^{(3)},B^{(3)}}(\sigma) = \begin{bmatrix} 0 & 1 & 2 \\ 2 & 0 & 1 \\ 3 & 1 & 0 \end{bmatrix} . \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix} = 10$$

Satisfiability

Lower bound of single clauses (A-clause, B-clause) :

$$Q_{A_3,B_3}(\sigma = (13)) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 2 \\ 0 & 2 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 1 & 0 & 0 \end{bmatrix} . \begin{bmatrix} 0 & 1 & \text{M} & \text{M} & 1 \\ 1 & 0 & \text{M} & \text{M} & 1 \\ \text{M} & \text{M} & 0 & \text{M} & \text{M} \\ \text{M} & \text{M} & \text{M} & 0 & \text{M} \\ 1 & 1 & \text{M} & \text{M} & 0 \end{bmatrix}^{\sigma}$$

$$= \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 2 \\ 0 & 2 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 1 & 0 & 0 \end{bmatrix} . \begin{bmatrix} 0 & \text{M} & \text{M} & \text{M} & \text{M} \\ \text{M} & 0 & 1 & \text{M} & 1 \\ \text{M} & 1 & 0 & \text{M} & 1 \\ \text{M} & \text{M} & \text{M} & 0 & \text{M} \\ \text{M} & 1 & 1 & \text{M} & 0 \end{bmatrix} = 10$$

Indeed any σ s.t. $\sigma(\{2,3,5\}) = \{1,2,5\}$, is an optimal solution

Satisfiability

Lower bound of single clauses (A-clause, B-clause) :

$$Q_{A_3,B_3}(\sigma = (13)) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 2 \\ 0 & 2 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 1 & 0 & 0 \end{bmatrix} . \begin{bmatrix} 0 & 1 & M & M & 1 \\ 1 & 0 & M & M & 1 \\ M & M & 0 & M & M \\ M & M & M & 0 & M \\ 1 & 1 & M & M & 0 \end{bmatrix}^{\sigma}$$

$$= \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 2 \\ 0 & 2 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 1 & 0 & 0 \end{bmatrix} . \begin{bmatrix} 0 & M & M & M & M \\ M & 0 & 1 & M & 1 \\ M & 1 & 0 & M & 1 \\ M & M & M & 0 & M \\ M & 1 & 1 & M & 0 \end{bmatrix} = 10$$

Clause $Q_{A_i,B}$ satisfied when the lb is reached : $\exists\sigma \; Q_{A_i,B}(\sigma) = \text{lb}(A_i)$

$Q_{A,B}$ satisfied when all clauses are satisfied : $\exists\sigma \; Q_{A,B}(\sigma) = m \; \text{lb}(A_i)$

Example of satisfiability : $m = 2$, and $m_1 = 2$

$$A = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 2 \\ 0 & 2 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 1 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 2 \\ 0 & 0 & 2 & 0 & 1 \\ 0 & 0 & 3 & 1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 2 \\ 0 & 2 & 0 & 1 & 3 \\ 0 & 0 & 2 & 0 & 1 \\ 0 & 3 & 4 & 1 & 0 \end{bmatrix}$$

$$B = \begin{bmatrix} 0 & 1 & M & M & 1 \\ 1 & 0 & M & M & 1 \\ M & M & 0 & M & M \\ M & M & M & 0 & M \\ 1 & 1 & M & M & 0 \end{bmatrix} \odot \begin{bmatrix} 0 & 1 & 1 & M & M \\ 1 & 0 & 1 & M & M \\ 1 & 1 & 0 & M & M \\ M & M & M & 0 & M \\ M & M & M & M & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 1 & M & 1 \\ 1 & 0 & 1 & M & 1 \\ 1 & 1 & 0 & M & M \\ M & M & M & 0 & M \\ 1 & 1 & M & M & 0 \end{bmatrix}$$

$$B^\sigma = \begin{bmatrix} 0 & M & M & M & M \\ M & 0 & 1 & M & 1 \\ M & 1 & 0 & M & 1 \\ M & M & M & 0 & M \\ M & 1 & 1 & M & 0 \end{bmatrix} \odot \begin{bmatrix} 0 & M & M & M & M \\ M & 0 & M & M & M \\ M & M & 0 & 1 & 1 \\ M & M & 1 & 0 & 1 \\ M & M & 1 & 1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & M & M & M & M \\ M & 0 & 1 & 1 & 1 \\ M & 1 & 0 & 1 & 1 \\ M & 1 & 1 & 0 & 1 \\ M & 1 & 1 & 1 & 0 \end{bmatrix}$$

$$\sigma = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 4 & 5 & 2 & 3 & 1 \end{pmatrix} \quad Q_{A,B}(\sigma) = 20, \; Q_{A,B} \text{ is satisfiable}$$

Random QAP-SAT instances

QAP-k-SAT

All clauses have the same size k

For each clause (A-clauses, and B-clauses),
- Select randomly and independently k different variables
- Use $A_{(3)}$, and $B_{(3)}$ to complete the clause indexed by the var.

Complete matrix B values $d > 1$ s. t. proportions follow $p_d = p_1^d$

$V_A = \{2, 3, 5\}$, $V_B = \{1, 2, 5\}$

$$A^{(3)} = \begin{bmatrix} 0 & 1 & 2 \\ 2 & 0 & 1 \\ 3 & 1 & 0 \end{bmatrix} \quad B^{(3)} = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}$$

Python code (generator), instances, data :

`https://gitlab.com/verel/qap-sat`

Experimental setup

Instance generation

	Description	Values
n	Problem dimension	$\{8, 9, \ldots, 17\}$ $\{18, 19\}$
k	Size of clause	3
m_1	Num. of B-clauses	$\{3, 6, 9, \ldots, 27\}$ $\{3, 9, 15, \ldots, 57\}$
m	Num. of A-clauses	$\{1, 2, 3, \ldots, 40\}$ $\{1, 3, 9, 15, \ldots, 57, 63\}$

50 instances for each parameter triplet (n, m_1, m)

Branch & Bound algorithm by Fujii *et al.* [7]

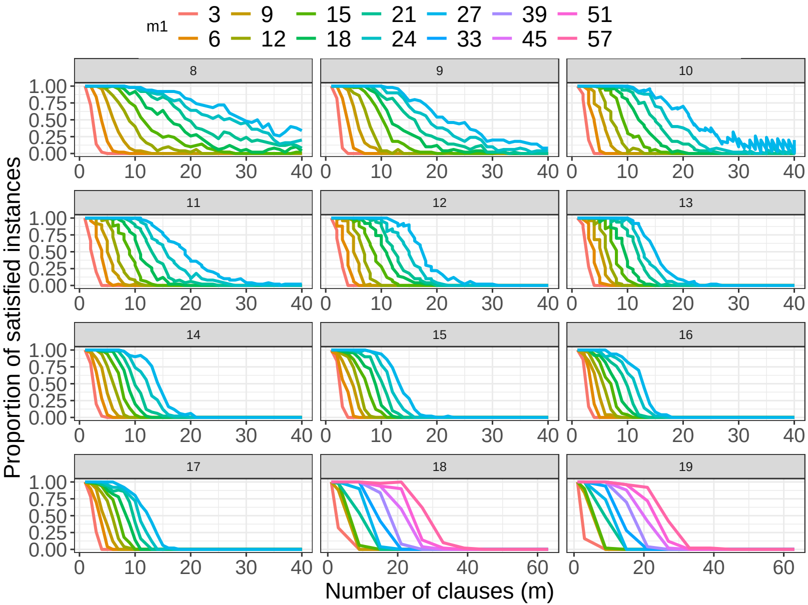
Lagrangian doubly non-negative relaxation and Newton-bracketing MATLAB code available.

Notice that : full enumeration is possible for $n \leq 13$

Tabu search

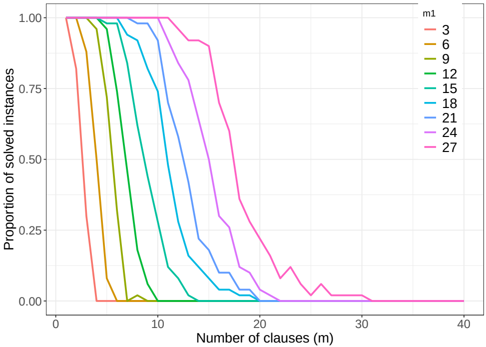
Baseline "classical" Robust Tabu Search of Taillard

Proportion of satisfiable instances



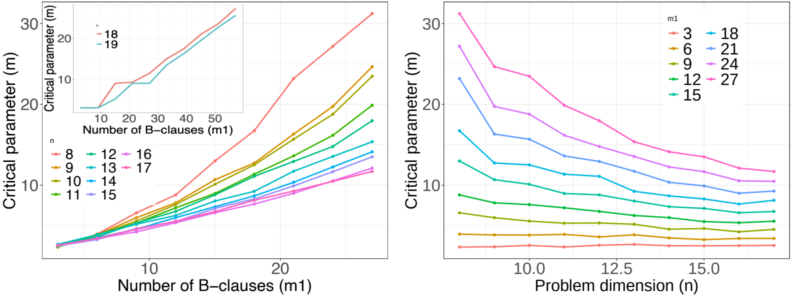
Proportion of satisfiable instances

$n = 12$



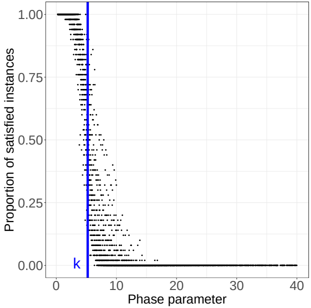
- When m_1 is fixed, fast drop "around" $m \approx m_1$
- Same shape for every problem dim. n
- Faster drop when n is larger

Phase transition parameter



- Critical parameter m_c of logistic model, estimated by logit regression (high R^2 values > 0.9)
- Regression of m_1 when n is given : $m_c = \beta_0 + \beta_1 m_1 + \epsilon$
R^2 over 0.97 Slope β_1 decreases with n

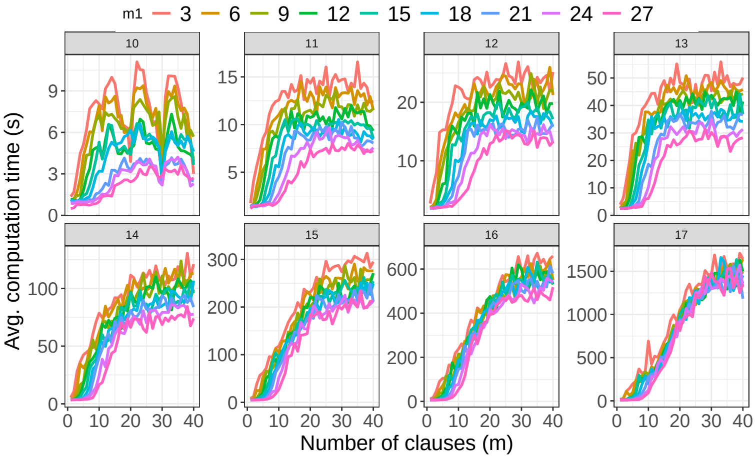
Phase transition parameter



$$m_c = k n^{\alpha_1} m_1^{\alpha_2} + \epsilon$$

Adding a scaling factor n^{α_1} (such as TSP)
Estimation using $\log(m_c)$, $R^2 = 0.947$ ($R^2 = 0.898$ without log)
$\alpha_1 = -0.75999$: negative $\in [-1/\sqrt{n}$, and $-1/n]$
$\alpha_2 = 0.90365$: close to 1. $\log(k) = 1.65453$
Hypothesise on phase trans. param. : $m \; n^{-\alpha_1} m_1^{-\alpha_2}$

B & B computation time

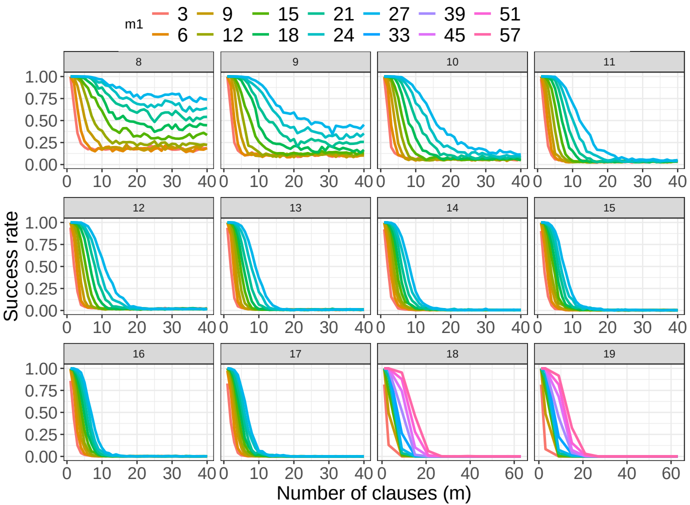


Sigmoid regression model : $t(m) = \frac{L}{1+e^{-r(m-m_t)}}$

$L \approx \gamma(2.043 + 0.476(n-8))$ max. value, r rate, and m_t inflexion

Median value regressions of $R^2 = 0.969$

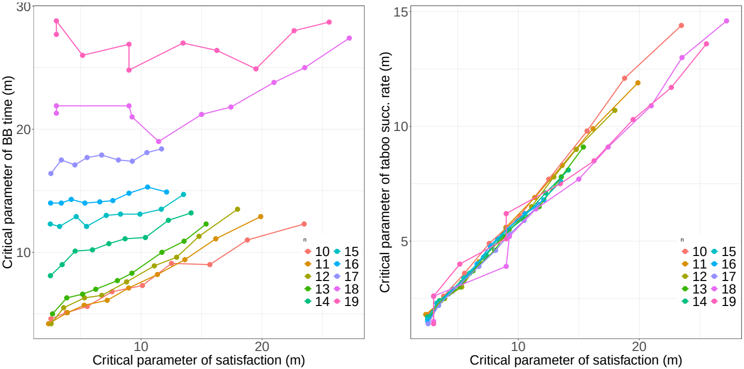
Tabu search success rate



Analysis using sigmoid regression model :

High regression quality again, follow the shape of m_c

Critical parameter m_c *v.s.* B & B, and Tabu critical param.



High linear correlation between m_c, and critical param. of algorithm
Correlation for tabu search : seems not depend of problem dim. n

Conclusions

Summary

- Propose new QAP benchmark :
  Difficulty related to the link between A, and B matrices
- Show phase transition across the instances
- Hypothesis of phase transition parameter model

Perspectives

- Large instances
- Compare QAP-SAT with QAPLib,
  decompose real-world instances into "clauses"
- Fitness landscape analysis, theoretical investigation
  QAP-2-SAT (graph matching), etc.
- Different k, clauses, relax the satisfiability condition, etc.

$$A^{(3)} = \begin{bmatrix} 0 & 1 & 2 \\ 2 & 0 & 1 \\ 3 & 1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & ? & ? \\ ? & 0 & ? \\ ? & ? & 0 \end{bmatrix} \quad B^{(3)} = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 2 \\ 1 & 0 & 1 \\ 2 & 1 & 0 \end{bmatrix}$$

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