Iterative Methods for Nonnegative and Box
Constrained Least Squares Problems and
Their Applications

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In this thesis, we mainly focus on iterative methods for large sparse nonnegative constrained least squares (NNLS) and box constrained least squares (BLS) problems, which arise in many scientific computing and engineering applications, e.g., image restoration with nonnegative or bounded pixel values, reconstruction problems in geodesy and tomography, contact problems for mechanical systems, and modeling of ocean circulation. We aim to design efficient algorithms to meet the demands for solving large scale and sparse practical problems. The main contribution of this thesis is the proposal of new iterative methods, especially based on the modulus variable transformation and active set strategy. Theoretical analysis on the convergence of the proposed methods is presented. Also, numerical experiments show that the proposed methods outperform previous methods in terms of computational time and storage requirement under suitable conditions with reasonable parameters. The ideas and techniques developed in this thesis could be valuable when extending them to other problems.

First, we briefly review numerical methods for the solution of NNLS and BLS problems. Moreover, the advantages and the disadvantages of different methods are discussed, which motivate one to design new iterative algorithms for large sparse problems.

Secondly, we consider the solution of the general NNLS problem. A new iterative method is proposed which uses the CGLS method for the inner iteration and the
modulus iterative method for the outer iteration to solve the linear complementarity problem resulting from the Karush-Kuhn-Tucker condition of the NNLS problem. Theoretical convergence analysis including the optimal choice of the parameter matrix is presented for the proposed method. In addition, the method can be further enhanced by incorporating the active set strategy, which contains two stages: the first stage consists of modulus iterations to identify the active set, while the second stage solves the reduced unconstrained least squares problems only on the inactive variables, and projects the solution into the nonnegative region. Numerical experiments show the efficiency of the proposed methods compared to projection gradient-type methods with less iteration steps and CPU time.

Thirdly, we consider the solution of large sparse BLS problems using a new class of iterative methods based on modulus transformations, which converts the solution of the BLS into a sequence of unconstrained least squares problems. The inner unconstrained least squares problems can be solved using CGLS. We also discuss the solution of saddle point inner systems. Numerical experiments show the efficiency of the proposed methods in comparison of the projection gradient methods.

Fourthly, we consider the solution of the nonnegative constrained ill-posed problem, especially the image restoration problem. The problem can be formulated as an NNLS problem, which can be solved by the modulus-type inner outer iteration method and the hybrid two-stage iteration method proposed previously. We also consider combining our methods with two regularization techniques: discrepancy principle and Tikhonov regularization. Computed examples illustrate the performances of these methods.

Fifthly, we consider the solution of nonnegative matrix factorization (NMF), which is a low rank matrix approximation problem with nonnegative constraints, using a new alternating least squares method by utilizing the modulus method to solve the nonnegative constrained least squares problem in each iteration. We review some existing methods for the solution of NMF, then construct the alternating modulus nonnegative least squares method for solving NMF. Moreover, we propose a new matrix-based active set method by utilizing the component-wise operation. We also show that the proposed methods can be extended to solve the sparse NMF and regularized NMF. We compare the proposed method with the existing methods numerically on the synthetic data and ORL face image data. The proposed matrix-based active set method outperforms the active set with grouping technique in terms of computational time and
storage requirement.

Finally, by considering that the methods for NMF can be regarded as fixed-point iterations, whose rate of convergence is at best linear, the Anderson extrapolation is used to accelerate the algorithms for NMF. We proposed a new Anderson acceleration technique that can flexibly accelerate the fixed point iteration sequences, instead of accelerating the iteration sequence for every step. Numerical experiments show that the Anderson acceleration not only accelerates the classical stationary iterations for linear equations, but also outperforms the previous methods on nonlinear problems like the linear complementarity problem, NNLS and NMF with less iterations and CPU time.