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Saddle-Point Problems and Their Iterative Solution

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Preface

It is often rumored that a "saddle point" in mathematics derives its name from the fact that the prototypical example in two dimensions is a surface that curves up in one direction and curves down in a different direction, resembling a riding saddle or a mountain pass between two peaks forming a landform saddle, see Figs. P.1 and P.2. In this contribution, we deal with a solution of linear algebraic systems with a particular 2-by-2 block structure, whereas the lower diagonal block is a zero matrix, and one of the two off-diagonal blocks is the transpose to the other. Since such systems arise also as the first-order optimality conditions in equality-constrained quadratic programming and any of its solutions represents a saddle point in the abovementioned meaning, we use the term "saddle-point problem" for the whole class of such problems. If the (2, 2)-block of this matrix is nonzero, then we use the term "generalized saddle-point problem."

The importance of saddle-point problems or generalized saddle-point problems stems from the fact that they arise in many applications of computational science, engineering, and humanities. Although it is impossible to cover all existing applications that lead to the solution of saddle-point problems and that sometimes naturally overlap, an attempt to keep and to regularly update a collection of various application fields and mathematical disciplines has been made by Michele Benzi (see the schematic list in Fig. P.3).

A lot of attention has been paid to saddle-point problems and their solution in the last two or three decades. A wide variety of results together have appeared in journal articles and conference proceedings as well as in comprehensive surveys and monographs. The excellent survey on numerical solution of saddle-point problems was given by Michele Benzi, Gene Golub, and Jörg Liesen in [12]. Although its purpose was to review the most promising solution approaches for saddle-point problems with an emphasis on iterative methods for large sparse systems, it became the most cited publication in the field, and it still reflects the contemporary state of the art. This fact is clearly visible in the first part of this textbook that loosely follows the subdivision used in [12]. The extensions included here are pointed out in the outline below.

The book by Howard Elman, David Silvester, and Andy Wathen [25] with a particular focus on applications in incompressible fluid dynamics is used not only as the basic reference book in computational fluid dynamics, but it is considered as a fundamental contribution to general numerical linear algebra concepts for solution of saddle-point problems such as the convergence analysis of MINRES, the block-diagonal and block-triangular preconditioning, or the theory of preconditioned iterative methods of $\mathcal{H}$-symmetric saddle-point problems. However, in many applications the information from the origin of saddle-point problems is absolutely essential. Discretization of partial differential equations such as Stokes or Navier-Stokes equations leads often to saddle-point problems. A variety of iterative methods for their solution have been proposed that have rates of convergence independent of the mesh size used in discretization. In most cases, these methods require a preconditioner that is spectrally equivalent or norm equivalent to the system matrix. This is frequently achieved only by very advanced techniques such as multigrid methods that certainly belong to the most efficient methods for solving large discretized problems [9, 21, 24, 48, 49, 68].

The continuous formulation of the original problem leads directly to natural preconditioning that guarantees the fast convergence of iterative methods. This transformation is often called operator preconditioning, and it motivates the construction of practical preconditioners used to accelerate the convergence of iterative methods for solution of resulting discretized problems. The bounds on convergence of iterative methods developed using the norm or spectral equivalence on operator level are then independent of discretization, while traditional approach is based on equivalence of matrices from a particular discretization and a particular preconditioner. These ideas were developed, e.g., in [5, 6, 28, 41, 43], or [49]. Indeed, in the context of numerical solution of partial differential equations, the discretization and efficient preconditioning should be tightly linked due to the fact that a preconditioner can be seen as a transformation of the discretization basis in the finite-dimensional given Hilbert space (see the book by Josef Málek and Zdeněk Strakoš [56]).

As it is seen from previous discussion, saddle-point problems represent a very wide research area with a large amount of work devoted to various applications. In this textbook we focus on some linear algebra aspects of solving saddle-point problems with emphasis on iterative methods, their analysis, implementation, and numerical behavior. We concentrate mainly on algebraic techniques that lead to comprehensive solvers for various saddle-point problems. Nevertheless, each of them can be adapted to particular class of problems with a specific application in mind. A great progress has been made toward an effective preconditioning of iterative methods that in many of such cases leads to very efficient solvers. Although we here briefly discuss some selected applications leading to saddle-point problems, we do not give a detailed treatment of any particular application-based approach. This textbook is based on the course “saddle-point problems and their solution” that is since 2014 included into the education program at the Department of Numerical Mathematics, Charles University in Prague. The course attempts to cover not only classical results on the solution of saddle-point problems that appeared in books, articles, and proceedings, but it also contains the presentation of original results achieved by the author and his colleagues. In particular, we concentrate on numerical behavior issues that have attracted considerably less attention than many other topics related to solving saddle-point problems. We analyze the accuracy of approximate solutions computed by inexact saddle-point solvers, where the solution of certain subproblems is replaced by a cheap relaxation with a relatively modest and easy-to-fulfill requirements. We also look at numerical behavior of certain iterative methods when applied to saddle-point problems with indefinite preconditioning. As an illustration, we consider also the case study with an example from a real-world application. The main idea here is to compare three main solution approaches without any preconditioning that lead to the same asymptotic (but suboptimal) rate of convergence. The development of the solver with optimal convergence rate independent on the discretization parameter that would require to use the information from the underlying continuous problem is out of the scope of this textbook.

The course represents a collection of nine relatively self-contained lectures with separate lists of relevant references. This textbook contains also nine chapters, but the bibliography is extended, unified, and moved toward the end. The first chapter is devoted to introductory remarks on saddle-point matrices and their indefiniteness and to the already mentioned saddle-point motivation from equality-constrained quadratic programming problems and second-order elliptic equations. In Chap. 2, we recall three prominent application fields that lead to saddle-point problems as augmented systems in least squares problems, in the form of linear systems from discretizations of partial differential equations with constraints and as Kuhn-Karush-Tucker systems in interior-point methods. The first part gives some basic facts on least squares methods that are useful also in the context of constraint preconditioning and covers some generalizations leading to saddle-point problems. Instead of a specification of a particular continuous problem, the second part on saddle-point problems that arise from discretization of partial differential equations uses a general abstract framework and formulation as mixed variational problem in certain Hilbert spaces together with the discretization in their finite-dimensional subspaces. The first part of Chap. 3 formulates the necessary and sufficient condition for the saddle-point matrix to be nonsingular and gives a review of basic results on the inverse of a saddle-point matrix that form essentially a background for two main solution approaches. In the second part, a special attention is paid to the spectral properties of this particular class of symmetric indefinite matrices including also the results on their inertia and on eigenvalue inclusion sets. Some of them were developed quite recently as those in the case of a semi-definite diagonal block or a rank-deficient off-diagonal block. Two main solution approaches, the Schur complement method and the null-space method, are discussed in Chap. 4 including their schematic algorithms in the general inner-outer iteration setting. The notion of the Schur complement method and the null-space method reappears several times throughout this textbook. We consider these two approaches in the context of factorization of saddle-point matrices, stationary iterative methods with indefinite splitting matrix, constraint preconditioning, and numerical behavior of inexact saddle-point solvers. Chapter 5 is devoted to the direct solution of saddle-point problems with a focus on the LDL^T factorization of symmetric indefinite matrices. It appears that under standard assumptions, the saddle-point matrix admits such a factorization, there is no need for pivoting. In addition, the condition number of the triangular factor can be explicitly bounded in terms of the condition numbers of the whole saddle-point matrix and diagonal block. Next, two main solution approaches are recalled again from a perspective of the direct solution of saddle-point problems. The central idea of Chap. 6 on the iterative solution of saddle-point problems using stationary iterative methods and Krylov subspace methods is to distinguish between three different cases: solution of the whole saddle-point system, solution of the Schur complement system, and solution of the system projected onto the null-space of the off-diagonal block. Therefore, we briefly discuss the most widely known and used Krylov subspace methods applied to symmetric positive definite systems, symmetric indefinite systems, and nonsymmetric systems: CG, MINRES, and GMRES. In particular, preconditioned Krylov subspace methods are reviewed very carefully treating all relevant combinations of the symmetric positive definite or indefinite system with the symmetric positive definite, symmetric indefinite, or nonsymmetric preconditioner. We briefly cover also multigrid methods that are successfully used for solving saddle-point problems that arise from discretizations of partial differential equations and give links to stationary iterative methods that represent their key ingredient in the form of smoothing procedure. Chapter 7 gives a survey on block preconditioners for saddle-point problems including block-diagonal, block-triangular, and constraint preconditioners. The focus is put on the relation of constraint preconditioners to the Schur complement or null-space method as these can be seen as applications of indefinitely preconditioned Krylov subspace method on the saddle-point problem with a particular initial guess. In Chap. 8 we concentrate on the numerical behavior of the Schur complement reduction method and the null-space method. Without going too much into details and without rigorous proofs of main results, we discuss the effects of inexact solution of inner systems on the maximum attainable accuracy of approximate solutions computed in the Schur complement method and in the null-space method with respect to the back-substitution formula used for computing the other approximate solutions to saddle-point system. We point out the optimal implementations delivering high-accuracy approximate solutions that are used in practical computations. We also study the influence of the scaling of the diagonal block in the saddle-point system solved with the conjugate gradient method and preconditioned with the corresponding constraint preconditioner on the accuracy of approximate solutions computed by these variants of the Schur complement method and of the null-space projection method. The described phenomena occur universally for all problems. In each case they are illustrated on small saddle-point problems, where we can also monitor their conditioning. Finally, Chap. 9 contains the case study that comes from a real-world application of groundwater flow modeling in the area of Stráž pod Ralskem in northern Bohemia. We consider the potential fluid flow in porous media discretized by the mixed-hybrid finite element method using trilateral prismatic elements with a uniformly regular mesh refinement leading to large-scale saddle-point problems with a particular block structure. The convergence behavior of the unpreconditioned MINRES method applied to the whole saddle-point problem, the Schur complement systems, and the systems projected onto certain null-spaces without preconditioning is analyzed using the tools described in previous chapters of this textbook. Since in the general indefinite case with positive and negative eigenvalues it is difficult to get sharp and descriptive bounds using the Chebyshev polynomials as in the positive definite case, for comparison of all approaches, the asymptotic convergence factor is used as a first indicator for describing their convergence behavior. It follows that the bounds for these three solution approaches are comparable in terms of the discretization parameter, and in practical situations they require efficient preconditioning that would ideally lead to convergence rate independent of discretization. The developed results are illustrated on a simple potential fluid flow problem in an artificial cubic domain.

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Fig. P.1 Bone horse saddles from the fifteenth century, traditionally associated with King Sigismund of Luxembourg (1368–1437), King of Hungary and Croatia (1387–1437), King of Germany (1411–1437), King of Bohemia (1419–1437), King of Italy (1431–1437) and Holy Roman Emperor (1433–1437). Collections of Hungarian National Museum, Budapest. (Courtesy of D. Dvořáková: Kôň a človek v stredoveku, Vydavateľstvo Rak, Budmerice, 2007)

Fig. P.2 Priečne sedlo (saddle) (2352 m above sea level) located in High Tatras, Slovakia, is a narrow pass from Malá Studená dolina to Velká Studená dolina, two beautiful mountain valleys, connecting in fact Téryho chata and Zbojnícka chata cottages. Sedielko ("little saddle") (2376 m above sea level) is the highest tourist pass across the main mountain ridge of High Tatras, connecting Malá Studená dolina with Zadná Javorová dolina. Priečne sedlo and Sedielko are connected with the ridge that summits in the peak Široká veža (2462 m above sea level). (Photo taken by I. Bohuš, ml. Courtesy of I. Bohušová, Vydavateľstvo IB Tatry, Tatranská Lomnica)

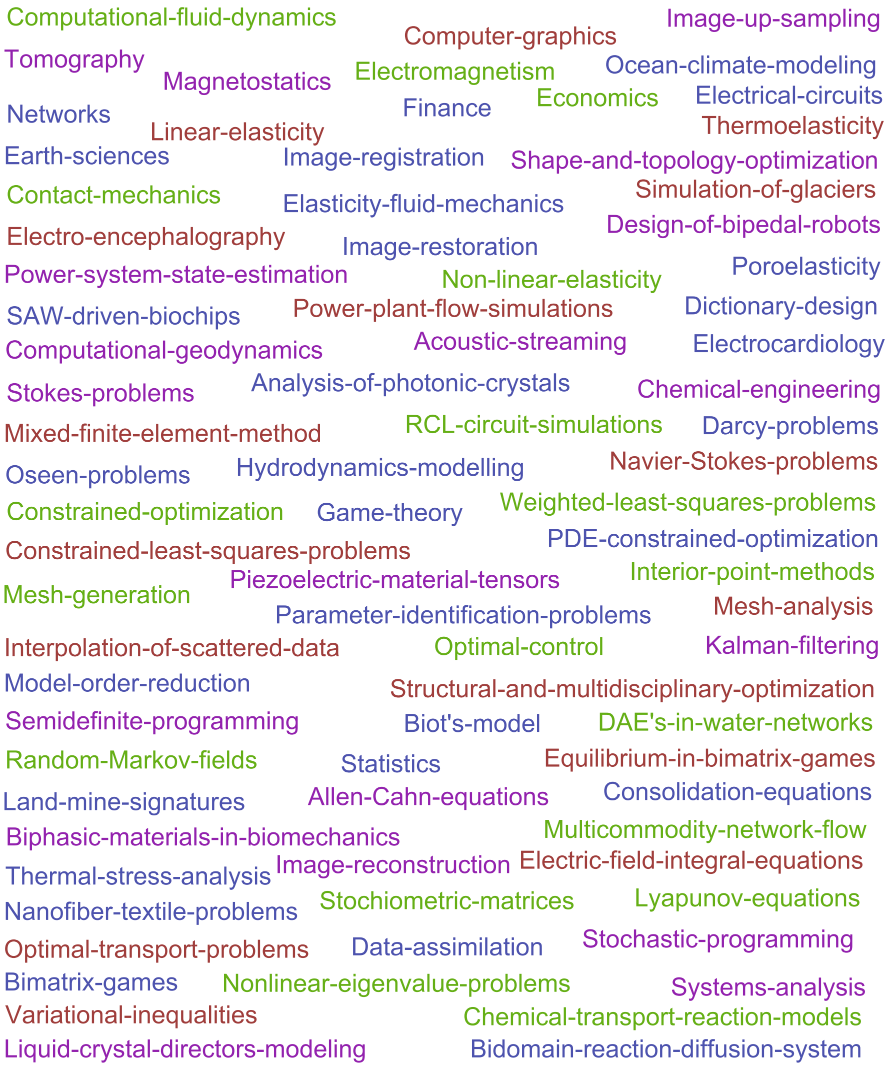

Fig. P.3 Collection of applications and mathematical disciplines leading to saddle-point problems. (Courtesy of M. Benzi)

Contents