Some global optimization problems on Stiefel manifolds *

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Abstract. Optimization on Stiefel manifolds was discussed by Rapcsák in earlier papers, and some global optimization methods were considered and tested on Stiefel manifolds. In the paper, test functions are given with known global optimum points and their optimal function values. A restriction, which leads to a discretization of the problem is suggested, which results in a problem equivalent to the well-known assignment problem.

Keywords: Nonlinear optimization; Quadratic equality constraints; Stiefel manifolds

1. Introduction

In 1935, Stiefel introduced a differentiable manifold consisting of all the orthonormal vector systems $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_k \in \mathbb{R}^n$, where $\mathbb{R}^n$ is the n-dimensional Euclidean space and $k \leq n$ (Stiefel, 1935-36). Bolla et al. analyzed the maximization of sums of heterogeneous quadratic functions on Stiefel manifolds based on matrix theory and gave the first-order and second-order necessary optimality conditions and a globally convergent algorithm (Bolla et al., 1998). Rapcsák introduced a new coordinate representation and reformed the original one to a smooth nonlinear optimization problem. Then, by using Riemannian geometry and the global Lagrange multiplier rule (Rapcsák, 2001; Rapcsák, 2002; Rapcsák, 2003), local and global, first-order and second-order nec-

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essary and sufficient optimality conditions were stated, and a globally convergent class of nonlinear optimization methods was suggested.

In the paper, some special global optimization problems on Stiefel manifolds are investigated and test functions are given for the global optimization tools. Consider the following optimization problem:

$$\min \sum_{i=1}^{k} \mathbf{x}_i^T A_i \mathbf{x}_i \tag{1}$$

$$\mathbf{x}_i^T \mathbf{x}_j = \delta_{ij}, \qquad 1 \le i, j \le k, \tag{2}$$
$$\mathbf{x}_i \in \mathbb{R}^n, \quad i = 1, \ldots, k, \qquad n \ge 2,$$

where A_i, $i = 1, \ldots, k$, are symmetric matrices, and δ_{ij} is the Kronecker delta. Furthermore, let $M_{n,k}$ denote the Stiefel manifold consisting of all the orthonormal systems of k vectors in the n-dimensional Euclidean space. Hence, we deal with the optimization of special type of quadratic functions subject to quadratic constraints. In the literature of optimization, not too many efficient methods giving a good approximate solution of this problem are known. It is also difficult to provide feasible solutions for it (Horst and Pardalos, 1995). This is the reason why special instances of the original problem are investigated.

In (Balogh et al., 2002), solution methods and techniques are given for the numerical optimization of problem (1)-(2). The structure of the optimum points is characterized in the lowest-dimensional interesting case and a criterion is given for the finiteness of the number of the optimum points on $M_{2,2}$ of (1)-(2). The case of diagonal matrices A_i, $i = 1, \ldots, k$, where all coordinates of the optimum points are from the set $\{0, +1, -1\}$, is dealt with separately (except the extreme case when all feasible points are optimum points, as well).

Some reduction steps and numerical results are presented in (Balogh et al., 2002) for the numerical optimization of (1)-(2). To illustrate them, a numerical study was attached, in which the computational costs were demonstrated by the number of functions (also gradient and constraint) evaluations and CPU time to measure the complexity of the problems. In other words, we studied problem (1)-(2) numerically to understand the structure of the problem and investigated an example with a diagonal coefficient matrix by using a stochastic method (Csendes, 1988) and a reliable procedure (Corliss and Kearfott, 1999; Kearfott, 1999). The aim of the application of the last one was to obtain verified solutions. It is worth mentioning that the GlobSol program (Corliss and Kearfott, 1999; Kearfott, 1999) provided verified solutions only by using spherical substitutions. Without such transformations, a similar problem on $M_{3,3}$ required a few days of running time — and without obtaining a verified solution. Thus, it seems indispensable to use some reduction steps to make the numerical tools reliable, effective and efficient. Some accelerating modifications are suggested in the paper. We focused again on a special problem instance where the coefficient matrices in the objective function are diagonal.

Since the results can easily be non optimal as it was seen, in the paper, we generate a series of test problems of arbitrary size (with n and k as parameters). These problems belong to an important area of global optimization (see (Floudas et al., 1990) and (Floudas et al., 1999)), to the constrained test problems which are used in several industrial applications.

In the paper, a theoretical investigation is completed on a discretization of the problem (1)-(2), which results in the well-known assignment problem. It can be easily seen that instead of the objective function (1), we can use a different one, e.g. the quadratic function

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{t=1}^{n}\sum_{r=1}^{n} a_{ij}\mathbf{x}_{it}\mathbf{x}_{jr}b_{tr}.$$

The respective restriction to the values give an NP-hard problem, the quadratic assignment problem, see (Pardalos et al., 1994) or (Sahni and Gonzalez, 1996).

2. Test functions on $M_{n,k}$ with known minimum points and minimum value

In this section, first, special constrained test functions are given with known optimum points and optima on each $M_{n,k}$ Stiefel manifold. This field, defining test functions, plays an important role in the literature of global optimization, for example, in theory and algorithm design, and naturally, in their tests (see (Floudas et al., 1990; Horst and Pardalos, 1995)). The handbook of Pardalos and Floudas does not contain a lot of constrained problems of global optimization, and the appearing test examples are, generally, from industrial applications (Horst and Pardalos, 1995).

As reported in (Balogh et al., 2002), a simple example of (Rapcsák, 2002), given on $M_{2,2}$ with diagonal coefficient matrices requires about 3 million function evaluations (out of which 2.9 million ones are the dense constraint evaluations) by using the GlobSol software (Corliss and Kearfott, 1999; Kearfott, 1999). The reason for this large computational effort is that the algorithm aims to verify the solutions with sophisticated interval arithmetic based techniques. Furthermore, the received boxes could not be verified, we know that they do not contain the optimal solution. Only the version with the polar form gives verified solutions. A not too complicated optimization problem on $M_{3,3}$ required about 3.5 days of CPU time on our computer and gave 36 different non-verified solutions with different function values through using the GlobSol program (Corliss and Kearfott, 1999; Kearfott, 1999). However, the hull of the non-verified boxes is about 10^{-24} times smaller than that of the starting one. The correctness of these values is very hard to be checked, because this question is equivalent to the original problem. This is why it makes sense to provide special problems on $M_{n,k}$ to test the efficiency and reliability of our algorithms. The advantage of the consideration of test problems like this is that we can handle objective functions more easily: the optimum points and optimum values are known on an arbitrary $M_{n,k}$ Stiefel manifold. For instance, on $M_{3,3}$ we can give a problem with 8 a priori known global optimal solutions. Let us consider minimization problem (1)-(2) on $M_{3,3}$, which is given by the diagonal coefficient matrices

$$A_1 = \mathrm{diag}(-1, 2, 3), \quad A_2 = \mathrm{diag}(4, -5, 6), \quad A_3 = \mathrm{diag}(7, 8, -9).$$

This is a good test function for the optimization methods, because all its global optimum points are easy to determine. Constraints (2) express that x_i, $(i = 1, 2, 3)$ are on the unit sphere. It follows that $0 \leq x_{ij}^2 \leq 1$ for all $1 \leq i, j \leq n$, and a lower bound can be obtained for the objective function value as follows:

$$f(\mathbf{x}) = (-1)x_{11}^2 + 2x_{12}^2 + \ldots + (-9)x_{33}^2 \geq (-1) \cdot 1 + 2 \cdot 0 + \ldots + (-9) \cdot 1$$

for $\mathbf{x} \in M_{3,3}$. It is easy to see that this optimum value is realized at the points

$$\pm 1, 0, 0; \quad 0, \pm 1, 0; \quad 0, 0, \pm 1,$$

and the optimum value is equal to -15. Here, all the possible combinations of values ± 1 give minimum points. The minimum value cannot be attained at another point of $M_{3,3}$, since at different points, the function values are obviously greater.

This method creating test functions on $M_{3,3}$ can be generalized for arbitrary values n, k $(n \geq k \geq 2)$ with the same property, i.e., the minimum points and the minimum value can be determined in an easy way. These problems are formulated for every possible pair n, k on $M_{n,k}$ as follows:

Example 1 Let us consider problem (1)-(2), where

$$\begin{aligned} A_1 &= \mathrm{diag}(l_1, 2, 3, \ldots, n), \\ A_2 &= \mathrm{diag}(n+1, l_2, n+3, n+4, \ldots, 2n), \\ &\ldots, \\ A_i &= \mathrm{diag}(n(i-1)+1, \ldots, n(i-1)+i-1, l_i, n(i-1)+i+1, \ldots, ni), \\ &\ldots, \\ A_k &= \mathrm{diag}(n(k-1)+1, \ldots, nk-1, l_k) \end{aligned} \tag{3}$$

are the diagonal coefficient matrices and $l_i < 0$, $i = 1 \ldots k$.

The above problem is a special case of Example 1 where $n = 3$, $k = 3$; $l_1 = -1, l_2 = -5$ and $l_k = l_3 = -9$. A further choice could be $l_i = -1, i = 1, \ldots k$ and keep the other values. In this case, the function value is the sum of all l_i, i.e., $-k$. The next statement shows that the places of the minima can be determined in a similar way to that of in Example 1. Let us introduce some notations.

Let $\pm E_{n,k}$ denote all the orthonormal systems of k number of n-vectors where the i-th vector ($i = 1, \ldots, k$) is the i-th unit vector (or multiplied by -1). In this way, each vector has only one non-zero coordinate, the i-th one of the i-th vector, the value of which is either 1 or -1 ($i = 1, \ldots, k$). It follows that $\pm E_{n,k}$ is a set of 2^k orthonormal vector systems. If e_i denotes the i-th unit vector, then

$$\pm E_{n,k} = \{(\pm e_1, \ldots \pm e_k) \mid \pm e_i \in \{e_i, -e_i\}\}.$$

Proposition 1 *The set of the minimum points of (1)-(2)-type problems with coefficient matrices (3) and constraints (2) is exactly* $\pm E_{n,k}$.

Proof It is sufficient to prove that an $\mathbf{e}^* \in \pm E_{n,k}$ is a feasible solution, furthermore, that at any other feasible point $\mathbf{x} \notin \pm E_{n,k}$, the objective function value is greater than the optimum, i.e., $f(\mathbf{x}) > f(\mathbf{e}^*)$.

A) To see that a vector $\mathbf{e}^* \in \pm E_{n,k}$ is a feasible point of the given problem, it must be shown that it satisfies equations (2). It is obvious that all the vector systems in $\pm E_{n,k}$ are on the unit circle and they are orthogonal, hence, they satisfy constraints (2) (see the earlier argumentation), and hence they are feasible.

B) Let us show now that the function value at any other feasible point is greater than the minimum. Consider a vector system $(\mathbf{y}_1, \ldots \mathbf{y}_k) \in M_{n,k}$ for which $(\mathbf{y}_1, \ldots \mathbf{y}_k) \notin \pm E_{n,k}$. Let us separate the index set $\{1, \ldots, k\}$ into two disjoint parts: $S \cup T = \{1, \ldots, k\}$ such that S contains all the indices of the vectors for which either $\mathbf{y}_s = \mathbf{e}_s$, or $\mathbf{y}_s = -\mathbf{e}_s$. Then, T contains the rest of the indices, thus $\mathbf{y}_t \neq \pm\mathbf{e}_t$ holds for any $t \in T$. Due to the assumption, $T \neq \emptyset$ must hold. Thus, the objective function value at the chosen point $\mathbf{y}$ is

$$\begin{aligned}\sum_{m\in\{1,\ldots,k\}} \mathbf{y}_m^T A_m \mathbf{y}_m &= \sum_{s\in S} \mathbf{y}_s^T A_s \mathbf{y}_s + \sum_{t\in T} \mathbf{y}_t^T A_t \mathbf{y}_t \\ &= \sum_{s\in S} \mathbf{e}_s^T A_s \mathbf{e}_s + \sum_{t\in T} \mathbf{y}_t^T A_t \mathbf{y}_t.\end{aligned}$$

Now, consider the difference from the minimum value:

$$\sum_{s\in S} \mathbf{e}_s^T A_s \mathbf{e}_s + \sum_{t\in T} \mathbf{y}_t^T A_t \mathbf{y}_t - \sum_{s\in S} \mathbf{e}_s^T A_s \mathbf{e}_s - \sum_{t\in T} \mathbf{e}_t^T A_t \mathbf{e}_t =$$

$$\sum_{t\in T} \mathbf{y}_t^T A_t \mathbf{y}_t - \sum_{t\in T} \mathbf{e}_t^T A_t \mathbf{e}_t = \sum_{t\in T} \left(\mathbf{y}_t^T A_t \mathbf{y}_t - \mathbf{e}_t^T A_t \mathbf{e}_t\right) = \sum_{t\in T} \sum_{i=1}^{n} a_{ii}^t (y_{ti}^2 - e_{ti}^2) =$$

$$\underbrace{\underbrace{\sum_{i=1,\ldots,n,} \underbrace{a_{ii}^i}_{<0} \underbrace{(y_{ii}^2 - 1)}_{\leq 0}}_{\geq 0} + \underbrace{\sum_{t\in T} \sum_{i=1,\ldots,n;\, i\neq t} \underbrace{a_{ii}^t y_{ti}^2}_{\geq 0}}_{\geq 0}}_{\geq 0} \geq 0.$$

Because of the assumptions, at least one term in the above sum is different from zero, thus part B) and hence the whole proposition is proved. □

2.1. Some technical notes

We have produced an infinite sequence of constrained global optimization test problems. Each is defined on an $M_{n,k}$ Stiefel manifold, $(n \geq k \geq 2)$, with 2^k solutions, thus the number of the minimum points is exponential in k. Moreover, the minimum value is easy to calculate: it is equal to the sum of the negative coefficients in A_i, $(i = 1, \ldots, k)$. This feature is advantageous in testing some optimization codes, e.g., those ones which can utilize the known minimum value (Casado et al., 2000).

The difficulty in these test problems caused by the great number of global (and local) minima which can be decreased by the addition of well chosen $x_{ij} \cdot x_{ik}$ terms to the objective function. By subtracting all $x_{ij}x_{il}$, $i = 1, \ldots, k; j, l = 1, \ldots, n; j \neq l$, for example, only two solutions remain (all non-zero coordinates are either $+1$, or -1, one coordinate per dimension, and all other values are 0). Unfortunately, the obtained problem, is no more of a diagonal type. To obtain a maximization problem, a matrix $-A_i$ must be applied, instead of A_i, for every index i.

Example 2 Let us consider problem (1)-(2) where

$$\begin{aligned} A_1 &= \mathrm{diag}(-1, 2), \\ A_2 &= \mathrm{diag}(3, -1). \end{aligned}$$

The objective function is then

$$f(\mathbf{x}) = -x_{11}^2 + 2x_{12}^2 + 3x_{21}^2 - x_{22}^2,$$

and the set of solution points is given by

$$\mathbf{x}^* = ((\pm 1, 0)^T, (0, \pm 1)^T)$$

consisting of $2^2 = 4$ points. The optimum value is the sum of the negative values in the diagonal, i.e., -2 in accordance with the above discussion.

3. Restriction of the feasible points

In this section, we impose a special restriction on the set of feasible points $M_{n,k}$. In the case of a special $0 - 1$ discretization of (2) and a quadratic objective function, an NP-hard problem, the quadratic assignment problem (Sahni and Gonzalez, 1996) is obtained.

In (Balogh et al., 2002) and the previous section, several instances have optimal solutions where every vector lies on an n-dimensional coordinate axis (that is, one of their coordinates is 1 or -1, and the $n-1$ other coordinates are zero). It was shown that on $M_{2,2}$ the optimal solutions' type is the above in the case of diagonal coefficient matrices (the only exception if the function is constant on the whole $M_{2,2}$). In cases like this, all solutions are from the set of the crossing points of the n-dimensional hypersphere and the coordinate axes. In other words, not only the given problems and test problems have solutions of this type, but also other problems can be included in this class. The common feature of these problems is that the objective function has only squared terms.

This fact served as motivation to restrict the feasible solution set of the problem. Consider the following restriction: if the set of the feasible points is a subset of $M_{n,k}$, the feasible solutions should also contain all

k vectors on an n-dimensional coordinate axis. We will perform this investigation in three steps: first, only $n \times n$ problems are considered in which there are square components only (the case of diagonal matrices). Then, we study the problems of the same type of $n \times k$ size, and finally, the general problem. All these cases will be considered on this restricted feasible set. If, however, the objective function is not of type (1), the structure of the solution set is an open question even on this restricted set of feasible points denoted by L'.

What can these restrictions be applied to? On the one hand, they can be used to approximate the optimum value f^* and this approximation can also be applied in some optimization methods to accelerate their convergence (see, e.g., (Casado et al., 2000)).

Let us return to the mentioned three-step-procedure. The above restriction of set (2) of feasible points to L' leads us back to the well-known assignment problem, as stated in the next proposition.

Proposition 2 *If the set of the feasible points $M_{n,k}$ in problem (1)-(2) is restricted to L' defined as the set of the crossing points of the n-dimensional unit sphere, the problem determined by (1) and the restriction of (2) to L' is equivalent to an assignment problem.*

Proof The proof needs a three-step-procedure. We start with the first special case on $M_{n,n}$, containing only diagonal coefficient matrices A_i $(i = 1, \dots, k = n)$ in the objective function (1). Then, using the first statement, the above fact can be generalized easily for $M_{n,k}$ with diagonal form matrices as well. Using the first and second statements in the third phase, we give the proof of the whole proposition. It is the case of the general form matrices of (1) on $M_{n,k}$.

1. Problem (1)-(2) on $M_{n,n}$ is equivalent to the assignment problem if the coefficient matrices are diagonal, and the set of the possible solutions L' is the set of crossing points of the n-dimensional unit sphere and the coordinate axes of R^n.

The well-known assignment problem is as follows:

$$\min \sum_{i=1}^{n} \sum_{j=1}^{n} x_{ij} a_{ij} \tag{4}$$

subject to

$$\sum_{t=1}^{n} x_{it} = 1 \quad (i = 1, \dots, n), \tag{5}$$

$$\sum_{t=1}^{n} x_{tj} = 1 \quad (j = 1, \dots, n), \tag{6}$$

$$x_{ij} \in \{0, 1\} \quad (i = 1, \dots, n;\ j = 1, \dots, n), \tag{7}$$

where the coefficients a_{ij} form an $n \times n$ matrix A'. We have to show that the objective function (1) and constraints (2) result in (4-7) on the new restricted set L'. Notice first that each x_i has $n-1$ zero components, and exactly one component is equal to one.

Let the elements a_{ij} of the A' matrix of the assignment problem be the matrix-elements $(A_i)_{jj}$ of (1). Furthermore, let the assignment problem's x_{ij} variables be the j-th elements of $\mathbf{x}_i$ in (1). Under these assumptions, constraints (5)-(7) of the assignment problem imply constraints (2) of the original problem, and the objective function (4) provides the original one in (1).

2. The above statement can be generalized for the Stiefel manifolds $M_{n,k}$. A problem (1)-(2) on $M_{n,k}$ with the previous restriction is equivalent to an assignment problem.

To show this, consider an assignment problem with an $n \times n$ matrix instead of the $k \times n$. Fill the missing $n-k$ rows with the value of $M+1$, where M is the sum of the absolute values of the first k columns. After solving the obtained assignment problem, e.g., by the Hungarian method, and leaving out the last $n-k$ vectors, there remains a system of k n-vectors which is exactly the solution of the original problem, as it can be seen easily.

Let us return now to the general case from the objective functions' point of view: we will consider problem (1)-(2), but on the restriction of $M_{n,k}$ to the vectors of the coordinate axes (5)-(7).

3. It is sufficient to show that the latter problem is equivalent to a problem the objective function of which contains the terms $x_i x_i$ multiplied by their coefficient $(A_i)_{ii}$ for every i. This problem is equivalent to the assignment problem which has been proved above.

Let us examine (1) on the subset L'. Each vector in L' is of a special property, namely, each coordinate except one of these is 0. Thus, in the objective function (1), each term $x_{ij}x_{jl}$ is zero, except the terms x_{ii}^2.

Formally:

$$\sum_{i=1}^{k} \mathbf{x}_i^T A_i \mathbf{x}_i = \sum_{i=1}^{k} (\sum_{j=1}^{n} \sum_{l=1}^{n} x_{ij}(A_i)_{jl} x_{il}) = \sum_{i=1}^{k} x_{ii}(A_i)_{ii} x_{ii} = \sum_{i=1}^{k} x_{ii}^2 (A_i)_{ii}.$$

It follows that we have obtained a problem which is equivalent to the problem of the previous proposition. □

Returning to the general case, a question can be raised: how can a general problem (the objective function of which is not necessarily given in the form (1)) be solved, considering the above restriction to the L' subset of $M_{n,k}$. In this case, if $n = k$, we have a special assignment problem, in which the $0-1$ value restriction of the problem is considered.

By the $0-1$ restriction on the set of feasible points defined by (2), instead of the $\{0, \pm 1\}$ restriction, we obtain a set of constraints of an assignment problem. This can also be obtained by writing 1 into the appropriate place, and writing 0 into all the other ones.

If the objective function is arbitrary quadratic, a quadratic assignment problem is obtained which is an NP-hard problem (Sahni and Gonzalez, 1996). Several relevant theoretical results can be found in the literature, for example, Pardalos et al. cite 254 related publications in their survey (Pardalos et al., 1994). The linear assignment problem is an LP-problem having many special cases (e.g., transportation problem).

On the one hand, it is interesting in itself to examine our problem with the restriction L' of $M_{n,k}$, on the other hand, this may have some advantages. As we have seen above, the solutions can be provided in the case of diagonal coefficient matrices. In general, this technique can be applied to arbitrary coefficient matrices by obtaining an approximation for the optima. The solution of the problem, subject to the set L' of feasible points, can be arbitrarily far from the solution of the original problem on $M_{n,k}$.

Another open question, regarding the last observation, is whether a good heuristic can be given regarding the approximation of the optimum value f^* with the restriction of the feasible points of the problem to the points of the coordinate axis, just like regarding the problems having square components only.

Example 3 Consider an example on the manifold $M_{3,2}$ with the objective function

$$3x_{11}^2 + 6x_{12}^2 + 4x_{13}^2 + 7x_{11}x_{12} - 4x_{11}x_{13} - 18x_{12}x_{13} -$$

$$3x_{21}^2 + 5x_{22}^2 + 3x_{23}^2 - 6x_{21}x_{22} + 7x_{21}x_{23} - 12x_{22}x_{23}$$

to be minimized on the restricted set of 0-1 valued coordinates.

This problem can be related to a problem (1)-(2) with the matrices

$$A_1 = \begin{pmatrix} 3 & 7/2 & -2 \\ 7/2 & 6 & -9 \\ -2 & -9 & 4 \end{pmatrix},$$

$$A_2 = \begin{pmatrix} -3 & -3 & 7/2 \\ -3 & 5 & -6 \\ 7/2 & -6 & 3 \end{pmatrix}.$$

According to the last result, the optimal solution is

$$\mathbf{x}^* = ((0,0,1)^T, (1,0,0)^T),$$

and the optimum value is 1.

4. Conclusions

It has been demonstrated earlier that a simple (9-variable) problem on $M_{3,3}$ runs for more than 3 days on an average computer if we require reliable results. That is why the possible speed up improvements should be theoretically investigated both in geometrical reductions and in numerical tools. Hence, appropriate testing examples should be necessary. The paper suggests test examples with known optimal solutions to measure the efficiency of the numerical tools. In a special case, the diagonal matrices A_i $(i = 1, \ldots, k)$ have been analyzed in details. Furthermore, an interesting special restricted problem was presented which is equivalent to an assignment problem where the number of minimum points is finite, although it is exponential in the size of the input. An interesting question is how to characterize the criterion of the finiteness of the number of the optimum points on $M_{n,k}$ in the studied problems. We intend to try other computational tools such as an interval based constraint handling global optimization method (Markót et al., 2003).

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