Final Report
of the
STSM in University of Seville

1 Purpose of the STSM

This Short Term Scientific Meeting was an exploratory visit whose main aim was to collaborate with the research group led by Emilio Carrizosa at the University of Seville, Spain, on Mixed Integer Nonlinear Programming (MINLP). I had not worked in the past with Emilio Carrizosa or any of his collaborators, so the scientific plan was to identify research topics of common interest and to develop new tools which may lead to publications in prestigious and high-impact journals in Operations Research.

2 Description of the work carried out during the STSM

Global Optimization is the branch of Mathematical Optimization addressing optimization problems which may have local (not globally) optimal solutions, and the global optimum is sought. Global Optimization methods are of two types: deterministic, which attempt to find (up to numerical accuracy) the globally optimal value in finite time, and stochastic, which, using random numbers, provide solutions which hopefully converge to the global optimum in probability.

We have addressed challenging Global Optimization problems which are of MINLP type: the functions involved are nonconvex and some of the decision variables are constrained to take integer values. Two research projects have been considered:

1. Multifacility location problems on networks.

2. Inference of stoichiometric matrices in chemical reactions.

In multifacility location problems on networks, one seeks the location of p points on a network optimizing a certain function of the distances from such points to the nodes or edges of the network. While the models studied so far in the literature allow to reduce the search of optima solutions to a finite set, we have addressed models in which no reduction to a discrete set is known, and thus analyzed as a continuous problem. I have addressed covering problems, where the demand to be covered is continuously distributed over the edges of a given graph. The aim is to locate p facilities on the graph with the maximal expected covering, where a facility covers every point within a prespecified distance. I have also collaborated in the work on locating p-facilities on graphs in a competitive environment using the well-known Huff model.

The second research line I have collaborated is part of an industrial project running in the University of Seville: given a set of species, whose concentrations are measured at given instants, the chemical reactions are sought. Due to chemical laws, the problem reduces to finding the stoichiometric matrix (in integer numbers) and reaction rates of the reactions governing the process.

3 Description of the main results obtained

For the multifacility location problems, we have designed a branch and bound strategy, in which one has to decide which edges from the network are to be selected, and, for edges fixed, the location of the facilities. The branch and bound method we have designed to solve the covering problem uses a special data structure, called superset, which is a set of disjoint edgesets, together with the numbers of facilities that every edgeset contains. Starting with the superset that contains only one edgeset, the whole graph, and p as the number of facilities, the algorithm divides the supersets and obtains upper bounds on the maximal covering over the new supersets. We have designed three different procedures to compute upper bounds of the objective function. The first one is an interval arithmetic type approach where every point that could be covered is added to the expected covering. It gives nice bounds when the superset is relatively small. The second bound is obtained computing the discrete maximal covering problem, where decision is made on locating on an edge or not and the expected covering is computed as the sum of the overall demand of every edge in the prespecified distance from the chosen edge. The third bound can be computed as the sum of the maximal 1-covering bounds over the given edgesets. This bound is very useful for small radius, but when the covered sets has large intersection, it doesn't provide a good bound. Combining the three bounding rules lead to an efficient method to tackle the above hard to solve problem for small number of facilities.

This branch-and-bound strategy, already successfully tested in many instances, has also been adapted to the Huff location problem. The implementation is now ongoing research.

With respect to the problem of inference of chemical reactions, I have collaborated in the modeling phase of the problem. First, we have explored in designing algorithms which fit properly empirical data of concentrations to mathematical functions. Since these fitting problems are rather multimodal but have a low dimension, an interval analysis branch and bound has been used to test different models. Second, the problem of reactions inference has been written as a MINLP. Due to the large dimension of the problem, the numerical tests performed with benchmark MINLP solvers did not succeed in solving the test instances available. Different reformulations have been developed and preliminary tests performed.

4 Future collaboration with the host institution

The first step will be to finish the research projects already open. The branch and bound strategy for location on networks can be extended to other models, which can be analyzed after submitting the papers started and partially written during my stay. I have settled strong links with the research group led by Emilio Carrizosa, and I am optimistic about future cooperation, not only with Emilio Carrizosa, but also with some other researchers, such as the young researcher (PhD student) Asunción Jiménez, who has received a strong training on Global Optimization during my stay.

5 Foreseen publications resulting from the STSM

The research done during my stay should lead to at least three papers: one on covering problems on networks, another one on competitive location on networks and a third one on inference of chemical reactions. It is my hope that these will be the three first papers with the group, since it is likely that more will come in a next future.

Budapest, 29th of January, 2014.

G.-Tóth Boglárka

Boglárka G.-Tóth
Visitor, Budapest University
of Technology and Economics

Confirmation by the host institution of the successful execution of the STSM

I have read the final report written by Boglárka G.-Tóth describing her STSM visit at the University of Seville to collaborate with my research group. I am extremely satisfied with the results of the visit. Not only have we successfully cooperated in some challenging MINLP problems, but Boglárka has been extremely collaborative in training PhD students in my group. I am willing to finish and submit the papers obtained from her visit and then we will plan further research lines, possibly involving also one or two PhD student from my group.

Seville, 30th of January, 2014.

Emilio Carrizosa
Host, University of Seville