Block Updating/Downdating Algorithms for Regularised Least Squares Problems and Applications to Linear Discriminant Analysis

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Abstract. Block updating and downdating algorithms for regularised least squares problems with multiple right-hand sides based on the economical *QR* decomposition are proposed. They exploit the initial coefficient matrix structure and use existing solution to establish a solution of the amended problem. Such an approach demonstrates its efficiency in terms of the memory required and the computational cost. Applications to linear discriminant analysis are considered and numerical experiments involving real-world databases show the efficiency of the methods.

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Key words: Block updating, block downdating, regularised least squares problem, economical *QR* decomposition, linear discriminant analysis.

1. Introduction

Consider the regularised least squares (RLS) problem with multiple right-hand sides

$$\min_{W \in \mathbb{R}^{m \times r}} \|AW - B\|_F^2 + \lambda^2 \|W\|_F^2,$$
(1.1)

where $A \in \mathbf{R}^{n \times m}$ is a data matrix with *n* samples from an *m*-dimensional feature space, $B \in \mathbf{R}^{n \times r}$ the corresponding response matrix and $\lambda > 0$ a regularisation parameter. The RLS problem (1.1), also called Tikhonov regularisation [50] or multivariate ridge regression [2], arises in linear ill-posed problems with multiple right-hand sides [8], pattern classification [18], regularised linear discriminant analysis [55, 56], least squares solutions of matrix equations [35], regularised nonnegative matrix factorisation for data representation [16, 54], component analysis [22, 34] and so on. Efficient solution of the problem (1.1) is

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crucial for many algorithms in statistical estimation, regularisation of ill-posed problems, regularised nonnegative matrix factorisation, signal processing, machine learning, and data mining.

It is well known that problem (1.1) has a unique solution — viz.

$$W^{*} = \left(A^{T}A + \lambda^{2}I_{m}\right)^{-1}A^{T}B = A^{T}\left(AA^{T} + \lambda^{2}I_{n}\right)^{-1}B,$$
(1.2)

where I_m is the $m \times m$ identity matrix. The solution W^* can be efficiently computed by the Cholesky factorisation of $A^T A + \lambda^2 I_m$ or $AA^T + \lambda^2 I_n$, rather than by the direct use of inverse matrices in (1.2). Nevertheless, for large m and n, this generally requires a large storage space and leads to a heavy computational burden. One approach to deal with such large-scale high-dimensional data is the Krylov subspace iteration methods [9, 27, 29, 43]. Despite their effectiveness, they all rely on data provided before the computations start and the computation of W^* should start from the very beginning if new data are added to A and B (updating) or some existing data are deleted from A and B (downdating). From the view of perturbation theory, new solutions to the RLS problem (1.1) should be close to the old one. Therefore, efficient algorithms for dynamical updating/downdating the solution of (1.1) are of practical interest.

Substantial efforts have been made to modify the existing matrix factorisations while adjusting the solution of linear least squares problems. Thus Björck and Duff [10] used LU decomposition in updating scheme when modifying solutions of least squares problems when extra equations are added. Gill et al. [28] described five methods to modify the Cholesky and QR factors for rank-one changes in the coefficient matrix. One of their methods was modified by Lawson and Hanson [39] and analysed by Bojanczyk et al. [12]. Bartels and Kaufman [6] used modified traditional Householder transformations to extend the methods [28] onto rank-2 matrix modifications. Using elementary reflection matrices and Gram-Schmidt processes with re-orthogonalisation, Daniel et al. [21] developed numerically stable updating/downdating algorithms for QR factorisation for rank-one matrix modifications. Olszanskyj et al. [42] extended the rank-one downdating method [21] to rank-k downdating method for least squares problems when several equations are deleted simultaneously. Based on Givens rotations, Kontoghiorghes [37, 38] proposed parallel strategies for block updating the QR decomposition if k rows are added. Block versions of Givens rotations have been used by Yanev and Kontoghiorghes [51] in downdating algorithms for least squares problems when few rows are deleted simultaneously. For QR factorisation, Yoo and Park [53] considered a downdating algorithm, which improves the Gram-Schmidt downdating algorithm when *Q*-factor columns are not orthonormal. Barlow *et al.* [5] presented modifications of downdating algorithm [53]. Barlow and Smoktunowicz [4] exploited the block Gram-Schmidt method in a reorthogonalised algorithm and evaluated its accuracy. Barlow [3] presented a block downdating for *QR* factorisation.

Let us note that the modification of the *R* factor in *QR* factorisation after a row is removed is equivalent to the downdating a Cholesky factorisation under a rank-one perturbation. Therefore, the downdating of Cholesky factorisation attracted substantial attention — cf. LINPACK downdating algorithm [47] and its modification [44], block downdating algorithms [24, 25, 48], a downdating algorithm based on the corrected seminor-

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