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Studies On Variation Data Assimilation

*Dr. Rajeev Kumar and **Gurpreet Kaur

*Assistant Professor, Department of Mathematics, OPJS University, Churu, Rajasthan (India)
**Research Scholar, Department of Mathematics, OPJS University, Churu, Rajasthan (India)
Email: shargun500@gmail.com; Contact No. +91-9996347359

Abstract: We introduce the Gauss-Newton 'incremental' and CVT techniques currently used for sc4DVAR. We then introduce the two wc4DVAR formulations. We then extend the theory of the Gauss-Newton and CVT concepts to both formulations and briefly discuss the structures of the two wc4DVAR Hessians. We conclude the chapter with a literature review of applications of wc4DVAR in NWP and current understanding of the conditioning of the wc4DVAR problem.
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Introduction

Bold upper-case letters denote partitioned matrices, meaning a matrix of matrices. In this thesis we refer to these partitioned matrices as 4-dimensional (4D) since they possess spatial and temporal information. Matrices with a normal font represent a standard N *x* N matrix as opposed to a partitioned 4D Nn x Nn matrix, for N, n £ N, where N refers to the spatial dimension and n denotes the temporal dimension. Similarly, we represent 4D partitioned vectors with bold lower-case letters and normal vectors of size N are written in normal font. Data assimilation is a major component of Numerical Weather Prediction. The data assimilation problem consists in using the available observations together with the model trajectory to provide an accurate description of the atmospheric state. This so-called "analysis" can then be used to initialize a forecast or on its own, for instance to help understand atmospheric properties or in the context of field experiments or re-analyses over long periods of time. There are mainly two different ways of performing data assimilation. The sequential way is using observations in small batches in time, as they become available. In contrast, the continuous way is working over time windows, using all the observations together. This is particularly well suited for re-analyses problems to obtain the best possible state of the atmosphere at time t using observations before and after this time. In general, for operational NWP, the time window of interest is typically 3 to 12 hours, due to the frequency of forecasts which are issued to the users.

We introduce the Gauss-Newton `incremental' and CVT techniques currently used for sc4DVAR. We then introduce the two wc4DVAR formulations. We then extend the theory of the Gauss-Newton and CVT concepts to both formulations and briey discuss the structures of the two wc4DVAR Hessians. We conclude the chapter with a literature review of applications of wc4DVAR in NWP and current understanding of the conditioning of the wc4DVAR problem. We begin by detailing the style of notation used in this thesis.

Notation and Assumptions

Matrices and Vectors

Bold upper-case letters denote partitioned matrices, meaning a matrix of matrices. In this thesis we refer to these partitioned matrices as 4-dimensional (4D) since they possess spatial and temporal information. Matrices with a normal font represent a standard N _ N matrix as opposed to a partitioned 4D Nn _ Nn matrix, for N; n 2 N, where N refers to the spatial dimension and n denotes the temporal

Operators

This notation also interlinks between operators and matrices. We denote non-linear operators using calligraphic font whereas a non-linear operator which has been differentiated and linearised around a point is denoted with normal font, which can then also be represented as a matrix. This also applies to 4D operators, so a linearised 4D operator for example would be bold. Letters with standard font denote linear or linearised operators, which can be represented in matrix form.

Condition Number

The condition number used throughout this chapter is the 2-norm condition number, composed of the ratio of the largest and smallest Eigen value of a symmetric positive-definite matrix. We formally introduce the condition number in Chapter 3 Section 3.1.

We now introduce the sc4DVAR problem.

Strong-Constraint 4DVAR

The aim of data assimilation is to merge the trajectory of a model with observational data from the process being modeled. In sc4DVAR the model is assumed to be perfect meaning each state is described exactly by the model equations. The errors therefore in the strong-constraint problem are the background, a previous forecast, and the observations. The objective is to seek the model initial conditions which minimizes the distance between the model trajectory and the background and observations.

We begin by writing the model evolution of the states as

Xi = Mi,i-i (xi-i), i = 1,...,n. (1.1)

The model is a discrete non-linear operator $M_{i)i}$-i: R^N —> R^N evolving the model state x_i £ R^N from time t_{i-1} to time t_i on the closed time interval [to, in] where $M_{i)i}$ = I_N. The model state can have several spatial points and contain additional parameters or boundary conditions that govern the behavior of the model. In this thesis we only consider models initialized by their respective states without any additional parameters.

The model integrations can be factorized into smaller integrations using the subscript time-stepping notation as follows

Mn,o (Xo) = Mn,n-1... (M2,l (Ml,o (Xo))). (1.2)

We utilize this notation throughout the thesis. Now that we have discussed the model, we briefly introduce the notion of observations in variational data assimilation related to NWP.

There is a wide network of observations gathered with the use of various instruments and methods for obtaining measurements in NWP. For example, radiosondes are attached to weather balloons, which are sent up through the layers of the atmosphere collecting data such as pressure, humidity and temperature. Observations are also obtained through satellite radiances, aircrafts and buoys in the ocean. The process of translating the observations into data which can be compared with the model presents its own inverse problem, but this is incorporated into the variational problem as we will see shortly. An example of such a complex problem is the translation of Atmospheric InfraRed Sounder (AIRS) radiance data, which involves characterizing the errors in the measured radiances and the radioactive-transfer model, [65]. In practice the number of the observations is ~ O (10^6) whereas the number of variables in the state is significantly larger ~ O (10^8), [51].

Let y_i £ R^p denote the raw observation value at time i and let $H_i(x_i)$ denote the non-linear observation operator, which maps the model equivalent of y_i from state space to observation space such that H_i: R^N — R^p. Therefore we have

Hi (xi) - yi = e^o, i = 0,n, (1.3)

where e^o £ R^p denotes the observation error at t_i. The errors in the observations are typically assumed to be uncorrelated with all other types of error, and of the form

e^o ~ N (0,Ri), i = 0,...,n, (1.4)

where R_i £ R^{pxp} is the observation error covariance matrix and the mean is equal to zero. The assumption of a normal distribution allows the distributions to be defined by the mean and covariance, which simplifies the problem. The Gaussian assumption in (1.4) is still currently used by leading weather centres' 4DVAR implementations, such as the Met Office and the ECMWF, [74], [75], [13].

Next, we consider model trajectory errors. Initial conditions x_o, produce a model trajectory by utilizing the non-linear model described in (1.1), with states at each time (x_1,...,x_n). The initial conditions that produce the previous forecast trajectory, is known as the 'background', denoted as The background is the solution of a previous 4DVAR application, since variational data assimilation is a cyclic process. We therefore have a background trajectory such that

x^b = Mi,i-i (x^b-i), i = 1,n, (1.5)

with initial conditions xo producing a trajectory (xl,...,x^). The error associated with the background is such that

xo - xo = eo, (1.6)

where the error is such that

eo ~ N (0,Bo). (1.7)

The background error eo £ R^N is assumed to be uncorrelated with all other types of error, have a zero mean and a background error covariance matrix such that.

So the aim of the variational problem is to minimize the errors in (1.6) and (1.3)

Conclusions

we have introduced the strong-constraint and weak-constraint variational data assimilation problems. We introduced concepts such as the Gauss-Newton incremental approach and the CVT technique for both sc4DVAR and wc4DVAR. We also discussed the structures of the weak-constraint Hessians. This was then followed by a review of the current literature detailing the applications and conditioning of the weak-constraint problem.

We now introduce the mathematical framework required to understand and solve the 4DVAR problem and the necessary tools used to obtain the results

Corresponding author:
Mrs. Gurpreet Kaur
Research Scholar, Department of Mathematics,
OPJS University, Churu, Rajasthan (India)
Contact No. +91-9996347359
Email- Email: shargun500@gmail.com

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