Modelling Rank Constraints in Mathematical Programming

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Several problems in optimization and control involve a matrix of decision variables to be subject to a rank constraint. Although semidefinite programming is used as a generalpurpose tool to provide strong relaxations of such problems, finding feasible solutions mostly relies on algorithmic techniques specific to the problem at hand. We present models for expressing rank constraints using mathematical programming, that provide a general-purpose method to find feasible solutions. Our models were tested against the classical Distance Geometry Problem.

1 Introduction

This paper presents modelling techniques for expressing the rank of a matrix $A \in \mathbb{M}^{m \times n}$ when this involves decision variables of a Mathematical Program (MP). Requiring linear independence of a set of vectors $\{v_i \mid i \in N\} \subseteq \mathbb{R}^m$ (with $N = \{1, \ldots, n\}$ and n < m) of decision variables is a nontrivial feat: the elementary definition, $\forall \alpha \in \mathbb{R}^n$, $\sum_{i \in N} \alpha_i v_i = 0 \Rightarrow \alpha = 0$, requires in general uncountably many nonlinear constraints, each involving either binary variables or complementarity terms. We explore an equivalent definition of the rank of A (its number of nonzero eigenvalues) to propose models consisting of a finite set of nonconvex constraints. We showcase our results on an application to the Distance Geometry Problem (DGP).

2 The Distance Geometry Problem

In the DGP [5], we are given an integer K > 0 and a weighted undirected graph G = (V, E, d)with $d: E \to \mathbb{R}_+$ and $|V| = n \ge K$, and we must find $y: V \to \mathbb{R}^K$ satisfying the polynomial system

$$\|y_i - y_j\|_2 = d_{ij} \quad \forall (i,j) \in E, \tag{1}$$

where $y(i) = y_i$ and $d((i, j)) = d_{ij}$. It was shown in [8] that the system above can be reformulated exactly as

$$(e_i - e_j)^\top X(e_i - e_j) = d_{ij}^2 \quad \forall (i, j) \in E$$

$$\tag{2}$$

subject to $X = Y^{\top}Y$, where $Y = [y_1 \ y_2 \ \dots \ y_n]$ is the matrix whose columns are the vectors y and $e_i \in \mathbb{R}^n$ is the canonical unit vector of all zeros except an 1 at the *i*th-position. The

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latter condition can also be written as $\mathsf{rk} X \leq K$ (with $\mathsf{rk} X = K$ if Y is required to span \mathbb{R}^K). The mapping between solutions of (1) and (2) is: if there exists X with rank K satisfying (2), there is $y_1, \ldots, y_n \in \mathbb{R}^K$ satisfying (1) with $\langle y_i, y_j \rangle = x_{ij}, \forall (i, j) \in E$. There are polynomial time algorithms to retrieve the vectors y associated to a solution X.

In [5] one finds the classical MP formulation used to solve the DGP. We however propose and use a simpler formulation w.r.t. nonlinearities. In order to derive the formulation equivalent to (2), we first expand the squared Euclidean norm term of (1) to obtain that $||y_i - y_j||_2^2 =$ $\langle (y_i - y_j), (y_i - y_j) \rangle = \langle y_i, y_i \rangle - 2\langle y_i, y_j \rangle + \langle y_j, y_j \rangle = x_{ii} - 2x_{ij} + x_{jj}, \forall (i, j) \in E$. Then, to each $(i, j) \in E$, we associate a continuous variable $s_{ij} = |x_{ii} - 2x_{ij} + x_{jj} - (d_{ij})^2|$ that measures the deviation from the respective given distance. All global optima of the DGP have zero total deviation. We can thus formulate the linear programming relaxation:

$$\min \sum_{(i,j)\in E} s_{ij} \tag{3}$$

s.t.
$$s_{ij} \ge x_{ii} - 2x_{ij} + x_{jj} - (d_{ij})^2, \quad \forall (i,j) \in E,$$
 (4)

$$s_{ij} \ge -x_{ii} + 2x_{ij} - x_{jj} + (d_{ij})^2, \ \forall (i,j) \in E.$$
(5)

It remains to formulate and adjoin to (3)-(5) the rank constraints over the matrix X. Contraints (4) and (5) together guarantee that the total deviation (objective function) tends to zero through positive values whenever $||y_i - y_j||_2^2 \neq (d_{ij})^2$ for any $(i, j) \in E$.

3 Modelling the rank

The rank is modeled as the number of nonzero eigenvalues of X using the eigensystem and eigendecompositon to encode eigenvalues and eigenvectors as decision variables.

Eigensystem: we assume that $\lambda_i(X) \subseteq [L_i, U_i]$ for $i \in N$ (with $L_i, U_i \in \mathbb{R}$) and that all nonzero eigenvalues have absolute value greater than a given $\epsilon > 0$. Define a sequence of binary decision variables like $z : N \to \{0, 1\}$. Moreover, let δ_{ij} be the Kronecker delta for $i, j \in N$. Consider the system of constraints:

$$\forall i, j \in N, \quad \sum_{k \in N} x_{ik} \vartheta_{kj} = \lambda_j \vartheta_{ij}, \tag{6}$$

$$\forall i, j \in N, \quad \sum_{k \in N} \vartheta_{ki} \vartheta_{kj} = \delta_{ij}, \tag{7}$$

$$\forall i \in N, \quad \lambda_i^2 \ge \epsilon^2 z_i, \tag{8}$$

$$\forall i \in N, \quad L_i z_i \le \lambda_i \le U_i z_i. \tag{9}$$

Constraints (6) represent the eigensystem. Constraints (7) state that the set $\{\vartheta_1, ..., \vartheta_n\}$ is an orthonormal eigenbasis of \mathbb{R}^n associated to X. Constraints (8)-(9) require that for all $i \in N, \lambda_i = 0 \Leftrightarrow z_i = 0$. By elementary linear algebra, the system above always has a solution whenever λ, ϑ are allowed to range over the complex numbers. The DGP as modeled in Section 2 actually require X to be a symmetric matrix. By adjoining symmetry constraints to X:

$$\forall i < j \in N, \quad x_{ij} = x_{ji},\tag{10}$$

we make sure the system can be solved over the reals. We call MES the model (6)-(10).

Eigendecomposition: the next model follows directly from substituting (6) by constraints that represent the eigendecomposition of X:

$$\forall i, j \in N, \quad x_{ij} = \sum_{k \in N} \vartheta_{ik} \vartheta_{jk} \lambda_k.$$
(11)

It is simple to see that constraints (11) implicitly guarantee that X is symmetric. Hence we do not need to adjoin constraints (10) to the model (11),(7)-(9), henceforth named MED. If we do add (10) to MED, the total number of constraints (11) are reduced as follows:

$$\forall i \le j \in N, \quad x_{ij} = \sum_{k \in N} \vartheta_{ik} \vartheta_{jk} \lambda_k, \tag{12}$$

to obtain a third model given by the constraints (12),(7)-(10), called MED_{RS}.

Rank constraint: finally, rank constraints can be constructed by means of the z variables:

$$\sum_{i \in N} z_i = r, \ r \in \mathbb{N}.$$
(13)

We remark that other types of constraints (e.g. the rank is bounded above by r) and objectives (e.g. the rank must be maximum) can be constructed similarly. In the DGP, r = K in (13).

Additional constraints: we make use of extra constraints that may improve the performance of the solver used. Namely, they are: the trace constraint (TC), symmetry breaking constraints (SBCs) [4] on the λ variables and complementary constraints (CCs) on the z and λ variables.

4 Computational experiments

The models MES, MED and MED_{RS} were combined either with a TC or with SBCs or with both. The formulations were solved using BARON 14.0.3 [9, 7] under the GAMS [6] environment, publicly available at the NEOS Server [1]. We adjoined CCs to all formulations because BARON may benefit from it [7]. Execution time was limited to 3 hours of wall clock time; we considered $\epsilon = 0.005$ and we set GAMS termination option *optca* [6] to 0.001. The eigenvalues' bounds ([3, Thm. 1]) were computed using Eigen [2], a C++ template library for linear algebra.

Table 1 reports the results for all MES, MED and MED_{RS} based formulations. Per instance and for each formulation, the table exhibits the best solution found, the elapsed wall clock time (in seconds), the number of nodes explored and the solver status (opt = optimal, feas = feasible, nsf = no solution found). Best values are emphasized in boldface.

The results obtained so far are too few (only 4 instances were submitted to testing) to draw definitive conclusions on which family of models performs the better, but we observe a slight advantage to the MED_{RS} based formulations: optimal solutions were found in 12 out of 16 runs, with 2 overall better performances (C0700odd.1 and lavor11) and a second place (C0700odd.2). On the other hand, the MES based formulations performed the worse: only in 8 of 16 runs an optimum was found, not even a feasible solution found for lavor11 and no overall better performance. Some execution times (particularly those for C0150alter.1 and the MES models) surpassed the pre-established time limit due to unknown reasons. In general, the only certainty we have so far is that it is unlike to solve big instances (all instances have at most 11 points except for C0150alter.1 that has 26) unless we either improve the modelling or the bounds on the x variables; the latter improvement would also yield an improvement in the bounds of the eigenvalues variables; theoretically, tighter bounds would favor BARON [7]. Another options would be to try other global optimization solvers or a VNS like heuristic.

Model	Instance	Best	Time	Nodes	St.	Instance	Best	Time	Nodes	St.
mes	C0700odd.1	0.00	74.62	3	opt	C0700odd.2	0.00	857.04	1255	opt
mes_trace	C0700odd.1	0.00	120.54	11	opt	C0700odd.2	0.00	570.58	724	$_{\rm opt}$
mes_sbcs	C0700odd.1	0.00	459.59	886	opt	C0700odd.2	0.00	760.26	684	opt
mes_trace_sbcs	C0700odd.1	0.00	10.40	1	opt	C0700odd.2	0.00	760.80	1439	$_{\rm opt}$
med	C0700odd.1	0.00	5.10	1	opt	C0700odd.2	0.00	11.69	1	opt
med_trace	C0700odd.1	0.00	50.92	49	opt	C0700odd.2	0.00	5.99	1	$_{\rm opt}$
med_sbcs	C0700odd.1	0.00	7.71	1	opt	C0700odd.2	0.00	104.35	46	opt
med_trace_sbcs	C0700odd.1	0.00	118.41	166	opt	C0700odd.2	0.00	79.00	56	$_{\rm opt}$
medrs	C0700odd.1	0.00	4.96	1	opt	C0700odd.2	0.00	7.98	1	opt
medrs_trace	C0700odd.1	0.00	11.23	6	opt	C0700odd.2	0.00	64.47	85	opt
medrs_sbcs	C0700odd.1	0.00	5.49	1	opt	C0700odd.2	0.00	8.77	1	$_{\rm opt}$
medrs_trace_sbcs	C0700odd.1	0.00	123.86	77	$_{\rm opt}$	C0700odd.2	0.00	40.99	6	opt
mes	lavor11	-	10800.00	145	nsf	C0150alter.1	-	14922.54	1	nsf
mes_trace	lavor11	-	10800.00	34	nsf	C0150alter.1	-	12962.56	1	nsf
mes_sbcs	lavor11	-	10800.00	65	nsf	C0150alter.1	-	10800.04	1	nsf
mes_trace_sbcs	lavor11	-	10800.00	82	nsf	C0150alter.1	-	10800.08	1	nsf
med	lavor11	0.00	598.25	46	opt	C0150alter.1	-	10999.20	1	nsf
med_trace	lavor11	0.00	363.20	46	opt	C0150alter.1	-	10810.50	1	nsf
med_sbcs	lavor11	0.00	1181.55	36	opt	C0150alter.1	-	10821.59	1	nsf
med_trace_sbcs	lavor11	0.00	912.91	46	opt	C0150alter.1	-	10800.41	1	nsf
medrs	lavor11	0.00	18.85	1	opt	C0150alter.1	-	10980.55	1	nsf
medrs_trace	lavor11	0.00	21.26	1	opt	C0150alter.1	-	10916.17	1	nsf
medrs_sbcs	lavor11	0.00	1353.86	285	opt	C0150alter.1	-	10800.04	1	nsf
medrs_trace_sbcs	lavor11	0.00	17.51	1	$_{\rm opt}$	C0150alter.1	-	10972.76	1	nsf

Table 1: Results obtained from all DGP formulations using BARON 14.0.3.

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