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A low-rank approach to the solution of weak constraint variational data assimilation problems

Melina A. Freitag *, Daniel L.H. Green

Department of Mathematical Sciences, University of Bath, Claverton Down, BA2 7AY, United Kingdom

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ABSTRACT

Weak constraint four-dimensional variational data assimilation is an important method for incorporating data (typically observations) into a model. The linearised system arising within the minimisation process can be formulated as a saddle point problem. A disadvantage of this formulation is the large storage requirements involved in the linear system. In this paper, we present a low-rank approach which exploits the structure of the saddle point system using techniques and theory from solving large scale matrix equations. Numerical experiments with the linear advection–diffusion equation, and the non-linear Lorenz-95 model demonstrate the effectiveness of a low-rank Krylov subspace solver when compared to a traditional solver.

1. Introduction

Data assimilation is a method for combining a numerical model with observations obtained from a physical system, in order to create a more accurate estimate for the true state of the system. One example where data assimilation is used is numerical weather prediction, however it is also applied in areas such as oceanography, glaciology and other geosciences.

A property which these applications all share is the vast dimensionality of the state vectors involved. In numerical weather prediction the systems have variables of order 10^8 [24]. In addition to the requirement that these computations to be solved quickly, the storage requirement presents an obstacle. In this paper we propose an approach for implementing the weak four-dimensional variational data assimilation method with a low-rank solution in order to achieve a reduction in storage space as well as computation time. The approach investigated here is based on a recent paper [38] which implemented this method in the setting of PDE-constrained optimisation. We introduce here a low-rank modification to GMRES in order to generate low-rank solutions in the setting of data assimilation.

This method was motivated by recent developments in the area of solving large sparse matrix equations, see [3,23,30,32,36,37], notably the Lyapunov equation

$$AX + XA^T = -BB^T$$

in which we solve for the matrix X, where A, B and X are large matrices of matching size. It is known that if the right hand side of these matrix equations are low-rank, there exist low-rank approximations to X [21]. There are a number of

* Corresponding author.
E-mail addresses: m.a.freitag@bath.ac.uk (M.A. Freitag), d.l.h.green@bath.ac.uk (D.L.H. Green).

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methods which iteratively generate low-rank solutions; see e.g. [13,26,30,32,36], and it is these ideas which are employed in this paper.

Alternative methods [14,31,39] have been considered for computing low-rank solutions, based on sequential data assimilation methods such as the Kalman filter [22,31]. Furthermore there have been developments in applying traditional model reduction techniques such as Balanced Truncation [29] and Principal Orthogonal Decomposition (POD) to data assimilation; e.g. [10,25]. In this paper we take a different approach, the data assimilation problem is considered in its full formulation, however the expensive solve of the linear system is done in a low-rank in time framework.

In the next section we introduce a saddle point formulation of weak constraint four dimensional variational data assimilation. Section 3 explains the connection between the arising linear system and the solution to matrix equations. We also introduce a low-rank approach to GMRES, and consider several preconditioning strategies. Numerical results are presented in Section 4, with an extension to time-dependent systems considered in Section 5.

2. Variational data assimilation

Variational data assimilation, initially proposed in [34,35] is one of two families of methods for data assimilation, the other being sequential data assimilation which includes the Kalman Filter and modifications [14,22,31].

We consider the discrete-time non-linear dynamical system

$$x_{k+1} = \mathcal{M}_k(x_k) + \eta_k, \tag{2.1}$$

where $x_k \in \mathbb{R}^n$ is the state of the system at time t_k and $\mathcal{M}_k : \mathbb{R}^n \to \mathbb{R}^n$ is the non-linear model operator which evolves the state from time t_k to t_{k+1} for $k = 0, \dots N-1$. The model errors are denoted η_k, and are assumed to be Gaussian with zero mean and covariance matrix $Q_k \in \mathbb{R}^{n\times n}$.

Observations of this system, $y_k \in \mathbb{R}^{p_k}$ at time t_k for $k = 0, \dots N$ are given by

$$y_k = \mathcal{H}_k(x_k) + \epsilon_k, \tag{2.2}$$

where $\mathcal{H}_k : \mathbb{R}^n \to \mathbb{R}^{p_k}$ is an observation operator, and ϵ_k is the observation error. In general, $p_k \ll n$. This observation operator $\mathcal{H}_k$ may also be non-linear, and may have explicit time dependence. The observation errors are assumed to be Gaussian, with zero mean and covariance matrix $R_k \in \mathbb{R}^{p_k\times p_k}$.

We assume that at the initial time we have an a priori estimate of the state, which we refer to as the background state, and denote x^b. This is commonly the result of a short-range forecast, or a previous assimilation, and is typically taken to be the first guess during the assimilation process. We assume that this background state has Gaussian errors with covariance matrix $B \in \mathbb{R}^{n\times n}$.

2.1. Four dimensional variational data assimilation (4D-Var)

Four dimensional variational data assimilation (4D-Var) is so called for three spatial dimensions, plus time, and to differentiate it from three-dimensional variational data assimilation (3D-Var), where we do not consider multiple observation times. In 4D-Var, we find an initial state which minimises both the weighted least squares distance to the background state x^b, and the weighted least squares distance between the model trajectory of this initial state x_k and the observations y_k for an assimilation window $[t_0, t_N]$. Mathematically, we can write this as a minimisation of a cost function, e.g. argmin $J(x)$, where

$$\begin{aligned} J(x) &= \underbrace{\frac{1}{2}(x_0 - x_0^b)^T B^{-1}(x_0 - x_0^b)}_{J_b} + \underbrace{\frac{1}{2}\sum_{i=0}^{N}(y_i - \mathcal{H}_i(x_i))^T R_i^{-1}(y_i - \mathcal{H}_i(x_i))}_{J_o} \\ &\quad + \underbrace{\frac{1}{2}\sum_{i=1}^{N}(x_i - \mathcal{M}_i(x_{i-1}))^T Q_i^{-1}(x_i - \mathcal{M}_i(x_{i-1}))}_{J_q}, \\ &= \frac{1}{2}\|x_0 - x_0^b\|^2_{B^{-1}} + \frac{1}{2}\sum_{i=0}^{N}\|y_i - \mathcal{H}_i(x_i)\|^2_{R_i^{-1}} + \frac{1}{2}\sum_{i=1}^{N}\|x_i - \mathcal{M}_i(x_{i-1})\|^2_{Q_i^{-1}}, \end{aligned} \tag{2.3}$$

where $x = [x_0^T, x_1^T, \dots, x_N^T]^T$, and x_k is the model state at each timestep t_k for $k = 0, \dots, N$. This is known as *weak constraint* 4D-Var. The assumption of a perfect model, gives rise to *strong constraint* 4D-Var, and a simplification of the cost function, notably the removal of the J_q term.

The additional cost of weak constraint 4D-Var, and the difficulties in computing Q_k mean that it is not widely implemented in real world systems. However, accounting for this model error (with suitable covariances) would lead to improved accuracy, and the added potential of longer assimilation windows [17,18].