Test functions and to test functions: a framework for global optimization on Stiefel manifolds

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Some methods of the global optimization are dealt and tested on Stiefel manifolds. The structure of the optimizer points is given theoretically and numerically for the lowest interesting dimensional case, as well as the criterion for the finiteness of the number of optimizer points. Some reduction tricks and numerical results are obtained, and test functions with known optimizer points and their optimal function value. A restriction, discretization of the problem is formulated which is equivalent to the well known assignment problem.

In 1935, Stiefel introduced a differentiable manifold consisting of all the orthonormal vector system $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_k \in \mathbb{R}^n$, where $\mathbb{R}^n$ is the n-dimensional Euclidean space and $k \leq n$ [1]. 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 [2]. Rapcsák introduced a new coordinate representation and reformulated it to a smooth nonlinear optimization problem, then by using the Riemannian geometry and the global Lagrange multiplier rule [3, 4], local and global, first-order and second-order, necessary and sufficient optimality conditions were stated, and a globally convergent class of nonlinear optimization methods was suggested.

In the present work, solution methods and techniques are investigated for optimization on Stiefel manifolds. Consider the following optimization problem:

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

$$\mathbf{x}_i^T \mathbf{x}_j = \delta_{i,j}, \qquad 1 \leq i, j \leq k, \tag{2}$$

$$\mathbf{x}_i \in \mathbb{R}^n, \quad i = 1, \ldots, k, \qquad n \geq 2,$$

where A_i, $i = 1, \ldots, k$, are given 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 n-vectors.

We characterize the structure of the optimizer points and give a criterion for the finiteness of the number of the optimizer points on $M_{2,2}$ of (1-2). The case of diagonal matrices A, $i = 1, \ldots, k$, is dealt separately where all coordinates of the optimizer points are from the set $\{0, +1, -1\}$ (except the extreme case when all feasible points are optimizer points, as well).

We have studied numerically the same problem to understand the structure of the problem and investigated an example with a diagonal coefficient matrix using a stochastic method [5] and a reliable one [6], [7]. The aim of the last one was to obtain verified solutions. It can be interesting that using the GlobSol program [6], [7], verified solutions are obtained only when making spherical substitutions, while for a similar problem on $M_{3,3}$ it runs a few days without providing verified solution – if no coordinate transformation or reduction of the variables was made. Thus, it seems indispensable to use some reduction tricks to make the numerical tools effective. Some accelerating changes are suggested in the present work.

Since the result can be non-verified as it have been seen, by reversing the process we give a series of test problems with arbitrary size (where n and k are parameters). These belong to an important area of the global optimization (see [8] and [9]), the constrained test problems which are generally related to industrial applications.

Theoretical investigation is given for the discretization of the problem (1-2), which is equivalent to the well-known assignment problem. It can be seen easily that instead of the objective function of (1), we can use another one, for example, the quadratic function

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

and the respective restriction to the values give an NP-hard problem, the quadratic assignment problem, see [10] or [11].

Acknowledgment: The support provided by the Hungarian National Research Foundation (project Nos. T 034350 and T029572) and by the APOLL Thematic Network Project within the Fifth European Community Framework Program (FP5, project No. 14084) is gratefully acknowledged.

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