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Block Conjugate Gradient Algorithms for Least Squares Problems

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Abstract

In this paper, extensions for the Conjugate Gradient Least Squares (CGLS) algorithm in block forms, so-called Block Conjugate Gradient Least Squares (BCGLS), are described. Block parameter matrices are designed to explore the block Krylov subspace so that multiple right-hand sides can be treated simultaneously, while maintaining orthogonality and minimization properties along iterations. Search subspace is reduced adaptively in case of (near) rank deficiency to prevent breakdown. A deflated form of BCGLS is developed to accelerate convergence. Numerical examples demonstrate effectiveness in handling rank deficiency and efficiency in convergence accelerations in these BCGLS forms.

Keywords: Block Krylov Subspace, Block Conjugate Gradient Least Squares, Rank Deficiency, Breakdown-Free, Deflation

1. Introduction

We consider the problem of stably finding the least squares solutions to a linear system of equations with multiple right-hand sides,

$$AX = B$$

where A is an $m \times n$ $(m \geq n)$ sparse, rectangular or square matrix with rank n, X is an $n \times s$ unknown matrix, B is an $m \times s$ right-hand side matrix, and s $(s \geq 1)$ is the number of right-hand sides. When A is large and sparse, block iterative methods are natural candidates for solving the least squares problem with multiple right-hand sides.

Using block methods to solve the least squares problems has three major advantages. First of all, solutions corresponding to multiple right-hand sides can be estimated simultaneously. This is particularly useful for applications such as multi-objective optimization [1] interested in finding solutions with respect to different right-hand side vectors. Secondly, compared to solvers with

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