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PRECONDITIONERS FOR PDE-CONSTRAINED OPTIMIZATION PROBLEMS WITH BOX CONSTRAINTS: TOWARDS HIGH RESOLUTION INVERSE ECG IMAGES

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Abstract. By combining the Minimal Residual Method and the Primal-Dual Active Set algorithm, we derive an efficient scheme for solving a class of PDE-constrained optimization problems with inequality constraints. The approach studied in this paper addresses box constrains on the control function, and leads to an iterative scheme in which linear optimality systems must be solved in each iteration. We prove that the spectra of the associate saddle point operators, appearing in each iteration, are well behaved: Almost all the eigenvalues are contained in three bounded intervals, not containing zero. In fact, for severely ill-posed problems, the number of eigenvalues outside these three intervals are of order $O(\ln(\alpha^{-1}))$ as $\alpha \to 0$, where α is the parameter employed in the Tikhonov regularization. Krylov subspace methods are well known to handle such systems of algebraic equations very well, and we thus obtain a fast method for PDE-constrained optimization problems with box constraints. In contrast to previous papers, our investigation is not targeted at analyzing a specific model, but instead covers a rather large class of problems. Our theoretical findings are illuminated by several numerical experiments. An example covered by our theoretical findings, as well as cases not fulfilling all the assumptions needed in the analysis, are presented. Also, in addition to computations only involving synthetic data, we briefly explore whether these new techniques can be applied to real world problems. More specifically, the algorithm is tested on a medical imaging problem with clinical patient data. These tests suggest that the method is fast and reliable.

Key words. PDE-constrained optimization, primal-dual active set, minimal residual method, real world applications.

1. Introduction

In the field of optimization many researchers have studied the minimization of quadratic cost-functionals with constraints given by partial differential equations. Several books have been written about this subject, see e.g [3, 5, 7, 15]. By using the Lagrange multiplier technique, one might derive a system of equations which must be satisfied by the optimal solution. After suitable discretization, this system, which typically is a saddle-point problem, can be solved by an all-at-once method. That is, a scheme in which the primal, dual and optimality conditions are solved in a fully coupled manner.

Such optimality systems are often ill-posed, which leads to bad condition numbers for the discretized systems, and regularization techniques must therefore be invoked. Typically, if Tikhonov regularization is employed, then the spectral condition number of the system is of order $O(\alpha^{-1})$, where $\alpha > 0$ is the regularization parameter. Hence one might expect that, for small values of α, the number of iterations required to solve the system, using e.g. Krylov subspace methods, would be large. However, in [11] the authors prove that the spectrum of the optimality system consists of three bounded intervals and a very limited number of isolated eigenvalues outside these three intervals. This result is established for a quite broad

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class of PDE constrained optimization problems and imply that the Minimal Residual Method (MINRES) will handle the associated algebraic systems very well. In fact, if the problem at hand is severely ill-posed, then the required number of iterations cannot grow faster than $O([\ln(\alpha^{-1})]^2)$ as $\alpha \to 0$, and in practice one often observes iterations counts of order $O(\ln(\alpha^{-1}))$.

Many real world problems are not only modeled by PDEs, but also involve inequality constraints. These are often given in the form of box constraints on the control function. In this paper we explore whether the method and analysis presented in [11] can be extended to handle such problems adequately.

Inequality constraints typically require the use of an iterative method to solve the overall optimization task. In consequence, since the linear systems arising in each iteration typically are ill-posed, we need to solve a sequence of algebraic systems with bad condition numbers.

For some specific state equations, such problems have been solved efficiently, see e.g. [4, 14]. These efficient techniques also combines the cherished PDAS method in [2] with different numerical techniques for solving saddle-point problems [1]. We will consider such optimization tasks in a more abstract and general setting. More precisely, our analysis concerns the class of problems that can be written on the form

$$\min_{(v,u)\in L^2(\Omega_v)\times U} \left\{ \frac{1}{2}\|Tu-d\|_Z^2 + \frac{1}{2}\alpha\|v\|_{L^2(\Omega_v)}^2 \right\}, \tag{1}$$

subject to

$$Au + Bv = 0, \tag{2}$$

$$v(x) \geq 0 \text{ a.e. in } \Omega_v, \tag{3}$$

where

- $L^2(\Omega_v)$ is the control space,
- U is the state space, $1 \leq \dim(U) \leq \infty$, and
- Z is the observation space, $1 \leq \dim(Z) \leq \infty$.

We assume that U and Z are Hilbert spaces. Further, $\Omega_v \subset \mathbb{R}^n$ is the domain the control function v is defined on, d is the given observation data, and $\alpha > 0$ is the regularization parameter. In Section 2 we will state the assumptions we need on the linear operators A, B and T. Also, there exists a solution to the problem (1)-(3) under fairly loose assumptions. For $\alpha > 0$, the solution is unique, see e.g. [5] for details.

For the problem (1)-(2), without the inequality constraint $v(x) \geq 0$, it was proven in [11] that for a sound discretization of the associated KKT system

$$\underbrace{\begin{bmatrix} \alpha I & 0 & B^* \\ 0 & T^*T & A^* \\ B & A & 0 \end{bmatrix}}_{=\mathcal{B}_\alpha} \begin{bmatrix} v \\ u \\ w \end{bmatrix} = \begin{bmatrix} 0 \\ T^*d \\ 0 \end{bmatrix}, \tag{4}$$

the eigenvalues of the discretized operator $\mathcal{B}_\alpha^h$ satisfies

$$\mathrm{sp}(\mathcal{B}_\alpha^h) \subset [-b, -a] \cup [c\alpha, 2\alpha] \cup \{\lambda_1, \lambda_2, ..., \lambda_{N(\alpha)}\} \cup [a, b]. \tag{5}$$

Here, a, b and c are constants, independent of the regularization parameter α, and $N(\alpha) = O(\ln(\alpha^{-1}))$ for severely ill-posed problems. Krylov subspace methods handle problems with spectra on the form (5) very well, and, since we have an indefinite system, the Minimal Residual (MINRES) method [12] is well suited for solving (4).