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# To Lay Out or Not To Lay Out?

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# To Lay Out or Not To Lay Out?

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**Abstract.** This paper seeks to raise awareness of some negative phenomena in science. It happens more and more frequently that somebody carries out research in one field but finds that the results are not strong enough for publication and then submits them to be published in a related but not identical field as an application. The Quadratic Assignment Problem (QAP) is known as one of the most difficult problems in integer programming, and it has a nice combinatorial formulation. Therefore, it is a suitable experimental field for many algorithmic ideas including artificial intelligence methods. On the other hand, these methods must compete with the special methods of QAP. The latter are far better in many cases. Thus, the experimental methods cannot be published in their own right. Their authors try to convert them to layout problems because QAP is well known as a basic model in that application area. However, it is easy to show by data analysis methods that the problems solved by some layout authors are not truly layout problems.

# 1 Introduction

The quantity of scientific research produced has increased significantly over the last few decades. The number of SCI journals is far above 8,000. The en masse production of science has contributed to some negative phenomena. It happens more and more frequently that a researcher carries out research in one field but finds that the results are not strong enough to publish in that field. The author then publishes them in a related but not identical field as an application. As a consequence of this practice, the authors do not know or even do not care of the results of the original field.

The Quadratic Assignment Problem (QAP) is known as one of the most difficult problems in integer programming, although it has a nice combinatorial formulation. Therefore, it is a suitable experimental field for many algorithmic ideas, including artificial intelligence methods. However, these methods must compete with the special methods of QAP. The latter are far better in many cases. Moreover, it is easy to get information on the most recent developments in QAP from [QAPLIB], where the most important benchmark problems are also available.

The main reason why QAP specific methods are superior to AI methods is that they are based on the careful analysis of the structure of QAP, while AI methods are quite general and are unable to exploit the special properties of QAP to the same extent. Thus, the experimental methods cannot be published in their own right. Their authors try to convert them to layout problems because QAP is well known to be a basic model in that application area.

However, it is easy to show by data analysis methods that the problems solved by some layout authors are not really layout problems. A special optimization model and a well-known statistical method called Multi-Dimensional Scaling (MDS) can be used for this purpose. The former can be used for exploring the geometric structure if the distances are $l_1$ distances (also called rectangular or Manhattan distances). MDS can be applied for Euclidean distances.

The next section describes the problems in QAPLIB. Section 3 discusses the reconstruction model in the case of $l_1$ distances. A very short description of MDS can be found in Section 4. Section 5 covers the computational experiments, including both the exact solution of QAP problems and the reconstruction of layout configurations. Some recent papers are critiqued in Sections 6 and 7. Section 6 gives a criterion for a QAP to be a layout problem. The contribution of AI methods to the solution of NP-complete problems is analyzed in Section 7. Section 8 concludes the paper.

# 2 QAPLIB

The QAPLIB library was established in April, 1996 by R. Burkard, E. Çela, S.E. Karisch, F. Rendl in Graz, Austria [Burkard et al. 1997]. Since August 2002, it has been updated by P. Hahn at Pennsylvania State University [QAPLIB]. The problems it contains have very different origins. For example, the problems of Burkard, under the code names Bur26a through Bur26h, concern the speed of typing the 26 letters of the alphabet in different languages. The set of real layout problems constitutes only a minority of the problems in QAPLIB. They are summarized in Table 1. The name of a problem consists of two or three parts. The first indicates the author(s) of the problem. The second is the size of the problem. Finally, if the same author has several problems of the same size, then another letter is used to distinguish them. For example, Bur26a indicates Burkard's problem of size 26, as 26 is the number of letters in the alphabet, and the 'a' designates the first problem in this series.

| Author(s) | problem name(s) | type of distance | optimal solution in QAPLIB |
|---|---|---|---|
| AN Elshafei | Els19 | n.a. | YES |
| SW Hadley, F Rendl, H Wolkowicz | Had12, Had14, Had16 Had18, Had20 | $l_1$ | YES |
| J Krarup, PM Prazan | Kra30a, Kra30b, Kra32 | weighted $l_1$ | YES |
| CE Nugent, TE Vollmann, J Ruml | Nug12, Nug14, Nug15, Nug16a Nug16b, Nug17, Nug18, Nug20 Nug21, Nug22, Nug24, Nug25 Nug27, Nug28, Nug30 | n.a. | YES |
| M Scriabin, RC Vergin | Scr12, Scr15, Scr20 | $l_1$ | YES |
| J Skorin-Kapov | Sko42, Sko49, Sko56, Sko64 Sko72, Sko81, Sko90, Sko100 | $l_1$ | NO |
| L Steinberg | Ste36a | $l_1$ | YES |
| L Steinberg | Ste36b, Ste36c | $l_2$ | YES |
| UW Thonemann, A Bölte | Tho30 | $l_1$ | YES |
| UW Thonemann, A Bölte | Tho40, Tho150 | $l_1$ | NO |
| MR Wilhelm, TL Ward | Wil50, Wil100 | $l_1$ | NO |

**Table 1.** Layout problems in QAPLIB. In all cases where the distance type is not available, the data are integers; therefore, it can be supposed that they are not l2 distances.

QAPLIB contains many types of useful information besides numerical problems. The results of heuristics and lower bounds on the numerical problems are also reported with the best-known or optimal solution. Codes for computer programs as well as a long list of important papers are also available. The interested reader can find news on promising new results and ongoing research.

# 3 The reconstruction model of $l_1$ distances

Reconstruction consists of finding proper positions in the plane or in space for the points. It can be done by solving a mixed integer linear programming problem. The model is discussed here for the case of the plane; the extension to 3 dimensions is obvious.

Assume that the $l_1$ distances among $n$ points are known. If $1 \leq j, k \leq n$ then let $d_{jk}$ be the distance between the $j$-th and $k$-th points. Their configuration is to be reconstructed in the plane, in the square $[0,h][0,h]$, where $h > 0$. Let $(x_j, y_j)$ be the co-ordinates of the $j$-th point. The value of $h$ must be at least the highest distance, but this may still not be sufficient for the existence of a reconstruction.

The first set of constraints is that the points must lie in the square, i.e.,

$$0 \leq x_j, y_j \leq h, \quad j = 1, \dots, n. \tag{1}$$

In general if $(a,b)$ and $(c,d)$ are two points in the plane then their $l_1$ distance is

$$\begin{aligned} l_1((a,b),(c,d)) &= |a-c| + |b-d| \\ &= \max\{a-c+b-d, a-c+d-b, c-a+b-d, c-a+d-b\}. \end{aligned}$$

Hence, the next set of constraints claims that for each pair of points, none of the four sums is greater than the distance between the two points:

$$\left.\begin{aligned} x_j - x_k + y_j - y_k &\leq d_{jk} \\ x_j - x_k + y_k - y_j &\leq d_{jk} \\ x_k - x_j + y_j - y_k &\leq d_{jk} \\ x_k - x_j + y_k - y_j &\leq d_{jk} \end{aligned}\right\} \quad 1 \leq j < k \leq n. \tag{2}$$

The third set of constraints claims an opposite inequality, that is, at least one of the above mentioned quantities is at least as great as the distance between the two points. The maximum of the four quantities must be selected, with the help of binary variables. Let $M$ be a large number; $M = 4h$ is a good choice. Then the inequalities are

$$\left.\begin{aligned} x_j - x_k + y_j - y_k + Mu_{jk1} &\geq d_{jk} \\ x_j - x_k + y_k - y_j + Mu_{jk2} &\geq d_{jk} \\ x_k - x_j + y_j - y_k + Mu_{jk3} &\geq d_{jk} \\ x_k - x_j + y_k - y_j + Mu_{jk4} &\geq d_{jk} \end{aligned}\right\} \quad 1 \leq j < k \leq n, \tag{3}$$

where

$$u_{jk1}, u_{jk2}, u_{jk3}, u_{jk4} \in \{0,1\} \quad 1 \leq j < k \leq n. \tag{4}$$

The quantity $Mu_{jkt}$ is a correction term to the $t$-th inequality of (3). If $u_{jkt} = 1$ then the t-th inequality is satisfied. If the j-th and k-th points are positioned properly, then at most three out of the four inequalities require the correction term. Therefore, the objective function is to minimize the number of correction terms used, i.e.,

$$\min \sum_{j=1}^{n-1} \sum_{k=j+1}^{n} (u_{jk1} + u_{jk2} + u_{jk3} + u_{jk4}) \tag{5}$$

Notice that the (1)-(5) problem always has a feasible solution: $x_j = y_j = 0$ $(j = 1, \dots, n)$ and $u_{jk1} = u_{jk2} = u_{jk3} = u_{jk4} = 1$. Its objective function value is $4n$. However, if the reconstruction is successful, then the optimal objective function value is at most 3n. If the optimal value is greater than 3n, then the reconstruction is not possible. If two points are on the same horizontal or vertical line, then two of the ujk s can be zero. For example, if $x_j = x_k$ and $y_j > y_k$ then if $d_{jk} = y_j - y_k$ then $u_{jk1} = u_{jk3} = 0$ in the optimal solution. Thus if the optimal value is at most $3n$ but there is a pair of points, say $j$ and $k$, such that $u_{jk1} = u_{jk2} = u_{jk3} = u_{jk4} = 1$ then a cut

$$u_{jk1} + u_{jk2} + u_{jk3} + u_{jk4} \leq 3 \tag{6}$$

has to be introduced. The procedure must be repeated until one of the following outcomes is achieved:

(i) a reconstruction is obtained,

(ii) the optimal objective function value is greater than 3n and

(iii) there is no feasible solution.

# 4 Multi-dimensional scaling

Multi-dimensional scaling is a well-known method used in statistics to explore the hidden dependency among data. In that sense, it serves the same purpose as factor analysis. A short summary of the method can be found in [MDS] and [STAT].

Assume that there are n comparable objects. The similarity of the objects is described by a nonnegative similarity matrix $(s_{ij})_{i,j=1,\ldots,n}$. The similarity value $s_{ij} = 0$ means that the two objects are identical, and the higher the value of sij is, the more dissimilar the objects are. The similarity matrix is supposed to be symmetric, i.e. $\forall\, 1 \leq i,j \leq n : s_{ij} = s_{ji}$. If the objects are described by a sufficiently high number of parameters and the similarity is measured by the Euclidean distance, then it is possible to find parameter values such that each similarity value is equal to the appropriate Euclidean distance. Thus, the hidden structure of the objects is revealed only if they are described by a lower number of parameters. However, complete equality of similarity numbers and geometric distances cannot be expected in that case.

MDS works as follows. First, the number of parameters, say $k$, must be determined. The objects will be represented by $k$-dimensional vectors, say $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$. Then, the parameter vectors are determined such that the total squared error is minimal, i.e., by the following unconstrained optimization problem:

$$\min_{\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_n} \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} (||\mathbf{x}_i - \mathbf{x}_j||_2 - s_{ij})^2. \tag{7}$$

The value of $k$ is either 2 or 3 in most applications. These low dimensions are selected so that the final results of MDS can be graphically represented and the hidden structure, if any, can be recognized by human intelligence. On the other hand, if the final result is a ”random cloud” of points, then no hidden structure is detected.

If a distance matrix contains Euclidean distances on a plane, then MDS is able to reconstruct the relative positions of the points completely. Notice that distances are invariant under rotation and shifting of the whole set of points in any direction. Thus, if it is supposed that the distances of a QAP claimed to be a layout problem are Euclidean distances, then MDS is a perfect tool to use to see whether the problem is a layout problem.

If MDS is executed by an automatic system, then the system selects the lowest dimension $d$ such that the loss of information compared to the case if the points are projected into the $d+1$ dimensional space is not significant.

## 5 Computational results

The Had14 problem of QAPLIB has been solved by the program called qapbb.f [Burkard et al. 1980]. It is also downloadable from QAPLIB. The program was running on a computer with an Intel Pentium Dual 2 GHz processor and 1024 Mb Ram. It solved the problem optimally in 5 seconds. Had14 was selected because it is the only problem that is experimentally discussed in [Kuan-Phen 2010].

To test the abilities of this approximately 30-year-old program, three further problems have been solved. Interestingly, in all three cases, an alternative optimal solution has been found that is not included in QAPLIB. They are contained in Table 2. In the case of the Els19 problem, the only difference is that the facilities 18 and 19 are interchanged. The CPU time was less than 1 second for both Els19 and Chr22a. It was 75 seconds for Chr25a. The optimal solutions found for the latter two problems are significantly different from the ones stored in QAPLIB. No further attempt to solve problems by qapbb.f was made, as the systematic reevaluation of earlier computer software is beyond the scope of the current research.

| Problem | Location | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Els19 | Assigned Dept. | 9 | 10 | 7 | 19 | 14 | 18 | 13 | 17 | 6 | 11 |
| | Location | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | |
| | Assigned Dept. | 4 | 5 | 12 | 8 | 15 | 16 | 1 | 2 | 3 | |
| Chr22a | Location | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| | Assigned Dept. | 6 | 2 | 15 | 16 | 11 | 13 | 7 | 4 | 19 | 21 |
| | Location | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 |
| | Assigned Dept. | 14 | 22 | 10 | 9 | 1 | 5 | 12 | 8 | 18 | 17 |
| | Location | 21 | 22 | | | | | | | | |
| | Assigned Dept. | 3 | 20 | | | | | | | | |
| Chr25a | Location | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| | Assigned Dept. | 18 | 22 | 4 | 6 | 3 | 12 | 24 | 8 | 25 | 10 |
| | Location | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 |
| | Assigned Dept. | 20 | 2 | 17 | 11 | 13 | 7 | 21 | 5 | 16 | 9 |
| | Location | 21 | 22 | 23 | 24 | 25 | | | | | |
| | Assigned Dept. | 19 | 23 | 14 | 15 | 1 | | | | | |

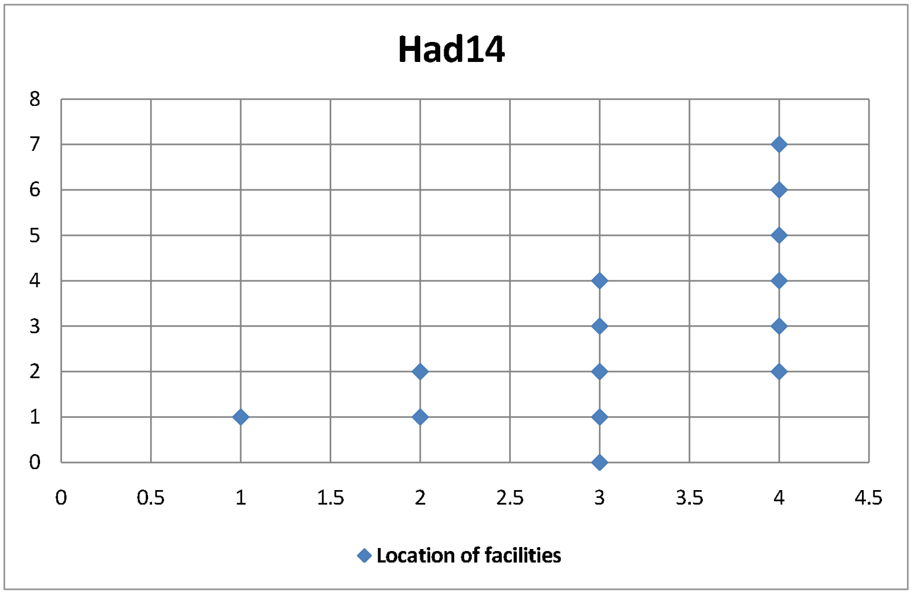


Figure 1: Reconstruction of the $l_1$ distances of the Had14 problem. The reconstruction is perfect in the sense that all $l_1$ distances are exactly the same as in the original problem.

**Table 2.** The alternative optimal solutions found by qapbb.f.

It is important to emphasize that the reconstruction methods determine only the relative positions of the points even in the case of perfect reconstruction. Then, to obtain the original structure, the reconstructed structure may need rotation and/or shifting.

The reconstruction is not successful in the case of the MDS method if the resulting set of points form a random cloud. This means that either the underlying geometrical structure does not exist, or $l_2$ is not the proper distance. If we suppose that the distances are of type $l_1$, then the reconstruction is made by problem (1)-(5). There is no reconstruction if there is no feasible solution, even assuming constraints (6). In such a case, if the problem is solved without constraints (6), the optimal solution may contain pairs of points that coincide and other pairs with the wrong distance. It is also likely, according to the computational experiments of the authors, that many points are on the same vertical or horizontal line, as shown in Figure 6. The distances of Rou12 in QAPLIB do not satisfy the triangle inequality.

The results of the reconstruction are not necessarily congruent geometrically to the original structure. If a distance matrix has a clear underlying geometric structure, then the reconstructed problem will have such a structure as well, but the reconstructed structure may depend on the dimension of the space into which the points are projected and the type of the distance, which may be $l_1$ or $l_2$. What is important is that the generated figure shows a structure. A sequence of figures illustrates this principle. Figure 1 shows the Had14 problem. The reconstruction is perfect in the sense that the $l_1$ distances are exactly equal to

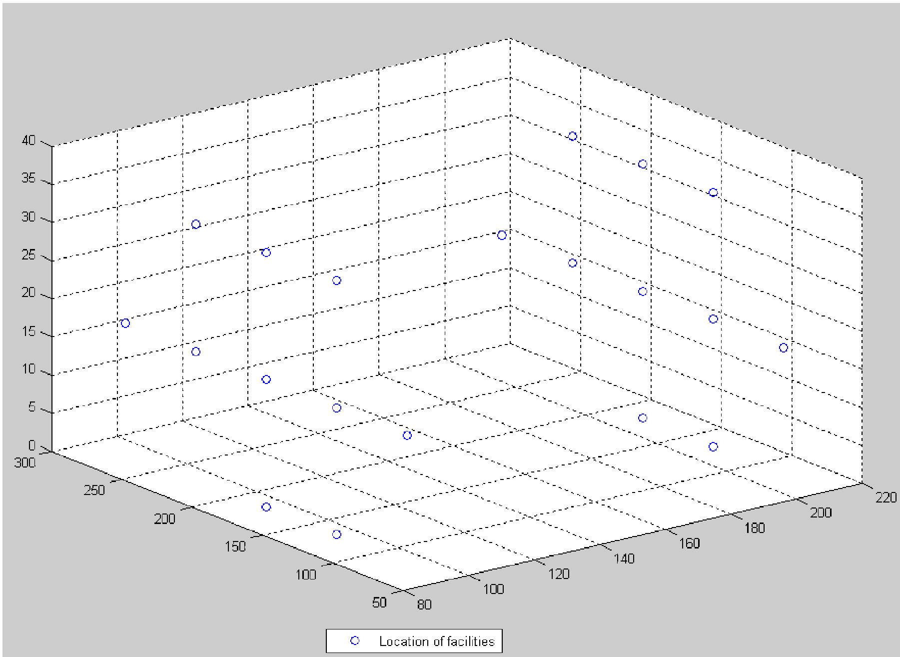


Figure 2: Reconstruction of the structure of the Kra30a problem by the model of type (1)-(5) in the 3-dimensional space. The reconstruction is not perfect, as the weights applied in the $l_1$ type distance are unknown. Note that the levels of the building are clearly recognizable.

the distances in the problem. Both methods give a good quality reconstruction for Kra30a in 3 dimensions. In the plane, the reconstructions are different but still have recognizable structure (see Figures 2 to 5). Kra30a has been selected because it a benchmark problem and was not solved exactly for 27 years [Hahn-Krarup 2001].

# 6 To lay out or not to lay out

The Traveling Salesman Problem (TSP) is another important problem in combinatorial optimization. The literature on this problem is even richer than that of QAP. There are many computational studies on TSP. They can give hints as to what can be expected in the

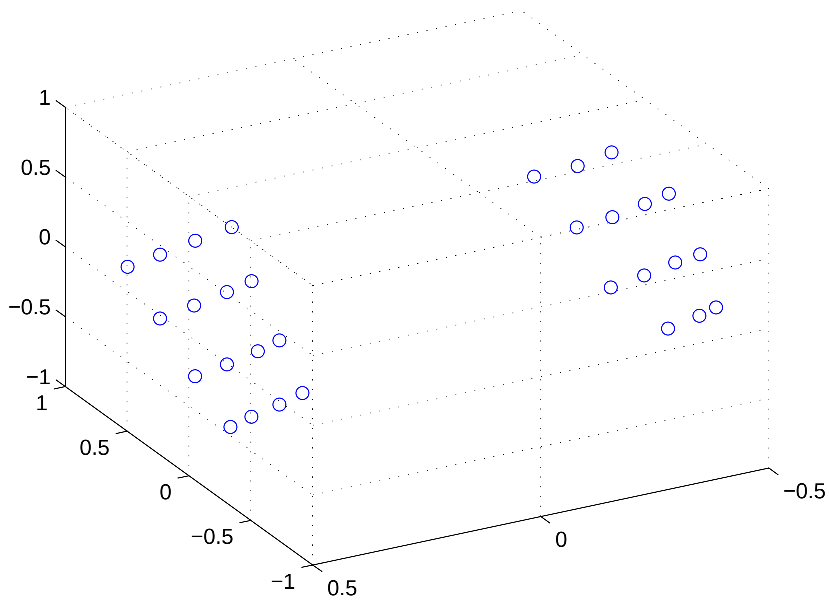


Figure 3: Reconstruction of the structure of Kra30a problem in 3-dimensional space by the MDS method. The configuration must be rotated to obtain the real positions.

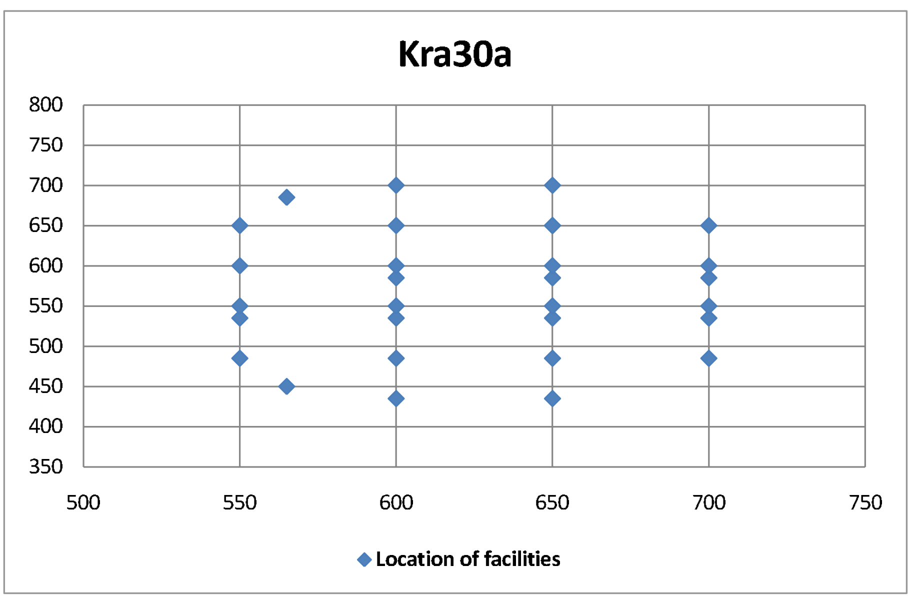


Figure 4: Reconstruction of the structure of the Kra30a problem in the plane by model (1)-(5). The configuration has some symmetry and regularity properties.

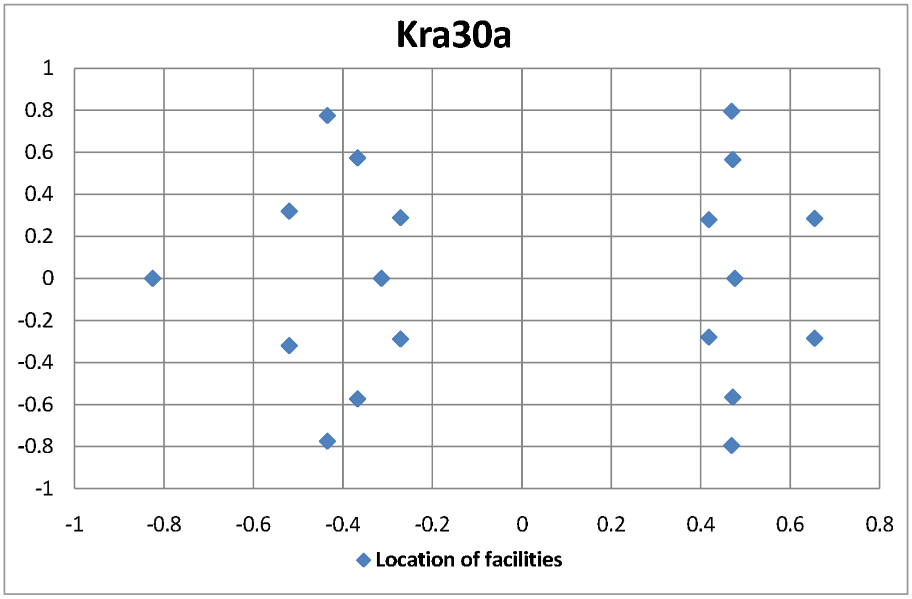


Figure 5: Reconstruction of the structure of Kra30a problem in the plane by the MDS method. This configuration also has some symmetry and regularity properties.

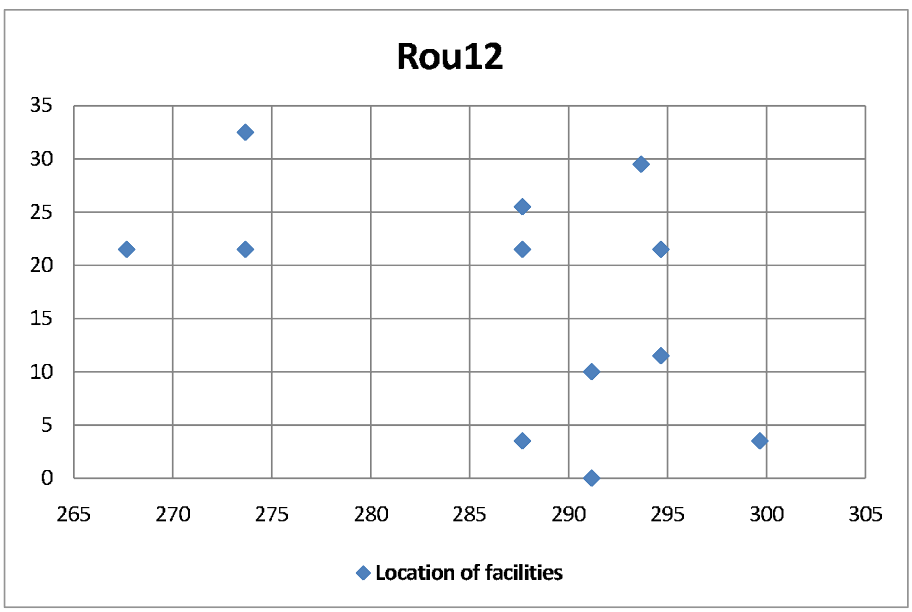


Figure 6: The problem Rou12 in QAPLIB. Its reconstruction is not possible. The attempt was made by the model (1)-(5).

case of other problems, like QAP. Moreover, TSP has many applications in very different areas, including transportation, design and production of integrated circuits, scheduling in chemical industry, minimization of set-up times, and automatic movements of robot arms and machines, to name just a few examples. These problems pose very different difficulties from the algorithmic point of view because the data sets of different practical problems have different structural properties. Not all of these properties are known and/or understood. Similarly, the instances of any other optimization problem may have different structural properties, depending on the origin of the practical problem to be modeled.

Any real layout problem can be reconstructed either in the plane, if the facilities must be positioned on a surface, or in 3-dimensional space, if the facilities must be assigned to positions in a building. In both cases, the reconstruction must show an easily recognizable geometric structure.

If a problem has no such reconstruction, then it is not a layout problem but another kind of problem that can also be modeled by QAP. There is no reason to suppose that their underlying QAPs have the same difficulty.

One can conclude that *if a paper deals with both reconstructable and non-reconstructable instances of QAP then that paper is a general purpose QAP paper regardless of whether it claims to be a layout paper.*

This is the case in the paper of [Ramkumar et al. 2009]. That paper provides computational results for almost all problem instances stored in QAPLIB. Only the three Thonemann-Bolte problems, the two Wilhelm-Ward problems and some very large scale problems from the classes Li-Pardalos, Skorin-Kapov, and Taillard are missing. However, the origins of the majority of the problems are not layout problems, as in the case, for example, of the problems of the Burkard-Offermann class (Bru26x) model typewriting, which was mentioned above.

[Ramkumar et al. 2009] does not give any information on the CPU times. Therefore, it is very difficult to evaluate its results in light of the results obtained by qapbb.f and mentioned in Section 5.

## 7 Further remarks

[Kuan-Phen 2010] discusses a hybrid ant colony-genetic algorithm for QAP. The application of the ant colony method to QAP is not a new idea. For some early publications, see [Coloni-Maniezzo 1999] and [Taillard-Gambardella 1997]. QAPLIB even contains a software system called FANT that was designed by Taillard. FANT is based on [Taillard 1998]. Unusually [Kuan-Phen 2010] does not refer to [Taillard 1998], but after the list of references, it offers another paper co-authored by Taillard as "Further reading" [Taillard-Gambardella 1997]. It is not an excuse for [Kuan-Phen 2010] if the authors did not know of QAPLIB. Ignorance of the literature cannot be an excuse. Moreover, [Kuan-Phen 2010] solves a single problem, namely, the Had14 problem contained in QAPLIB. Furthermore, they even use the optimal value that is also reported in QAPLIB. As a matter of fact, they refer to QAPLIB on page 124 in the second-to-last paragraph. Therefore, they would have had to refer to both [Taillard 1998] and the software FANT.

At this point a very serious question arises:

*What is the computational effort that the operations research community should expect from papers applying artificial intelligence methods to optimization problems?*

There are many questions connected to the main question. *Is the solution of a single problem enough?* Certainly not. The result of one measurement may reflect random effects. It is possible to draw conclusions on the properties of a method only if the method behaves in the same way for several problems. The more problems, the better. *Is it necessary that the new ideas must compete with all previous ideas?* Yes, it is. This principle concerns any kind of new results, not only AI methods. [Kuan-Phen 2010] finds the a priori known optimal solution of Had14 in 603 seconds but is unable to say anything about its optimality because of the nature of the method. Its optimality was recognized because it was already known. However, a branch and bound code, which is 30 years older, solved the problem in 5 seconds. If no further computational evidence is provided, then the only conclusion that can be drawn is that the new ant colony- genetic algorithm is useless. More generally, we can state the following principle: a *new method may be published only if the author is able to produce at least one case where the new method is superior to the known methods.*

*When can the application of AI methods be justified?* According to the present state of science, NP-complete problems can be solved exactly only by enumerative type methods, including dynamic programming. These methods have an exponential number of operations. Therefore, all of these methods/programs are subject to combinatorial explosion, so the problems larger than a certain threshold cannot be solved. The combinatorial explosion will be never eliminated. Smarter methods and faster computers only shift the threshold. The use of AI methods is justified beyond the threshold, as they control the CPU time required. To predict what can be expected in that region is an important problem. The only basis for prediction is the behavior of the AI methods within the exactly solvable region. Hence, for that purpose, the computational experiments must be exhaustive in that region of the problems.

# 8 Conclusions

The initial objective of the current paper was to show that results of general quadratic assignment problems appear under the name of layout problem. General quadratic assignment problems and layout problems can be distinguished according if a geometric structure of the position reconstructable. Two methods are used for reconstruction: a new mixed integer programming model and the MDS method of statistics. An unexpected result is that a 30 years old public program behaves very well in contemporary computers. Thus new methods must compete with that program as well.

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