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Approximate Gauss-Newton Methods Using Reduced Order Models

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Abstract

The Gauss-Newton (GN) method is a well known iterative technique for solving nonlinear least squares problems subject to dynamical system constraints. Such problems arise commonly from applications in optimal control and state estimation. Variational data assimilation systems for weather, ocean and climate prediction currently use approximate GN methods. The GN method solves a sequence of linear least squares problems subject to linearized system constraints. For very large systems, low resolution linear approximations to the model dynamics are used to improve the efficiency of the algorithm. We propose a new method for deriving low order system approximations based on model reduction techniques from control theory. We show how this technique can be combined with the GN method to retain the response of the dynamical system more accurately and improve the performance of the GN method.

Keywords Large-scale nonlinear least squares problems subject to dynamical system constraints; Gauss-Newton methods; variational data assimilation; weather, ocean and climate prediction.

1 INTRODUCTION

The Gauss-Newton (GN) method is a well known iterative technique for solving nonlinear least squares problems subject to strong dynamical constraints [5]. It is commonly applied to solve optimal control and optimal state estimation problems and is used in variational data assimilation for environmental systems [11, 9, 10, 3]. The Gauss-Newton method is essentially an approximation to the Newton method in which only the first order part of the Hessian is retained. We consider a general nonlinear least squares problem

$$\min_{\mathbf{x}} \phi(\mathbf{x}) = \mathbf{f}(\mathbf{x})^T \mathbf{f}(\mathbf{x}), \tag{1}$$

where $\mathbf{f}(\mathbf{x})$ is a nonlinear function of $\mathbf{x}$ and we define $\mathbf{J}(\mathbf{x})$ to be the Jacobian of $\mathbf{f}(\mathbf{x})$. Then the Gauss-Newton iteration method for solving this problem consists of the following steps:

$$\text{Solve for } \delta\mathbf{x}^{(k)}: \quad (\mathbf{J}(\mathbf{x}^{(k)})^{\mathrm{T}}\mathbf{J}(\mathbf{x}^{(k)}))\delta\mathbf{x}^{(k)} = -\mathbf{J}(\mathbf{x}^{(k)})^{\mathrm{T}}\mathbf{f}(\mathbf{x}^{(k)}), \tag{2}$$

$$\text{Update:} \quad \mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \delta\mathbf{x}^{(k)}, \tag{3}$$

for $k = 0, 1 \ldots$. For very large systems, such as arise in meteorology and oceanography, it is not generally possible to solve (2) directly. The solution $\delta\mathbf{x}^{(k)}$ is then found by an 'inner' minimization of the linear least squares function

$$\tilde{\phi}(\delta\mathbf{x}^{(k)}) = ||\mathbf{J}(\mathbf{x}^{(k)})\delta\mathbf{x}^{(k)} + \mathbf{f}(\mathbf{x}^{(k)})||_2. \tag{4}$$

In the case where strong dynamical constraints are imposed on the optimization problem, the objective function $\mathbf{f}(\mathbf{x})$ contains the dynamical system equations. In order to apply the GN method, the Jacobian of the function $\mathbf{f}(\mathbf{x})$ is needed and, hence, the Jacobian of the nonlinear system equations, known as the tangent linear model, is also required. The inner linear minimization problem (4) is then solved subject to the strong dynamical constraints imposed by the tangent linear model equations.

In order to make the GN method more efficient for large systems, a commonly used approach is to approximate the full tangent linear model by a linearized model at low spatial resolution, while still calculating $\mathbf{f}(\mathbf{x})$ and updating $\mathbf{x}$ at the highest spatial resolution. Thus in (4) the Jacobian $\mathbf{J}(\mathbf{x}^{(k)})$ is replaced by an approximate low resolution operator $\tilde{\mathbf{J}}(\mathbf{x}^{(k)})$. Whilst this leads to an algorithm that is practical to compute in real-time, the approximations made do not take into account whether the most important parts of the dynamical system are being retained. Thus it is difficult to quantify how much information is being lost due to the reduction in resolution.

In this work we propose a new method for approximating the inner step of the Gauss-Newton method, based on the ideas of model reduction. Model reduction has been used in the field of state-space control theory to approximate very large dynamical systems with low order models [1]. Employing the example of the balanced truncation technique we show how model reduction may be used in the inner step of the Gauss-Newton algorithm to give an approximate iteration procedure that retains the most important properties of the dynamical system response.

We demonstrate the application of this technique to the problem of variational data assimilation, which corresponds to an optimal state estimation problem. Experiments with a shallow-water model are used to show the benefit that may be obtained by using a reduced order model instead of a standard low resolution model within the GN algorithm. We show how the use of model reduction allows the system to be approximated by a system of much smaller dimension than can be used with a low resolution model.

In the next section we describe the application of approximate GN methods to the variational data assimilation problem and in Section 3 we present the model reduction techniques that we use here. In Section 4 the test model is defined and experimental results are shown. Conclusions are given in Section 5.

2 FOUR DIMENSIONAL VARIATIONAL DATA ASSIMILATION

The aim of variational data assimilation is to match the output response of a dynamical system model to observed measurements of the outputs over a specified time window. For a discrete dynamical system, we let $\mathbf{x}_j \in \mathbb{R}^n$

be the model state vector, $\mathbf{y}_j \in \mathbb{R}^{p_j}$ be a vector of p_j observations and $\mathbf{h}_j : \mathbb{R}^n \to \mathbb{R}^{p_j}$ be a nonlinear function that relates the system states to the observations at time t_j. The data assimilation problem is then defined as follows.

Problem 1. *Minimize, with respect to* $\mathbf{x}_0$*, the objective function*

$$\mathcal{J}[\mathbf{x}_0] = \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}_0^b)^T \mathbf{B}_0^{-1}(\mathbf{x}_0 - \mathbf{x}_0^b) + \frac{1}{2}\sum_{j=0}^{N}(\mathbf{h}_j(\mathbf{x}_j) - \mathbf{y}_j)^T \mathbf{R}_j^{-1}(\mathbf{h}_j(\mathbf{x}_j) - \mathbf{y}_j), \tag{5}$$

subject to $\mathbf{x}_j,\ j = 0, \ldots, N$*, satisfying the discrete dynamical system equations.*

The background estimate, $\mathbf{x}_0^b$, of the initial state, $\mathbf{x}_0$, is known. If the initial errors $(\mathbf{x}_0 - \mathbf{x}_0^b)$ and the observational errors $\mathbf{d}_j = \mathbf{h}_j(\mathbf{x}_j) - \mathbf{y}_j$ are assumed to be unbiased, Gaussian random vectors with covariance matrices $\mathbf{B}_0$ and $\mathbf{R}_j$, respectively, then the optimization delivers the best statistically linear unbiased estimate of the initial system states.

In practice the constrained minimization problem is solved iteratively by the GN method. At each step of this method the inner linear least squares problem (4) must be solved for the increment $\delta\mathbf{x}^{(k)}$. We write the linearized discrete system equations as

$$\delta\mathbf{x}_{j+1} = \mathbf{M}_j \delta\mathbf{x}_j, \qquad \mathbf{d}_j = \mathbf{H}_j \delta\mathbf{x}_j, \tag{6}$$

where the input $\delta\mathbf{x}_0 = \mathbf{B}_0^{\frac{1}{2}}\boldsymbol{\omega}$ with $\boldsymbol{\omega} \sim \mathcal{N}(0, \mathbf{I})$, and $\mathbf{M}_j$ and $\mathbf{H}_j$ are, respectively, the tangent linear system model and the Jacobian of the observation operator obtained by linearizing around the state $\mathbf{x}_j$. The inner minimization problem is then given by

Problem 2. *Minimize, with respect to* $\delta\mathbf{x}_0^{(k)}$*, the objective function*

$$\begin{aligned}\tilde{\mathcal{J}}^{(k)}[\delta\mathbf{x}_0^{(k)}] &= \frac{1}{2}(\delta\mathbf{x}_0^{(k)} - [\mathbf{x}^b - \mathbf{x}_0{}^{(k)}])^{\mathrm{T}} \mathbf{B}_0^{-1}(\delta\mathbf{x}_0^{(k)} - [\mathbf{x}^b - \mathbf{x}_0{}^{(k)}]) \\ &+ \frac{1}{2}\sum_{j=0}^{N}(\mathbf{H}_j\delta\mathbf{x}_j^{(k)} - \mathbf{d}_j^{(k)})^{\mathrm{T}} \mathbf{R}_j^{-1}(\mathbf{H}_j\delta\mathbf{x}_j^{(k)} - \mathbf{d}_j^{(k)}),\end{aligned} \tag{7}$$

subject to the states $\delta\mathbf{x}_j^{(k)}$ *satisfying the discrete linear system equations (6).*

Problem 2 is solved by an inner iteration process, such as the conjugate gradient method. Each inner iteration requires one forward solution of the tangent linear model equations (6), starting from the current best estimate of the initial states, and one backward solution of the corresponding linear adjoint equations to determine the gradient of the objective function. In order for this process to be operationally feasible for very large systems such as weather and ocean systems, which involve as many as 10^8 state variables, the computational cost is reduced by using low dimensional approximations to the linear models.

Low dimensional system models can be obtained by using low resolution approximations to the full dynamical system. Significant features of the system behaviour are often lost, however, in such approximations. In particular optimal error growth modes may not be captured by these models. In the next section we propose an alternative method for generating low order system approximations using techniques of model reduction.

3 MODEL REDUCTION BY BALANCED - TRUNCATION

To find low order approximations to the linearized system model (6), we project the system into a low dimensional subspace. We introduce linear restriction operators $\mathbf{U}_j^T \in \mathbb{R}^{r \times n}$ that project the state variables into the subspace $\mathbb{R}^r$ where $r << n$. We define variables $\delta\hat{\mathbf{x}}_j \in \mathbb{R}^r$, such that $\delta\hat{\mathbf{x}}_j = \mathbf{U}_j^T \delta\mathbf{x}_j$, and define prolongation operators $\mathbf{V}_j \in \mathbb{R}^{n \times r}$ that project the variables back into the original space $\mathbb{R}^n$. The restriction and prolongation operators $\mathbf{U}_j^T$ and $\mathbf{V}_j$ satisfy $\mathbf{U}_j^T \mathbf{V}_j = \mathbf{I}_r$ and $\mathbf{V}_j \mathbf{U}_j^T$ is a projection operator. We write the projected linear system as

$$\delta\hat{\mathbf{x}}_{j+1} = \mathbf{U}_j^T \mathbf{M}_j \mathbf{V}_j \delta\hat{\mathbf{x}}_j, \qquad \hat{\mathbf{d}}_j = \mathbf{H}_j \mathbf{V}_j \delta\hat{\mathbf{x}}_j. \tag{8}$$

The reduced-dimension inner minimization problem then becomes

Problem 3. *Minimize, with respect to* $\delta\hat{\mathbf{x}}_0^{(k)}$*, the objective function*

$$\begin{aligned} \hat{\mathcal{J}}^{(k)}[\delta\hat{\mathbf{x}}_0^{(k)}] &= \frac{1}{2}(\delta\hat{\mathbf{x}}_0^{(k)} - \mathbf{U}_0^T[\mathbf{x}^b - \mathbf{x}_0{}^{(k)}])^{\mathrm{T}} \hat{\mathbf{B}}_0^{-1} (\delta\hat{\mathbf{x}}_0^{(k)} - \mathbf{U}_0^T[\mathbf{x}^b - \mathbf{x}_0{}^{(k)}]) \\ &+ \frac{1}{2}\sum_{i=0}^{N} (\mathbf{H}_j \mathbf{V}_j \delta\hat{\mathbf{x}}_j^{(k)} - \mathbf{d}_j^{(k)})^{\mathrm{T}} \mathbf{R}_j^{-1} (\mathbf{H}_j \mathbf{V}_j \delta\hat{\mathbf{x}}_j^{(k)} - \mathbf{d}_j^{(k)}), \end{aligned} \tag{9}$$

subject to the states $\delta\hat{\mathbf{x}}_j^{(k)}$ *satisfying the discrete linear system equations (8).* The prolongation operator $\mathbf{V}_0$ is then applied to lift the solution $\delta\hat{\mathbf{x}}_0^{(k)}$ back into the space $\mathbb{R}^n$. Here the matrix $\hat{\mathbf{B}}_0 = \mathbf{U}_0^T \mathbf{B}_0 \mathbf{U}_0$ models the background error statistics in the reduced space.

The projection matrices are chosen to ensure that the low order linear model (8) accurately approximates the output response of the linear system (6) to the input data over a full frequency range. Specifically the aim of the model reduction is to design a model of order $r << n$ of the form (8) such that the expected value of the distance between the system outputs $\mathbf{d}_j$ and the reduced order model outputs $\hat{\mathbf{d}}_j$, written as

$$\lim_{i\to\infty} \mathcal{E}\left\{\|\hat{\mathbf{d}}_j - \mathbf{d}_j\|_2^2\right\} = \lim_{i\to\infty} \mathcal{E}\left\{\left[\hat{\mathbf{d}}_j - \mathbf{d}_j\right]^T \left[\hat{\mathbf{d}}_j - \mathbf{d}_j\right]\right\}, \tag{10}$$

is minimized over all white noise input errors $\boldsymbol{\omega}$ of normalized unit length, with $\mathcal{E}\left\{\frac{1}{n}\|\boldsymbol{\omega}\|_2^2\right\} = 1$, where $\mathcal{E}\{\cdot\}$ denotes the expected value.

The response of a discrete linear system is represented by its Hankel matrix and a good approximation to the optimal reduced order system can be found by matching the Hankel singular values of the reduced order model to those of the full linear system model. The projection matrices $\mathbf{U}_j$ and $\mathbf{V}_j$ are therefore selected to ensure that the maximum Hankel singular values of the full system are retained by the reduced order model. A global error bound on the expected error between the frequency responses of the full and reduced systems, based on the neglected Hankel singular values, then exists [1]. A reduced order system derived by this method is therefore expected to capture well the modes of optimal error growth. Efficient and accurate numerical techniques are readily available for finding the restriction and prolongation operators for systems of moderately large size based on balanced-truncation methods ([8, 2]), and for very large systems, Krylov subspace methods and rational interpolation methods can be implemented ([4, 6]). (See [12] for further details and preliminary results.)

4 NUMERICAL EXPERIMENTS

To illustrate the benefit of using reduced order models we apply the method of balanced truncation to a discrete model of the nonlinear 1D shallow water equations with rotation and compare the results to those obtained using a low resolution model of the system. The continuous system is given by

$$\frac{\partial u}{\partial t} + (U_c + u)\frac{\partial u}{\partial x} - fv = -g\frac{\partial (h + \bar{h})}{\partial x},$$

$$\frac{\partial v}{\partial t} + (U_c + u)\frac{\partial v}{\partial x} + fu = 0, \quad \frac{\partial h}{\partial t} + \frac{\partial h(U_c + u)}{\partial x} = 0, \tag{11}$$

where u denotes the departure of the velocity in the x-direction from a known constant forcing mean flow, U_c , $\bar{h} = \bar{h}(x)$ is the height of the orography, f is the Coriolis parameter and g is the gravitational force. The model domain is periodic in the x-direction. The system is discretized as described in [7] using a semi-implicit semi-Lagrangian integration scheme.

The data for the problem is also given in [7]. An initial perturbation $\delta\mathbf{x}_0$ is defined and the outputs $\mathbf{d}_j$ satisfying the discrete linear equations (6) are determined. A time-invariant linear model that approximates the tangent linear model of the system is used in the experiments. The solution in $\mathbb{R}^r$ of the reduced inner minimization problem, Problem 3, is found using (i) a low resolution model and (ii) a reduced order model obtained by balanced-truncation. In case (i) the corresponding solution in $\mathbb{R}^n$ is found by interpolation, whilst in case (ii) the solution in $\mathbb{R}^n$ is found by applying the prolongation operator.

The results are compared to the exact solution to the full linear least squares problem, Problem 2, in $\mathbb{R}^n$. For the example where $n = 1500$ and

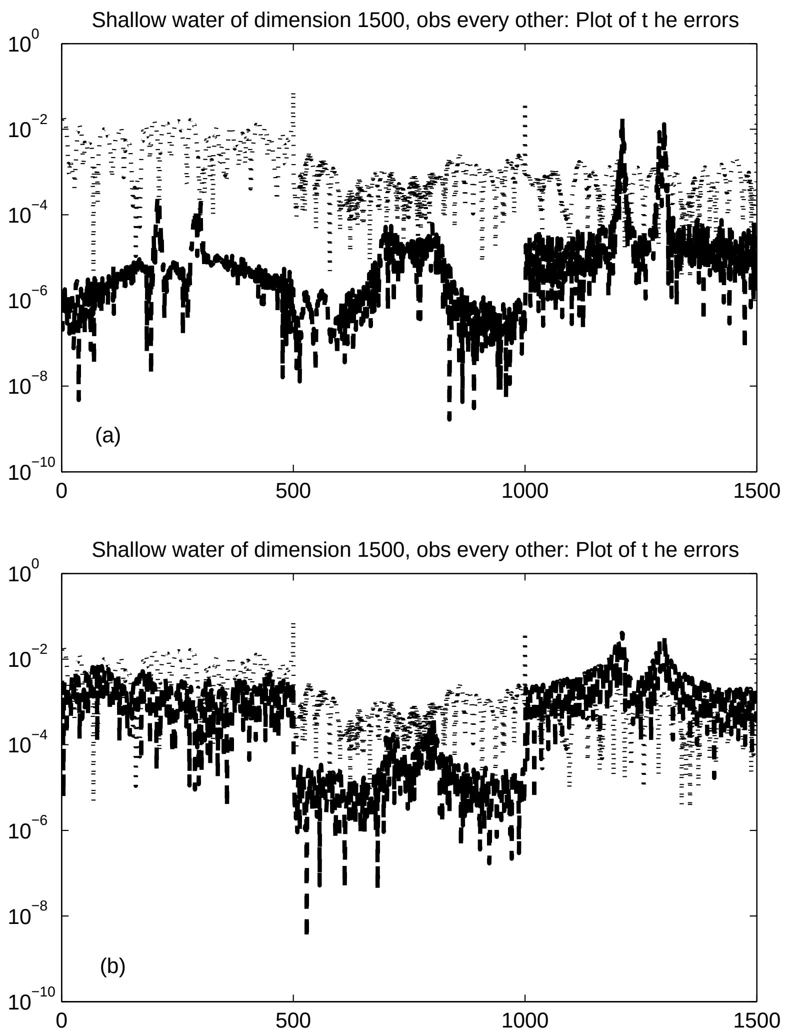

Figure 1: Errors in solutions to reduced linear least squares problem for low resolution model (dotted) of order $r = 750$ and optimal reduced order model (dashed) of order (a) $r = 750$ and (b) $r = 250$.

$r = 750$, the errors between the exact solution and the solutions obtained using the two different low dimensional models are shown in Figure 1(a). The least square norms of the errors in the two cases are given, respectively, by (i) 0.0396 and (ii) 0.0057. It is clear that for the same model size, the optimal reduced order models are significantly more accurate than the low resolution models. This benefit can be explained in part by examining the eigenstructure of the reduced dimensional systems. More of the significant eigenvalues of the optimal reduced order model match those of the full system than is the case for the low resolution model, showing that the modes of the system are more accurately captured by the balanced-truncation method than by using low resolution models.

Solutions to the reduced least squares problem obtained for smaller values of r demonstrate that balanced-truncation can be applied to find much smaller systems with accuracy equal to that of the low resolution model. A comparison of the errors obtained with the low resolution model of dimension $r = 750$ and an optimal reduced order model of dimension $r = 250$ is shown in Figure 1(b). The least square error norm obtained using the optimal reduced order model is now 0.0288. This demonstrates that an optimal reduced order model with one-third the dimension can achieve the same accuracy as a low resolution model. This represents a considerable increase in computational efficiency in practice.

5 CONCLUSIONS

We have described a new approach to finding low dimensional linear models that can be used to improve the efficiency of approximate Gauss-Newton methods for solving nonlinear least squares problems. The new approach applies techniques of optimal reduced order modelling from control theory and is shown to give better accuracy with significant improvement in performance in solving the inner linear least squares problem. The challenge is now to develop these techniques to apply to the very large problems arising in environmental systems.

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