Global Solutions of Nonconvex Standard Quadratic Programs via Mixed Integer Linear Programming Formulations

E. Alper Yıldırım

Koç University
Department of Industrial Engineering
Istanbul, Turkey

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Outline

1. Introduction
   - Standard Quadratic Programs
2. Two MILP Formulations
   - KKT-Based Reformulation
   - Upper Bounds on Big-M Parameters
   - An Alternative MILP Formulation
   - Valid Inequalities
3. Computational Results
4. Conclusions

Standard Quadratic Program

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A **standard quadratic program** involves minimizing a (nonconvex) quadratic form (i.e., a homogeneous quadratic function) over the unit simplex.

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$$(\mathrm{StQP}) \quad \nu(Q) = \min\{x^T Q x : x \in \Delta_n\},$$

where

- $\Delta_n = \{x \in \mathbb{R}^n : e^T x = 1, \quad x \in \mathbb{R}^n_+\}$ (the unit simplex),
- $Q \in \mathcal{S}^n$, where $\mathcal{S}^n$ denotes the space of $n \times n$ real symmetric matrices,
- $x \in \mathbb{R}^n$,
- $e \in \mathbb{R}^n$ denotes the vector of all ones, and
- $\mathbb{R}^n_+$ denotes the nonnegative orthant in $\mathbb{R}^n$.

Applications

- Portfolio optimization [Markowitz, 1952]
- Quadratic resource allocation problem [Ibaraki and Katoh, 1988]
- Population genetics [Kingman, 1961]
- Evolutionary game theory [Bomze, 2002]
- Social network analysis [Bomze et al., 2018]
- Copositivity detection (a matrix $M \in \mathcal{S}^n$ is copositive iff $\nu(M) = \min\{x^T Mx : x \in \Delta_n\} \geq 0$)
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- Maximum (weighted) stable set problem [Motzkin and Straus, 1965], [Gibbons et al., 1997]
- NP-hard in general

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- DC-based branch-and-bound [Bomze, 2002]; clique-based branch-and-bound [Scozzari and Tardella, 2008], [Liuzzi et al.,2017]; spatial branch-and-bound with cutting planes [Bonami et al., 2016]; KKT-based branch-and-bound [Burer and Vandenbussche, 2009], [Chen and Burer, 2012]

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- General purpose solvers (e.g., BARON [Sahinidis, 1996], COUENNE [Belotti, 2000], CPLEX 12.6.0+)

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- Our MILP reformulations are aimed at exploiting the specific structure of standard quadratic programs.

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KKT Conditions

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- By the Karush-Kuhn-Tucker optimality conditions, if $x \in \Delta_n$ is an optimal solution of (StQP), then there exist $s \in \mathbb{R}^n$ and $\lambda \in \mathbb{R}$ such that

$$\begin{aligned} Qx - \lambda e - s &= 0, && (1)\\ e^T x &= 1, && (2)\\ x &\in \mathbb{R}^n_+, && (3)\\ s &\in \mathbb{R}^n_+, && (4)\\ x_j s_j &= 0, \quad j = 1, \ldots, n. && (5) \end{aligned}$$

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- $x \in \Delta_n$ is a KKT point of (StQP) if there exists $(s, \lambda) \in \mathbb{R}^n \times \mathbb{R}$ such that (1) – (5) are satisfied.

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- $x \in \Delta_n$ is a KKT point of (StQP) if there exists $(s, \lambda) \in \mathbb{R}^n \times \mathbb{R}$ such that (1) – (5) are satisfied.
- By (1), (2), and (5), if $x \in \Delta_n$ is a KKT point of (StQP), then $\nu(Q) = x^T Qx = \lambda$.

KKT-Based MILP Reformulation

$$
\begin{array}{lrcll}
\text{(MILP1)} & \min & & \lambda & \\
& Qx - \lambda e - s & = & 0, & \\
& e^T x & = & 1, & \\
& x_j & \leq & K_j y_j, & j = 1, \ldots, n, \\
& s_j & \leq & M_j (1 - y_j), & j = 1, \ldots, n, \\
& x & \geq & 0, & \\
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- How big should K_j and M_j be?

Big-M Parameters

- Recall

$$\begin{aligned} x_j &\leq K_j y_j, & j &= 1, \ldots, n, \\ s_j &\leq M_j(1 - y_j), & j &= 1, \ldots, n. \end{aligned}$$

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- Choose $K_j = 1, \; j = 1, \ldots, n$.
- By the first constraint $Qx - \lambda e - s = 0$, which implies,
$$s_j = e_j^T Qx - \lambda, \quad j = 1, \ldots, n,$$
where $e_j \in \mathbb{R}^n$ denotes the jth unit vector, $j = 1, \ldots, n$.

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- Since $x \in \Delta_n$, we have $e_j^T Qx = x^T Qe_j \leq \max_{i=1,\ldots,n} Q_{ij}$.

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- Since $x \in \Delta_n$, we have $e_j^T Qx = x^T Qe_j \leq \max_{i=1,\ldots,n} Q_{ij}$.
- Recall that $\lambda \geq \nu(Q)$ on the feasible region.

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- Since $x \in \Delta_n$, we have $e_j^T Qx = x^T Qe_j \leq \max_{i=1,\ldots,n} Q_{ij}$.
- Recall that $\lambda \geq \nu(Q)$ on the feasible region.
- If we can obtain a lower bound on $\nu(Q)$, then we can use it to obtain an upper bound on $s_j, \; j = 1, \ldots, n$.

Two Lower Bounds

- Two lower bounds on $\nu(Q)$:

$$\nu(Q) \quad \geq \quad \ell_1(Q) = \min_{1 \leq i \leq j \leq n} Q_{ij} \left(+ \frac{1}{\sum_{k=1}^{n} (1/(Q_{kk} - \min_{1 \leq i \leq j \leq n} Q_{ij}))} \right),$$

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- For other lower bounds, see, e.g., [Nowak, 1999], [Bomze and de Klerk, 2002], [Anstreicher and Burer, 2005], and [Bomze et al., 2008] for a comparison.
- In (MILP1), we can use $M_j := \max_{i=1,\ldots,n} Q_{ij} - \ell, \; j = 1, \ldots, n$, where $\ell \in \{\ell_1(Q), \ell_2(Q)\}$.

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Lemma

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Furthermore, if $x \in \Delta_n$ is a KKT point of (StQP), then

$$\min_{j \in \mathcal{P}(x)} e_j^T Qx = x^T Qx = \max_{j \in \mathcal{P}(x)} e_j^T Qx.$$

A Min-Max Characterization

Proposition

Given an instance of (StQP),

$$\nu(Q) = \min\{x^T Qx : x \in \Delta_n\} = \min_{x \in \Delta_n} \max_{j \in \mathcal{P}(x)} e_j^T Qx.$$

A Min-Max Based MILP Formulation

$$
\begin{array}{llrcll}
\text{(MILP2)} & \min & \alpha & & & \\
& & e_j^T Qx & \leq & \alpha + z_j, & j = 1, \ldots, n, \\
& & e^T x & = & 1, & \\
& & x_j & \leq & K_j y_j, & j = 1, \ldots, n, \\
& & z_j & \leq & U_j(1 - y_j), & j = 1, \ldots, n, \\
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Remark

Given an instance of (StQP), (MILP2) is an equivalent reformulation of (StQP) if $K_j \geq 1, \ j = 1, \ldots, n$ *and*

$$U_j \geq M_j = \max_{i=1,\ldots,n} Q_{ij} - \ell, \quad j = 1, \ldots, n,$$

where ℓ *is any valid lower bound on* $\nu(Q)$.

A Comparison of Two Formulations

- There is a one-to-one correspondence between feasible solutions (x, y, s, λ) of the KKT-based formulation (MILP1) and KKT points of (StQP).

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- On the other hand, for any $x \in \Delta_n$, we can construct a feasible solution (x, y, z, α) of the min-max formulation (MILP2) such that $\alpha \geq x^T Qx$, with equality if x is a KKT point of (StQP).

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- On the other hand, for any $x \in \Delta_n$, we can construct a feasible solution (x, y, z, α) of the min-max formulation (MILP2) such that $\alpha \geq x^T Qx$, with equality if x is a KKT point of (StQP).
- Therefore, (MILP2) is an *exact relaxation* of (MILP1).

Convexity Graph and Valid Inequalities

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Definition

A graph $G = (V, E)$ is called the *convexity graph* of Q if $V = \{1, \ldots, n\}$ and

$$E = \{(i, j) : Q_{ii} + Q_{jj} - 2Q_{ij} > 0, \quad 1 \leq i < j \leq n\}.$$

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Theorem (Scozzari and Tardella, 2008)

There exists a globally optimal solution $x^* \in \Delta_n$ of (StQP) such that the vertices corresponding to $\mathcal{P}(x^*)$ form a clique in the convexity graph $G = (V, E)$ of Q (or, equivalently, a stable set in the complement of G).

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Theorem

The following inequalities are valid for both (MILP1) and (MILP2):

$$y_i + y_j \leq 1, \quad 1 \leq i < j \leq n \text{ s.t. } Q_{ii} + Q_{jj} - 2Q_{ij} \leq 0.$$

Outline

Computational Setup I

- Two MILP formulations: KKT Based (MILP1) and Min-Max Based (MILP2)

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- We add the following bound constraints to (MILP1) and (MILP2):

$$\ell \leq \left\{ \begin{array}{c} \lambda \\ \alpha \end{array} \right\} \leq \min_{k=1,\ldots,n} Q_{kk}.$$

Computational Setup II

- We compare the performances of our MILP formulations with three other global solution approaches:
  (i) MILP formulation of [Xia, Vera, Zuluaga, 2015] (denoted by QP-IP)
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- 64-bit HP workstation with 24 threads (2 sockets, 6 cores per socket, 2 threads per core) running Ubuntu Linux with 48 GB of RAM and Intel Xeon CPU E5-2667 processors with a clock speed of 2.90 GHz

Set of Instances

We conducted extensive experiments on the following set of instances from the literature:

(i) *BLST Instances* [Bonami et al., 2016]: Randomly generated instances with $n \in \{30, 50\}$.

(ii) *ST Instances* [Scozzari and Tardella, 2008]: Randomly generated instances with a prespecified convexity graph density with $n \in \{100, 200, 500, 1000\}$.

(iii) *DIMACS Instances*: Subset of maximum clique instances from the DIMACS collection with $n \in [28, 300]$.

(iv) *BSU Instances* [Bomze et al., 2018]: Specifically constructed hard instances with $n \in [5, 24]$ and the number of strict local minimizers between $(1.38)^n$ and $(1.49)^n$.

Summary

Instance Family	Number of Instances	n	δ
BLST30	134	30	[0.10,1.00]
BLST50	138	50	[0.11,1.00]
ST100	24	100	[0.25,0.90]
ST200	18	200	[0.25,0.75]
ST500	11	500	[0.25,0.50]
ST1000	1	1000	0.25
DIMACS1	8	[28,171]	[.35,.93]
DIMACS2	22	[200,300]	[.08,.97]
BSU	20	[5,24]	[.6,1]

Table 1: Summary of Instances

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Table 1: Summary of Instances

- δ denotes the density of the convexity graph.
- 376 instances in total

BLST30 Instances

	Total Time	OPT	Time Limit	Average Gap
MILP1-L1	26.97	**134**	0	–
MILP1-L1-VI	30.71	**134**	0	–
MILP2-L1	30.50	**134**	0	–
MILP2-L1-VI	33.80	**134**	0	–
MILP1-L2	34.67	**134**	0	–
MILP1-L2-VI	**24.10**	**134**	0	–
MILP2-L2	25.65	**134**	0	–
MILP2-L2-VI	29.28	**134**	0	–
QP-IP	38.10	**134**	0	–
CPLEX QP	39370.66	124	10	6.14%
BARON	188005.68	96	38	115.91%
DNN	14.33	134	–	–

Table 2: Performance on BLST30 (134 instances; $n = 30$)

BLST50 Instances

	Total Time	OPT	Time Limit	Average Gap
MILP1-L1	50.30	**138**	0	–
MILP1-L1-VI	50.46	**138**	0	–
MILP2-L1	49.91	**138**	0	–
MILP2-L1-VI	55.54	**138**	0	–
MILP1-L2	45.06	**138**	0	–
MILP1-L2-VI	41.32	**138**	0	–
MILP2-L2	**30.48**	**138**	0	–
MILP2-L2-VI	35.25	**138**	0	–
QP-IP	85.85	**138**	0	–
CPLEX QP	77072.98	124	14	13.74%
BARON	431110.51	19	119	246.14%
DNN	99.44	138	–	–

Table 3: Performance on BLST50 (138 instances; $n = 50$)

ST 100 Instances

	Total Time	OPT	Time Limit	Average Gap
MILP1-L1	38.21	**24**	0	–
MILP1-L1-VI	52.95	**24**	0	–
MILP2-L1	20.78	**24**	0	–
MILP2-L1-VI	28.16	**24**	0	–
MILP1-L2	44.22	**24**	0	–
MILP1-L2-VI	63.88	**24**	0	–
MILP2-L2	**10.84**	**24**	0	–
MILP2-L2-VI	16.87	**24**	0	–
QP-IP	135.01	**24**	0	–
CPLEX QP	70894.32	6	18	38.18%
BARON	86404.50	0	24	1131.58%
DNN	388.39	24	–	–

Table 4: Performance on ST100 (24 instances; $n = 100$)

ST200 Instances

	Total Time	OPT	Time Limit	Average Gap
MILP1-L1	576.13	**18**	0	–
MILP1-L1-VI	512.49	**18**	0	–
MILP2-L1	189.45	**18**	0	–
MILP2-L1-VI	226.08	**18**	0	–
MILP1-L2	463.57	**18**	0	–
MILP1-L2-VI	417.84	**18**	0	–
MILP2-L2	**37.96**	**18**	0	–
MILP2-L2-VI	124.83	**18**	0	–
QP-IP	1197.43	**18**	0	–
CPLEX QP	64804.65	0	18	44.63%
BARON	64807.69	0	18	4249.18%
DNN	7729.80	18	–	–

Table 5: Performance on ST200 (18 instances; $n = 200$)

ST100 & ST 200 Instances

	Total Time	OPT	Time Limit	Average Gap
MILP1-L1	38.21	**24**	0	–
MILP1-L1-VI	52.95	**24**	0	–
MILP2-L1	20.78	**24**	0	–
MILP2-L1-VI	28.16	**24**	0	–
MILP1-L2	44.22	**24**	0	–
MILP1-L2-VI	63.88	**24**	0	–
MILP2-L2	**10.84**	**24**	0	–
MILP2-L2-VI	16.87	**24**	0	–
QP-IP	135.01	**24**	0	–
CPLEX QP	70894.32	6	18	38.18%
BARON	86404.50	0	24	1131.58%
DNN	388.39	24	–	–

Table 6: Performance on ST100 (24 instances; $n = 100$) and ST200 (18 instances; $n = 200$)

ST500 Instances

	Total Time	OPT	Time Limit	Average Gap
MILP1-L1	6583.05	**11**	0	–
MILP1-L1-VI	8960.10	**11**	0	–
MILP2-L1	**2519.94**	**11**	0	–
MILP2-L1-VI	3802.81	**11**	0	–
QP-IP	20291.34	6	5	6.97%
CPLEX QP	39603.91	0	11	44660285.88%
BARON	39600.13	0	11	11376.00%

Table 7: Performance on ST500 (11 instances; $n = 500$)

ST1000 Instance

	Total Time	OPT	Time Limit	Average Gap
MILP1-L1	3600.31	0	1	7.63%
MILP1-L1-VI	3609.65	0	1	46.74%
MILP2-L1	**2100.22**	**1**	0	–
MILP2-L1-VI	3600.18	0	1	11.59%
QP-IP	3607.88	0	1	22.05%
CPLEX QP	3600.95	0	1	86423971.55%
BARON	3601.03	0	1	18020.23%

Table 8: Performance on ST1000 (1 instance; $n = 1000$)

DIMACS1 Instances

	Total Time	OPT	Time Limit	Average Gap
MILP1-L1	3697.94	7	1	72.80%
MILP1-L1-VI	52.31	**8**	0	–
MILP2-L1	3624.48	7	1	72.80%
MILP2-L1-VI	59.72	**8**	0	–
MILP1-L2	3731.06	7	1	9.46%
MILP1-L2-VI	140.79	**8**	0	–
MILP2-L2	3616.89	7	1	9.46%
MILP2-L2-VI	**51.82**	**8**	0	–
QP-IP	4863.33	7	1	100.00%
CPLEX QP	29449.29	0	8	61.79%
BARON	28804.96	0	8	83.13%
ILP	**16.17**	**8**	0	–
DNN	356.74	8	–	–

Table 9: Performance on DIMACS1 (8 instances; $n \in [28, 171]$)

DIMACS2 Instances

	Total Time	OPT	Time Limit	Average Gap
MILP1-L1	57676.31	7	15	81.91%
MILP1-L1-VI	**21463.40**	**18**	4	71.60%
MILP2-L1	55529.78	7	15	82.38%
MILP2-L1-VI	25214.24	17	5	79.65%
MILP1-L2	56047.95	7	15	18.29%
MILP1-L2-VI	27944.05	17	5	9.40%
MILP2-L2	55127.62	8	14	20.60%
MILP2-L2-VI	30903.19	15	7	**7.65%**
QP-IP	61884.01	5	17	99.98%
CPLEX QP	77391.14	1	21	84.68%
BARON	75616.99	1	21	92.79%
ILP	**4672.59**	**21**	1	14.07%
DNN	25071.78	22	–	–

Table 10: Performance on DIMACS2 (22 instances; $n \in [200, 300]$)

BSU Instances

	Total Time	OPT	Time Limit	Average Gap
MILP1-L1	6.75	**20**	0	–
MILP1-L1-VI	5.99	**20**	0	–
MILP2-L1	8.77	**20**	0	–
MILP2-L1-VI	7.39	**20**	0	–
MILP1-L2	7.02	**20**	0	–
MILP1-L2-VI	**4.92**	**20**	0	–
MILP2-L2	7.04	**20**	0	–
MILP2-L2-VI	7.45	**20**	0	–
QP-IP	11.96	**20**	0	–
CPLEX QP	63194.15	5	15	14.82%
BARON	58022.22	5	15	54.53%
DNN	**0.51**	20	–	–

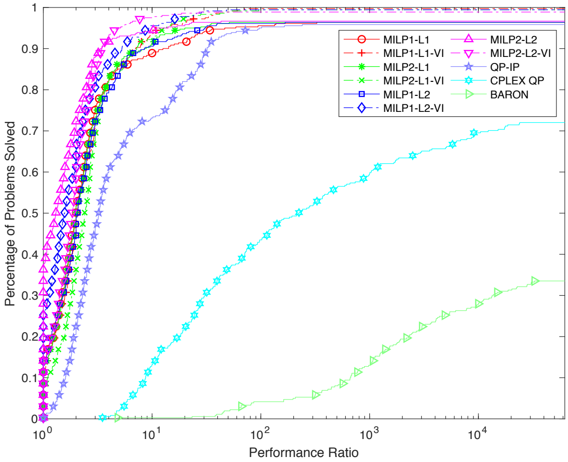
Table 11: Performance on BSU (20 instances; $n \in [5, 24]$)

Overall Comparison

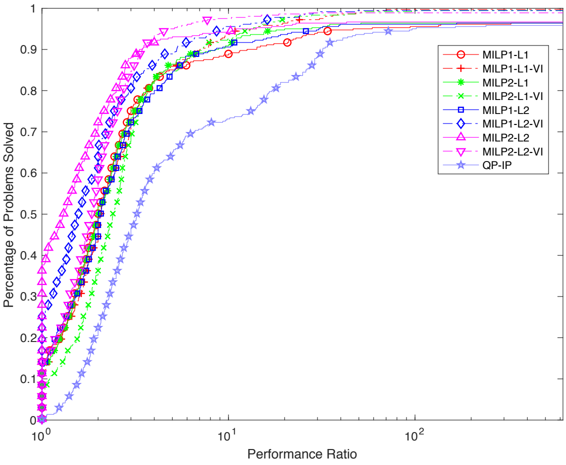
	IS1			IS2		
	Total Time	OPT	Time Limit	Total Time	OPT	Time Limit
MILP1-L1	62072.61	348	16	10183.36	11	1
MILP1-L1-VI	**22168.31**	**360**	4	12569.75	11	1
MILP2-L1	59453.67	348	16	**4620.16**	**12**	0
MILP2-L1-VI	25624.93	359	5	7402.99	11	1
MILP1-L2	60373.55	348	16	–	–	–
MILP1-L2-VI	28636.90	358	5	–	–	–
MILP2-L2	58846.48	349	15	–	–	–
MILP2-L2-VI	31168.69	357	7	–	–	–
QP-IP	68215.69	346	18	23899.22	6	6
CPLEX QP	422177.19	260	104	43204.86	0	**12**
BARON	932772.55	121	243	43201.16	0	**12**
DNN	33660.99	364	–	–	–	–

Table 12: Overall performance comparison (IS1: 364 instances; $n \in [5, 300]$; IS2: 12 instances; $n \in [500, 1000]$)

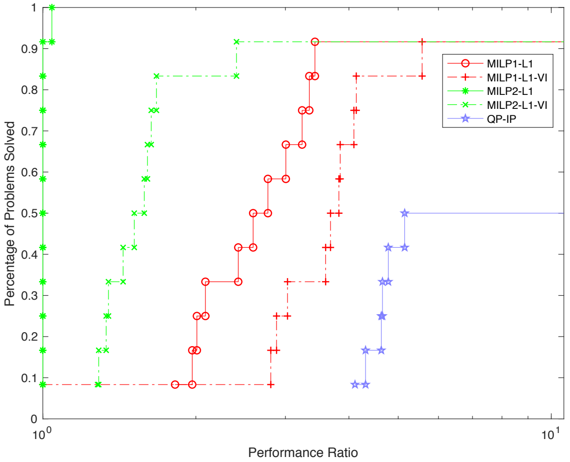
Performance Profile on IS1



Performance Profile on IS1 (w/o CPLEX QP and BARON)



Performance Profile on IS2 (w/o CPLEX QP and BARON)



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- Tight MILP formulations for other classes of quadratic programs?

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- Irene Klein, Vera Lehmwald, Markus Leitner, Ivana Ljubic, and Werner Schachinger
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- School of Mathematics, University of Edinburgh
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HAPPY BIRTHDAY, MANUEL!