Appendix

Appendix A

Future Perspectives

We think that deterministic algorithms for global optimization of nonconvex mixed-integer nonlinear programs will become an increasingly important research area in the future. This view is also supported by other authors interested in the future perspectives of optimization (Grossmann and Biegler, 2002).

The concept of the BCP framework presented here for general MINLPs is quite similar to modern BCP methods for MIPs. However, our current BCP-solver for MINLP is still in its infancy, and there is still much room for improvement in order to make it more efficient. The following list includes a number of things that would facilitate the development of a reliable large-scale general purpose MINLP solver:

1. Nonconvex polyhedral outer and inner approximations and an MIP master problem can be used, as described in Section 13.6.
2. Faster solution of (Lagrangian) subproblems: Specialized sub-solvers can be used for solving particular subproblems, such as separable MINLP, convex MINLP, concave NLP or MIP. In particular, LP-based branch-and-bound methods seem to be quite efficient. Since similar subproblems have to be solved, a sub-solver should be able to perform a warm-start.
3. The column generation based *fixing heuristic* of (Borndörfer et al., 2001) can be used to simultaneously generate columns and to fix binary variables.
4. Generation of block-separable reformulations: Instead of black-box representations of MINLPs, *expression trees* or *directed acyclic graph* (DAG) representations Schichl and Neumaier, 2004 can be used to generate splitting schemes and subproblems in a flexible way.
5. Rigorous bounds: Rigorous underestimators can be computed using interval methods, as discussed in Section 6.5.1. Moreover, predefined convex underestimators for special functions, such as Bézier-underestimators defined in Section 6.2, can be used.

6. Box reduction: The described box-reduction methods can be applied to each node produced by the BCP method. Furthermore, constraint propagation tools, such as used in the *Constrained Envelope Scheduling* approach (Boddy and Johnson, 2003), can be included in the MINLP-BCP framework.
7. Parallelization: A parallel MINLP-BCP framework, based on the structure of COIN-BCP (IBM, 2003), can be developed.
8. Support of user-knowledge: Similar to the open outer approximation MINLP solver AIMMS-OA (Bisschop and Roelofs, 2002), an *open BCP algorithm* can be developed, which allows users to tune solution strategies for specific problems.
9. Support of discretized optimization problems: Based on the ideas of Chapter 9, a tool for simultaneously solving and updating discretized stochastic programs and optimal control problems can be implemented.

Appendix B

MINLP Problems

B.1 Instances from the MINLPLib

The MINLPLib is a recently created library of MINLP instances (Bussieck et al., 2003a). These problems come from a very wide variety of applications. Table B.2 shows 49 instances of the MINLPLib that were used in our numerical experiments. The corresponding columns are described in Table B.1. Almost all problems are block-separable and have a small maximum block-size. Moreover, 14 problems are convex, and 19 problems are quadratic.

name	The name of the problem
n	The number of variables
$\lvert B\rvert$	The number of binary variables
m	The number of constraints
box diam	The diameter of $[\underline{x}, \overline{x}]$
avg. block size	The average block size
max. block size	The maximum block size
p	The number of blocks
max nr.var	The maximum number of nonlinear variables of the objective or a constraint function
conv	Indicates if the problem is a convex MINLP or not
probl type	The type of the problem: 'Q' means MIQQP and 'N' means MINLP

Table B.1: Descriptions of the columns of Table B.2.

name	n	$\|B\|$	m	box diam.	block size avg	block size max	p	max nl.var	conv	probl type
alan	9	4	7	∞	1.3	3	7	3	yes	Q
batch	47	24	73	1567.64	1.3	2	36	2	yes	N
batchdes	20	9	20	∞	1.3	2	15	2	no	N
elf	55	24	38	∞	1.1	2	52	2	no	Q
eniplac	142	24	189	∞	1.2	2	118	2	no	N
enpro48	154	92	215	∞	1.1	3	138	3	no	N
enpro56	128	73	192	∞	1.1	3	116	3	no	N
ex1221	6	3	5	14.2478	1	1	6	1	no	N
ex1222	4	1	3	1.77255	1	1	4	1	no	N
ex1223	12	4	13	17.5499	1	1	12	1	yes	N
ex1223a	8	4	9	17.4356	1	1	8	1	yes	Q
ex1223b	8	4	9	17.4356	1	1	8	1	yes	N
ex1224	12	8	7	3.31491	1.2	3	10	3	no	N
ex1225	9	6	10	6.16441	1.1	2	8	2	no	N
ex1226	6	3	5	10.4403	1.2	2	5	2	no	N
ex1252	40	15	43	5192.7	1.8	7	22	4	no	N
ex1263	93	72	55	63.8122	1.2	5	77	2	no	Q
ex1264	89	68	55	30.8869	1.2	5	73	2	no	Q
ex1265	131	100	74	35.3129	1.2	6	106	2	no	Q
ex1266	181	138	95	39.2428	1.2	7	145	2	no	Q
ex3	33	8	31	∞	1	1	33	1	no	N
ex4	37	25	31	∞	1	1	37	1	no	Q
fac1	23	6	18	1200	2.6	8	9	8	yes	N
fac3	67	12	33	7348.47	4.2	18	16	18	yes	Q
feedtray2	88	36	284	∞	3.4	63	26	17	no	Q
fuel	16	3	15	∞	1	1	16	1	no	Q
gastrans	107	21	149	∞	1.2	2	86	2	no	N
gbd	5	3	4	1.90788	1	1	5	1	yes	Q
gear2	29	24	4	96.1249	1.1	4	26	4	no	N
gkocis	12	3	8	∞	1	1	12	1	no	N
johnall	195	190	192	13.9284	1	3	193	3	no	N
meanvarx	36	14	44	∞	1.2	7	30	7	yes	Q
nous2	51	2	43	∞	3.4	8	15	5	no	Q
oaer	10	3	7	∞	1	1	10	1	no	N
ortez	88	18	74	∞	1.4	9	61	2	no	N
parallel	206	25	115	∞	3.7	151	56	131	no	N
procsel	11	3	7	∞	1	1	11	1	no	N
ravem	113	54	186	∞	1.1	3	101	3	yes	N
sep1	30	2	31	237.181	1.2	5	26	2	no	Q
space25	894	750	235	∞	1	43	852	7	no	Q
space25a	384	240	201	∞	1.1	43	342	7	no	Q
spectra2	70	30	73	∞	1.6	10	43	10	no	Q
stockcycle	481	432	97	1060.22	1	1	481	1	yes	N
synheat	57	12	64	∞	1.5	5	37	5	no	N
synthes1	7	3	6	3.4641	1.2	2	6	2	yes	N

synthes2	12	5	14	∞	1.1	2	11	2	yes	N
synthes3	18	8	23	6.55744	1.1	2	17	2	yes	N
util	146	28	168	∞	1	5	141	2	no	Q
waterx	71	14	54	∞	1.7	3	41	3	no	N

Table B.2: Instances from the MINLPLib

B.2 Random MIQQP problems

Algorithm B.1 shows a procedure for generating a random MIQQP of the form

$$\begin{array}{lll} \min & q_0(x) & \\ \text{s.t.} & q_i(x) \leq 0, & i = 1, \dots, m/2 \\ & q_i(x) = 0, & i = m/2+1, \dots, m \\ & x \in [\underline{x}, \overline{x}], & x_B \text{ binary} \end{array} \tag{B.1}$$

where $q_i(x) = x^T A_i x + 2a_i^T x + d_i$, $A_i \in \mathbb{R}^{(n,n)}$ is symmetric, $a_i \in \mathbb{R}^n$, $d_i \in \mathbb{R}$, $i = 0, \dots, m$. The functions q_i are block-separable with respect to the blocks $J_k = \{(k-1)l + 1, \dots, kl\}$, $k = 1, \dots, p$. Since $c_i = 0$ for $i = 0, \dots, m$, the point $x = 0$ is feasible for (B.1).

Input: (n,m,l)

Set $p = n/l$ (number of blocks).

Set $B = \{1, \dots, n/2\}$, $\underline{x} = -e$ and $\overline{x} = e$.

for $i = 0, \dots, m$

Compute symmetric dense matrices $A_{i,k} \in \mathbb{R}^{(l,l)}$ with uniformly distributed random components in $[-10, 10]$ for $k = 1, \dots, p$.

Compute vectors $b_i \in \mathbb{R}^n$ with uniformly distributed random components in $[-10, 10]$, and set $c_i = 0$.

end for

Algorithm B.1: Procedure for generating random MIQQPs

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