Numerical methods and experiments of global optimization problems on Stiefel manifolds

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Some global optimization methods are tested on Stiefel manifolds. The structure of the optimizer points is given theoretically and numerically for interesting lower dimensional cases. Some reduction tricks and numerical results are given as well.

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 $k \leq n$ [8]. 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 [3]. 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 [6, 7], 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:

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

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

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

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.

In the present talk, we optimize (1)-type quadratic functions with quadratic constraints. In the literature of optimization, there are not too many efficient methods which give a good approximation to this problem, moreover, to provide feasible solutions is also a difficult problem. Some important particular cases are considered in more details. In [2], we gave a series of test problems of arbitrary size (for different n and k values), as test functions with known optimizer points and optimal function value. Furthermore, in [2] a theoretical investigation is made for the discretization of the problem (1-2) which is equivalent to the well-known assignment problem.

We characterize the structure of the optimizer points on $M_{2,2}$ of (1-2), which is a generalization of a result of [1].

The case of diagonal matrices A_i, $i = 1, \ldots, k$, is dealt separately where all coordinates of the optimizer points are from the set $\{0, +1, -1\}$.

In the present talk we are focusing on the numerical investigation of the problem, and the results of it. This study is made by using a stochastic method [5] and a reliable one [4]. The aim of the last study was to obtain verified solutions. The result and difficulty of the numerical optimization will be discussed in the talk. If we require reliable solutions, the most of the computational effort in the numerical optimization is the so called "dense constrained" evaluation, i.e. to check whether a point is a feasible solution, according to the constraints (or not). Thus, it seems to be indispensable to use some reduction tricks in order to make the numerical tools effective. Some accelerating changes are suggested in the present work and on the results we obtained. Because of the big computational requirements, it can be interesting the using of non-reliable methods (heuristic-stochastic methods), for example by using penalty functions.

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