Relaxations for Convex Nonlinear Generalized Disjunctive Programs and their Application to Nonconvex Problems

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This seminar deals with the theory of reformulations and numerical solution of generalized disjunctive programming (GDP) problems, which are expressed in terms of Boolean and continuous variables, and involve algebraic constraints, disjunctions and propositional logic statements. We propose a framework to generate alternative MINLP formulations for convex nonlinear GDPs that lead to stronger relaxations by generalizing the seminal work by Egon Balas (1988) for linear disjunctive programs. We define for the case of convex nonlinear GDPs an operation equivalent to a basic step for linear disjunctive programs that takes a disjunctive set to another one with fewer conjuncts. We show that the strength of relaxations increases as the number of conjuncts decreases, leading to a hierarchy of relaxations. We prove that the tightest of these relaxations, allows in theory the solution of the convex GDP problem as an NLP problem. We apply the proposed theory for generating strong relaxations through an algorithm that involves preprocessing and application of basic steps following some rules to avoid incurring in an exponential increase of the size of the reformulated MINLP.. Results are presented for a dozen convex GDPs that are solved with a NLP-based branch and bound method. Compared to the reformulation based on big-M and the hull relaxation, the results show that significant improvements can be obtained in the predicted lower bounds, which in turn translates into a smaller number of nodes for the branch and bound enumeration.

We next address the extension of the above ideas to the solution of nonconvex GDPs that involve bilinear, concave and linear fractional terms. In order to solve these nonconvex problems with a spatial branch and bound method, a *convex GDP relaxation* is obtained by using suitable under- and over-estimating functions of the nonconvex constraints. In order to predict tighter lower bounds to the global optimum we exploiting the hierarchy of relaxations for convex GDP problems. We illustrate the application of these ideas in the optimization of several process systems to demonstrate the computational savings that can be achieved with the tighter lower bounds.

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Ignacio E. Grossmann is the R. R. Dean University Professor of Chemical Engineering, and former Department Head at Carnegie Mellon University. He obtained his B.S. degree at the Universidad Iberoamericana, Mexico City, in 1974, and his M.S. and Ph.D. at Imperial College in 1975 and 1977, respectively. After working at the Instituto Mexicano del Petróleo in 1978, he joined Carnegie Mellon in 1979. He is currently director of the "Center for Advanced Process Decision-making," an industrial consortium that involves about 20 petroleum, chemical, engineering and software companies.

Ignacio Grossmann is a member of the National Academy of Engineering, and associate editor of *AIChE Journal* and member of editorial board of *Computers and Chemical Engineering, Journal of Global Optimization, Optimization and Engineering,* and *Latin American Applied Research.* Major awards include the 1994 Computing in Chemical Engineering Award of the CAST Division of AIChE, the 1997 William H. Walker Award of AIChE, the 2000 Steven J. Fenves Award for Systems Research, the 2003 Computing Society Prize of INFORMS, the 2007 Kun Li Award for Excellence in Education at Carnegie Mellon, the 2009 Warren Lewis Award of AIChE, the 2011 Research Excellence in Sustainable Engineering Award of AIChE, and Luis Federico Leloir Award for International Cooperation, Argentina, 2012. In 2002 he received the Honorary Doctor in Technology from Åbo Akademi in Finland, in 2007 Doctor honoris causa from University of Maribor in Slovenia, and in 2012 Doctor in Engineering Honoris Causa, Technical University of Dortmund. He is Fellow of INFORMS and AIChE, Top 15 Most Cited Author in Computer Science by ISI, and was named "One of the Hundred Chemical Engineers of the Modern Era" by AIChE in 2008. He is recipient of the Best Technical Paper in 1988, 1996, 1998 and 2000 of *Computers and Chemical Engineering*. He was the 6th Robert Vaughn Lecturer at Caltech in 1986, the 18th Ashton Hall Cary Lecturer at Georgia Tech in 2002, the Kelley Lecturer at Purdue University in 2004, ExxonMobil Lecturer at University of Massachusetts in 2007, the 2011 Distinguished Basore Lecture at Auburn University, the 2012 Walter J. Weber, Jr. Distinguished Lecturer at the University of Michigan, the 2012 Chemical and Biochemical Engineering Distinguished Lecturer at Western University, Canada, the 2012 Texas Distinguished Faculty Lecturer at University of Texas, Austin, and the 2013 Agustin Vazquez Vera Lecturer at Instituto Tecnologico Celaya, Mexico. He was also the Mary Upson Visiting Professor at Cornell in 1986-87, and a Fulbright Senior Lecturer at the Universidad de Cantabria in Spain in 2003-2004. He is a member of the American Institute of Chemical Engineers, Institute for Operations Research and Management Science, and American Chemical Society. He was chair of the Chemical Engineering section of the National Academy of Engineering, was a member of the Technology Advisory Board of Engineering Sciences at Dow Chemical and has been consultant to ExxonMobil, Air Products and Instituto Mexicano del Petróleo.

The research interests of Ignacio Grossmann are in the areas of mixed-integer and logic-based optimization, process synthesis, energy integration, process flexibility, planning and scheduling of batch and continuous processes, and supply chain optimization. He has authored more than 400 papers, several monographs on design cases studies, and the textbook *"Systematic Methods of Chemical Process Design,"* which he co-authored with Larry Biegler and Art Westerberg. He has also organized the *Virtual Library on Process Systems Engineering*: http://cepac.cheme.cmu.edu/pasilectures.htm.

Professor Grossmann has graduated 47 Ph.D. and 7 M.S. students. He has taught short courses at PLAPIQUI, Bahía Blanca and INTEC, Santa Fé, Argentina; IIT, Bombay, India; Norwegian Institute of Technology, Trondheim, Norway; Instituto Tecnológico de Celaya, Mexico; ITESM, Mexico; Universidad de Santiago de Chile, Universidad de Antofagasta, Chile; Imperial College, London; Yonsei University, Seoul, Korea; Universidad Iberoamericana, Mexico City; Universidad Roviri e Virgili, Spain; Abo Akademi, Turku, Finland; University of Dortmund, Germany; Universidad de Cantabria and Universidad de Valladolid, Spain; ETH, Switzerland; National University of Singapore; Tsinghua University; Instituto Mexicano del Petróleo, Mexico; Petrobras, Rio de Janeiro.