Practical and Theoretical Aspects of Adjoint Parameter Estimation and Identifiability in Meteorology and Oceanography

By I. M. NAVON

Department of Mathematics

and Supercomputer Computations Research Institute

Florida State University

Tallahassee, FL 32306-4052

Dedicated to Professor Richard Pfeffer

Abstract

The present paper has two aims. One is to survey briefly the state of the art of parameter estimation in meteorology and oceanography in view of applications of 4-D variational data assimilation techniques to inverse parameter estimation problems, which bear promise of serious positive impact on improving model prediction. The other aim is to present crucial aspects of identifiability and stability essential for validating results of optimal parameter estimation and which have not been addressed so far in either the meteorological or the oceanographic literature.

As noted by Yeh(1986) in the context of ground water flow parameter estimation the inverse or parameter estimation problem is often ill-posed and beset by instability and nonuniqueness, particularly if one seeks parameters distributed in space-time domain. This approach will allow one to assess and rigorously validate results of parameter estimation, i. e., do they indeed represent a real identification of physical model parameters or just compensate model errors? A brief survey of other approaches for solving the problem of optimal parameter estimation in meteorology and oceanography is finally presented.

Introduction

While a sizable amount of research on adjoint parameter estimation was carried out in the last twenty years in fields such as groundwater hydrology and petroleum reservoirs for instance by Carrera and Neuman (1986a, b, c), Yeh(1986), Cushman-Roisin(1986), Seinfeld and Kravaris(1982), Sun and Yeh (1990a, b, 1992), matched by a major effort of the mathematical community started early by seminar work of Richard Bellman and collaborators(Bellman et al. 1965a, 1965b), Chavent and Lemonnier (1974) and Chavent et al. (1975), adjoint parameter estimation work in meteorology and oceanography is more recent and consists of fewer contributions lacking the in-depth approach for validation of the uniqueness of results taken in above mentioned research fields.

In this paper directed at the segment of the meteorological and oceanographic community which focuses on data assimilation by 4-D VAR or estimation theory, we aim to achieve two main goals:

The first is to present a brief review of the state of the art of parameter estimation in the meteorological and oceanographic community.

The second goal is to illuminate without recourse to the use of heavy mathematics the issue of ill-posedness of the problem of parameter estimation along with a description of the problems of identifiability and uniqueness which may preclude the possibility of a successful parameter estimation procedure. The rigorous mathematical background is provided in appendix A.

The paper plan is as follows. Section 2 as mentioned above provides a brief survey of state of the art parameter estimation in meteorology and oceanography along with the typical set-up for adjoint parameter estimation. Section 2. 3 describes issues of identifiability ill-posedness and regularization in a qualitative way and illustrates the issue with examples. An effort is made to point out the importance of these concepts for the adjoint parameter estimation procedure to be relevant and for the results to be uniquely validated. Chapter 3 describes an alternative approach to adjoint parameter estimation focusing on the maximum likelihood(ML) method. The use of total variation as a regularization method for parameters with discontinuities is presented in Chapter 4. Parameter estimation via the extended Kalman filter(EKF) is presented in Section 5. The issue of the regularization procedure is also discussed. Sensitivity analysis as an efficient tool in parameter estimation in meteorology and oceanography is discussed in Section 6. Summary and conclusions are then presented in Section 7. Mathematical results related to identifiability are presented in Appendix A for the sake of completion.

2. State of the art of adjoint parameter estimation in meteorology and oceanography

2. 1 Parameter estimation in meteorology

The research effort on adjoint parameter estimation in meteorology can be dated back to the work of Courtier(1986, 1987) on estimating orography using a shallow-water equations model.

An early detailed survey addressing also issues of adjoint parameter identification was provided by Le Dimet and Navon (1988). Early monographs treating inverse problems in geophysics are those of Menke (1984) and Tarantola (1987).

Zou et al. (1992) estimated the magnitude of the nudging coefficient in the NMC adiabatic version of the spectral MRF model, while Wang(1993) and Wang et al. (1995) estimated the same coefficient using the FSU adiabatic spectral model. Stauffer and Bao (1993) performed a parameter estimation of nudging coefficients in a 1-D linearized shallow water equations model.

Wergen (1992) used also a 1-D linearized shallow-water equations model to recover both initial state and a set of forcing parameters from the observations. Wergen found out that even with noisy observation the parameters were recovered to an acceptable degree of accuracy.

Louis and Živković (1994) carried out physical parameters estimation in a simplified single column model, and their effort presents a more comprehensive approach to parameter estimation, making it amenable to generalization to problems of parameter estimation involving 3-D numerical weather prediction models.

The research methodology used in adjoint parameter estimation in meteorology can be viewed to be an extension of the 4-D VAR approach for controlling initial or initial and boundary conditions.

Some authors determine which are the crucial physical package parameters to be optimally identified based either on experience or using a relative adjoint sensitivity analysis. Such an analysis enables one to rank a subset of chosen parameters according to their relative sensitivities adequately chosen model responses.

The usual procedure for assessing the impact of an optimized parameter, requires testing impact on the model for a sufficiently long period, thus ensuring that no degradation of the forecast is caused by the optimally estimated parameter.

Since some parameters are known to vary between given bounds, the minimization of the cost functional(to be described below) will by necessity be of the constrained minimization type. Several efficient constrained minimization procedures are available(for instance see Nash and Sofer, 1995 for details). For methods of unconstrained minimization see Navon and Legler (1987), Navon et al. (1992a, 1992b) and Zou et al. (1993b) along with an excellent review by Nocedal (1991).

An essential monograph explaining analysis and application of assimilation methods is the one by Daley (1991).

If an optimally estimated parameter attains unphysical values, one can deduce that either an overfitting of the data took place, or that this parameter is not identifiable with the data available. We will address this issue in detail in the section related to identifiability.

Stratification of groups of parameters to be optimally identified may proceed by either seasonal stratification or following a given physical process at a time. Due to the nonlinear feedbacks that exist between classes of physical parameters, one should proceed with caution when increasing the dimensionality of the problem, i. e., by adding a new class of physical parameters to be optimally identified.

2. 2 Parameter estimation in oceanography

In oceanography optimal control parameter estimation issues have been addressed in early work by Bennett and McIntosh(1982) and Prevost and Salmon(1986) using Sasaki's weak constraint formalism. Early adjoint parameter estimation work is also the one carried out by Panchang and O'Brien (1989) for bottom drag coefficient identification in a tidal channel, while phase speeds were estimated in the review article by Smedstad and O'Brien (1991) using the adjoint method in a reduced gravity model for the tropical Pacific Ocean. Yu and O'Brien (1991) carried out a wind stress coefficient estimation along with the estimation of the oceanic eddy viscosity profile.Heemink (1987) used estimation theory for shallow water flow identification.

Early reviews of data assimilation methods in oceanographic applications are the lectures by Miller (1987) and the special issue of Dynamics of Atmospheres and Oceans edited by Haidvogel and Robinson (1989).

The book of Bennett (1992) provides a mathematically advanced and thorough synthesis of oceanographic assimilation methodologies.

An important comprehensive review serving as a milestone in adjoint methodology in meteorology and oceanography and summarizing state-of-the-art for beginning of the 1990's, including issues of parameter estimation, is the excellent review by Ghil and Malanotte-Rizzoli (1991).

Typical recent advances related to assimilating data into complex, time-dependent ocean general circulation models are those of Fukumori et al. (1993), Tziperman et al. (1992).

Das and Lardner(1990, 1992) estimated bottom friction and water depth in a 2-D tidal model and related to the issue of the number of observations required for a given mesh resolution in order to achieve satisfactory parameter identification.

Richardson and Panchang (1992) are the first in oceanography to have noted the difficulties associated with parameter estimation(eddy viscosity) with adjoint methods(and inverse modeling techniques in general) due to their being beset by instabilities and nonuniqueness when identifying parameters distributed in the space time domain, especially when the data is noisy. To overcome these difficulties they proposed to insert and additional criterion in the cost functional formulation namely that the parameter profiles should be smoothly varying, i. e., a compromise between data - model misfit minimization and the solution smoothness. A similar approach was introduced in the context of ground water flow parameter estimation in the doctoral thesis of Cushman-Roisin(1986). Additional work on eddy viscosity profile parameter estimation in a 3-D tidal model was carried out by Lardner and his collaborators (See Lardner and Song (1995) and references therein).

Additional recent parameter estimation applications in oceanography include work of Tziperman and Thacker(1989), estimating friction and wind forcing in ocean circulation models, Marotzke(1992), Marotzke and Wunsch (1993), Chertok and Lardner (1996), Gunson (1995), Yu and O'Brien(1992) and ten Brummelhuis et al. (1993) which used parameter estimation for tidal models.

A recent book presenting a comprehensive picture of the state-of-the-art of data assimilation in oceanography in the mid 90s and addressing also in several chapters the topic of parameter estimation is the excellent monograph edited by Malanotte-Rizzoli (1996). In particular the contributions of Malanotte-Rizzoli and Tziperman and references therein and that of Hogg in the above monograph, represent modern lucid contributions to state-of-the-art in parameter estimation in oceanography.

The book by Wunsch(1996) is also a very well-written, lucid and useful contribution including Gauss-Markov estimation, sequential estimators and adjoint/ Pontryagin principle devoted to finite dimensional problems and methods along with a very useful subsection on parameter estimation geared towards the general topics of parameter estimation .

I would finally like to caution the reader that I only addressed in this subsection literature on the adjoint parameter estimation aspect in oceanography and thus covered but a narrow aspect of the vast literature on oceanographic adjoint applications. The monograph edited by Malanotte- Rizzoli (1996) is an authoritative source for references to these applications .

2. 3 Identifiability

The uniqueness problem in parameter identification is ultimately related to the issue of *parameter identifiability.*

The notion of identifiability addresses the question of whether it is at all possible to obtain unique solutions of the inverse problem for unknown parameters of interest in a meteorological/oceanic model from data collected in the spatial and temporal domains.

Simply put(see Kitamura and Nakarigi, 1977) the parameter identification problem can be formulated as the one-to-one property of mapping from the space of system outputs to the space of parameters. The uniqueness of such a mapping is extremely difficult to establish. A working definition of identifiability is as follows(Kitamura and Nakarigi, 1977): "We shall call an unknown parameter 'identifiable' if it can be determined uniquely in all points of its domain by using the input-output relation of the system and the input-output data".

An early review work in the field of identification of parameters was provided by Goodson and Polis (1979).

Chavent(1979, 1983, 1991) presented a definition of identifiability using the output least-squares error criterion as used in 4-D Var. If such a criterion is used for solving the inverse problem of parameter identification the parameter is said to be *output least-square identifiable* if and only if a unique solution of the optimization problem exists and the solution depends continuously on the observations.

We will now provide two simple illustrative examples related to identifiability(see Banks and Kunish, 1989).

The first is related to ill-posedness of parameter estimation problems - where there is a lack of a continuous inverse of the parameter-to-observation mapping.

Example 1 (Banks and Kunish, 1989):

Let Q be the set of parameters which guarantee that a chosen model equation has solution $u(q)$, let C be observation operator mapping from solution space of model to observation space Z. Using these mappings we have the parameter-to-output mapping $\Phi : Q \to Z$ with $\Phi(q) = Cu(q)$.

Let us assume our model is the 1-D equation

$$-(qu_x)_x = f \qquad \text{on } (0,1) \tag{1}$$

$$u(0) = u(1) = 0$$

Here f is assumed to be known and q is the unknown parameter.

Integrating (1) formally we obtain for $x_p \in (0,1)$

$$q(x) = \frac{u_x(x_p)}{u_x(x)} q(x_p) - \frac{1}{u_x(x)} \int_{x_p}^{x} f(s)ds \qquad \text{for} x \in [0,1] \tag{2}$$

If $u_x > 0$ (or $u_x < 0$) on [0, 1] then q is uniquely determined by (2) provided $q(x_p)$ is given for some $x_p \in [0,1]$. If u_x has precisely one root we may take this point as x_p and define from (1)

$$q(x_p) = \frac{f(x_p)}{u_{xx}(x_p)}$$

provided $u_{xx}(x_p) \neq 0$.

Then q is determined uniquely without specification of q at any point in its domain.

Also q can be bounded in terms of $u_x(q)$ provided that u_x can be bounded away from zero. However we cannot bound the inverse of

$$\Phi(q) = u(q)$$

as a mapping from C(0, 1) to C(0, 1) even in a neighborhood of some u^* satisfying $u_x^* > 0$.

To see this let

$$u_k(x) = x + \frac{1}{(2k+1)\pi} \sin 2k\pi x \qquad \textit{on } [0,1], k = 1, 2, ...$$

and assume $f = 0$ and $q(0) = 1$, are known, then

$$(u_k)_x = 1 - 2k/(2k+1),$$

$$u_k(0) > 0,$$

$$u_k(1) = 1 \qquad for\ all\ k$$

and $u_k \to u^*$ with $u^*(x) = x \qquad in\ C(0,1)$.

On the other hand by Eq. (2) we have for the corresponding parameters

$$q_k(x) = \frac{(u_k)_x(0)}{(u_k)_x(x)} = \frac{1 + \frac{2k\pi}{(2k+1)\pi}}{1 + \frac{2k\pi}{(2k+1)\pi} \cos 2k\pi x} \tag{3}$$

which is a *divergent* series in C(0, 1). This example illustrates the lack of a continuous inverse of the parameter-to-observation mapping of parameter estimation problems.

Example 2 (Banks and Kunish, 1989):

We consider the case of a parabolic model equation and show that the unknown parameters are identifiable. Then a spectral approximation to the model equation is performed for which the parameters are again identifiable.

Nevertheless it is not possible to use a spectral approximation in an output least squares(OLS) formulation to successfully estimate the unknown parameters.

The model equation is:

$$u_t = q_1 u_{xx} + q_2 u \qquad \text{for} t > 0, \quad 0 < x < 1 \tag{4}$$

$$u(0,x) = \Phi(x) \qquad 0 \le x \le 1$$

$$u(t,0) = u(t,1) = 0 \qquad t > 0$$

where Φ is the piecewise linear interpolant satisfying

$$\Phi(0) = \Phi(1) = 0, \qquad \Phi(\frac{1}{2}) = 1$$

The solution of (4) is given by

$$u(t,x,q_1,q_2) = \sum_{i=1}^{\infty} \tilde{u}_i exp((q_2 - q_1(i\pi)^2)t) \sin i\pi x \tag{5}$$

where $\tilde{u}_i$ are the Fourier coefficients of the sine series for Φ. Observe that

$$\tilde{u}_{2i} = 0, \qquad \text{for} i = 1, 2, ...$$

Let us assume that the observations are of the form

$$u(t^*, \cdot) \in L^2 \text{ for such} t^* \in (0, \infty)$$

and let

$$q^* = (q_1^*, q_2^*), \qquad q_1^* > 0$$

be the "true" parameters with corresponding observation

$$Z = u(t^*, ..., q^*)$$

Then if $u(t^*, \cdot, q^*) = u(t^*, \cdot, q), \qquad q = (q_1, q_2)$ it follows from (5) that $q = q^*$.

Now let us take an approximation to (5) of the form

$$u^N(t,x,q_1,q_2) = \sum_{i=1}^{N} u_i exp((q_2 - q_1(i\pi)^2 t) \sin i\pi x$$

Again $u^N(t^*, ..., q^*) = u^N(t^*, ..., q)$ implies $q = q^*$, provided $N \geq 3$.

Thus q is identifiable at q^* for the original as well as for the approximating model equation. Practically this is useless, however since for only moderately large t^* and i, the contribution of the term $exp((q_2 - q_1(i\pi)^2 t^*)$ to $u^N(t,x,q_1,q_2)$ is negligible.

Since $\tilde{u}^2 = 0$ we essentially estimate only $(q_2 - q_1\pi^2)t^*$ in an OLS formulation. Thus either q_1 or q_2 separately can be estimated successfully, but a simultaneous estimation of q_1 and q_2 fails.

2. 4 Mathematical background for parameter estimation

A typical cost functional in adjoint parameter estimation takes the form (Zou, Navon, and Le Dimet, 1992)

$$J(\mathbf{X},\mathbf{P}) = \int_{t_0}^{t_r} < W(\mathbf{X}-\mathbf{X}^{obs}), (\mathbf{X}-\mathbf{X}^{obs}) > dt +$$

$$+ \int_{t_0}^{t_r} K < \mathbf{P}-\hat{\mathbf{P}}, \mathbf{P}-\hat{\mathbf{P}} > \ dt \tag{6}$$

where vector $\mathbf{P}$, represents model parameters, $\hat{\mathbf{P}}$ is the vector of estimated parameters, K are specified weighting matrices, $\mathbf{X}^{obs}$ is the observation vector, $\mathbf{X}$ are the model output variables, W is a weighting matrix and, for the more realistic case, there is an interpolation operator H from the model space to the observation space.

The adjoint model equation for

$$\frac{\partial \mathbf{X}}{\partial t} = \mathbf{F}(\mathbf{X}) + K(\mathbf{P}-\hat{\mathbf{P}}) \tag{7}$$

The adjoint model equation is obtained from a formulation of an augmented Lagrangian, where

$$\nabla_P J = 2K(\mathbf{P}-\hat{\mathbf{P}}) - \int_{t_0}^{t_r} < \mathbf{P}, (\mathbf{X}-\mathbf{X}^{obs}) > \ dt \tag{8}$$

and the adjoint model equation is

$$\frac{\partial \mathbf{Q}}{\partial t} + \left[\frac{\partial \mathbf{F}}{\partial \mathbf{X}}\right]^T \mathbf{Q} - \mathbf{P}^T\mathbf{Q} = W(\mathbf{X}-\mathbf{X}^{obs}) \tag{9}$$

where $\mathbf{Q}$ is a vector of Lagrangian multipliers identified with the adjoint variables,

$\mathbf{X}$ is the discretized state variable,

$\mathbf{X}^{obs}$ is the observation vector, and we see that an additional term, namely:

$$-\mathbf{P}^T\mathbf{Q}$$

was added to the left hand side of the last equation.

We can assess sensitivity of forecast to model parameters in a simplistic way (i. e., without taking into account presence of data) by considering

$$\delta J = < \nabla_P J, \delta \mathbf{P} >$$

where $\delta\mathbf{P}$ is a small change in parameters vector resulting in a change δJ in forecast errors.

In a general set up the cost function is

$$J(\mathbf{X},\mathbf{P}) = \frac{1}{2}(\mathbf{X}-\mathbf{X}_b)^T \ B^{-1} \ (\mathbf{X}-\mathbf{X}_b) \ + \ \frac{1}{2}(H\mathbf{X}-\mathbf{X}^o)^T \ O^{-1} \ (H\mathbf{X}-\mathbf{X}^o) +$$

$$+ \ K(\mathbf{P}-\hat{\mathbf{P}})^T(\mathbf{P}-\hat{\mathbf{P}}) \tag{10}$$

where B is the background error covariance matrix, $\mathbf{X}^o$ is the set of observation whose error covariance is O, and H is the observation operator which computes the model equivalent $H\mathbf{X}$ of the observation $\mathbf{X}^o$.

Typical cost functional for parameter estimation

$$J(p) = J_h(p) + J_d(p) + J_f(p) + J_R(p) \tag{11}$$

$J_h(p)$ - weighted least-squares term between "measured" and model estimated parameters, with weight which are related to confidence in the data. They may be more reliable.

$J_f(p)$ - weight least squares error between "measured" and model estimated parameters at final time of assimilation - J_f optimizing improvements in data measurements made at later times.

$J_d(p)$ - A weighted prior data error term, which represents prior knowledge about the parameters with weights representing the confidence in the measured prior data.

$J_r(p)$ - A Tichonov regularization term - which deals with instabilities in values of parameter estimates that appear to be closely related to noise in measured data. This term smooths parameter estimates, by imposing a penalty on oscillations in parameter estimates.

Reduction in the dimensionality of parameters

If the number of distributed parameters to be estimated is large - we can approximate them by constructing (simple) sequences using simple polynomial basis functions according to

$$P^e(\mathbf{X}) = \sum_{j=1}^{N_1} \alpha_j \mathbf{X}^{j-1} \tag{12}$$

where estimates $\bar{p}^e(\mathbf{X}) \to p(\mathbf{X})$ as $N_1 \to \infty$. Parameter identification is now reduced to identifying a finite number of coefficients α_j such that the cost functional (11) is minimized.

2. 5 Ill-posedness of the problem of parameter estimation

Chavent(1974, 1979, 1983, 1991) was amongst the first to propose parameter estimation using the adjoint method in connection with the output least squares problem. He also recognized that this inverse problem is often ill-posed. This ill-posedness is characterized by

- nonuniqueness
- instability of the identified parameters.

Instability here means that small errors in data will cause serious errors in the identified parameters.

The uniqueness problem in parameter identification is intimately related to *identifiability.*

- The concept of identifiability addresses the question of whether it is at all possible to obtain unique solutions of the inverse problem for unknown parameters of interest in a mathematical model from data collected in the spatial and (temporal) time domains.

- The parameter estimation problem consist in finding an estimated value $\hat{\mathbf{P}}$ of the parameter $\mathbf{P}$ from knowledge of data $\mathbf{Z}$, of the parameter to output mapping ϕ and some '*a priori*' knowledge on the parameter which is condensed in a set C of admissible parameters C_{ad}

Due to measurement and forecast model errors the equation

$$\text{find} \quad \hat{\mathbf{P}} \in C_{ad}, \quad \phi(\hat{\mathbf{P}}) = \mathbf{Z} \tag{13}$$

has no analytic solution so the equation is solved approximatively using a least-squares formulation

$$\text{find} \quad \hat{\mathbf{P}} \in C_{ad}, \qquad \text{s. t.}$$

$$J\left(\hat{\mathbf{P}}\right) \leq J\left(\mathbf{P}\right) \qquad \forall \mathbf{P} \in C_{ad} \tag{14}$$

where $J\left(\hat{\mathbf{P}}\right)$ is the output or measurement error criterion

$$\forall \mathbf{P} \in C_{ad}, \qquad J(\mathbf{X}) = \|\phi(\mathbf{X}) - \mathbf{Z}\|_F^2 \tag{15}$$

for some norm in data space F and one attempts to minimize (15) over the set C using his favourite optimization routine.

Here C_{ad} is the admissible parameter set which is chosen as small as possible by taking into account largest possible amount of '*a priori*' information on the unknown parameter such as the following considerations: lower and upper bounds, trends and regularity.

In many instances of parameter estimation one finds that a) Instability occurs when the discretization of parameter is refined.

b) Lack of uniqueness of the estimated parameter $\hat{\mathbf{P}}$, and/or the optimization algorithm gets stuck in a local minimum.

2. 6 Identifiability, Ill-Posedness and Regularization of Parameter Estimation

The key difficulty in developing successful numerical techniques for identifying spatially-dependent parameters resides in the fact such problems are ill-posed.

Ill-posedness follows from the fact that the differentiation operator is not continuous with respect to any physically meaningful observation topology.

For instance, the problem of identifying spatially-dependent coefficients appearing in the differential operator of a P. D. E. is, in general, both nonlinear and ill-posed(Ewing et al., 1989).

Using the customary approach of output least-squares Chavent (1991) we minimize a cost functional

$$J_{LS} = \int_0^T \sum_{i=1}^{M} \left[U(x_i, y_i, \alpha, t) - Z_{d_i}\right]^2 dt \tag{16}$$

subject to model equations, initial and boundary conditions, where Z_{d_i} is a set of given observations (measurements) of $U(x_i, y_i, \alpha, t)$ at a set of discrete spatial locations, $i = 1, 2, ...M$.

When the number of parameters is kept small - a well behaved solution results.

However modeling error is significant - since corresponding subspace of parameter $\delta\alpha$ is too restricted to provide good approximation an arbitrary α.

As number of parameters is increased - numerical instabilities appear - manifested by spatial oscillation in estimated α, frequency and amplitude of which are not consistent with expected smoothness of α.

A typical symptom is a flat global minimum of J_{LS} (Yakowitz and Duckstein, 1980).

To alleviate problem one may incorporate '*a priori*' statistics concerning α by adding a Bayesian term to cost functional.

Numerical instabilities and ill-posed nature of problem strongly suggest a regularization approach.

"Regularization" of a problem refers generally to solving a related problem - called the "regularized problem", the solution of which is more regular in a sense than that of the

original problem - but which approximates solution of the original problem (Tichonov, 1963, and Tichonov and Arsenin, 1977).

When one refers to ill-posed problems - regularization is an approach to circumvent lack of continuous dependence on the data. The regularized problem is a well-posed problem whose solution yields a physically meaningful answer to the given ill-posed problem.

The idea of regularization was first proposed by Tichonov(1963) or earlier, and extended by Morozov(1968) and Morozov and Stessin(1993).

3. Maximum likelihood (ML) method for parameter estimation

In this inverse approach, each of the model parameters to be estimated is represented by a set of discrete "model parameters". Let us designate the "true" values of these model parameters by p, and their prior estimates(or "measured") values by p^*.

The purpose of the inverse model is to provide improved estimates of p, $\hat{p}$ by relying on model variables measurements - obtained at a set of observation locations at discrete time intervals.

The discrepancies between measured and true quantities such as $p^* - p$ are referred to as "measurement errors"' while differences between measured and computed quantities $p^* - p$ are called "residuals".

Maximum likelihood theory is developed in terms of "prior errors" which are usually taken to be measurement errors. In practice estimation is performed by minimizing a criterion expressed in terms of the residuals which are a combination of measurement errors and errors arising from the numerical model. Thus the prior statistics entering into the estimation criterion should reflect both types of errors.

Since prior errors in the model parameters are affected by a variety of cases we can assume that the prior errors can be considered Gaussian with zero mean. The covariance C_i, the prior errors associated with parameter type p_i can be written as

$$C_i = \sigma_i^2 V_i \tag{17}$$

where σ_i^2 is either a known or unknown positive scalar and V_i is a known symmetric positive-definite matrix.

We assume that the prior estimates of varies parameter types are naturally uncorrelated. The global covariance matrix of the model parameters to be estimated C_p is block diagonal, its diagonal components being C.

The prior errors can be written as

$$\epsilon^* = N(0, \sigma_i^2 V_i) \tag{18}$$

meaning ϵ^* is a Gaussian random vector with 0 mean and covariance matrix $\sigma_i^2 V_i$.

Let $Z^* = (\underline{x}^*, \underline{P}^*)$ be a vector incorporating model and parameter data and $\theta = (\sigma_x^2, \sigma_i^2, ...)^T$ be a vector of unknown statistical parameters characterizing prior errors. If $\beta = (p, \theta)^T$ is the vector of all the unknown parameters then the likelihood $L(\beta/Z^*)$ of a hypothesis regarding the value of β_1 given Z^* and a specific model structure such as numerical method parameterization etc. (see Carrera and Neuman, 1986) is proportional to $f(Z^*/\beta)$, the probability density of observing Z^* if β was true.

For a given model structure, the optimum parameter estimates are taken to be those that maximize $L(\hat{\beta}/Z^*)$, where $\hat{\beta}$ is an estimate of β. Based on an hypothesis that all data have been properly transformed to yield Gaussian distributions of the prior errors it becomes obvious that the likelihood function can be written as

$$L(\beta^*/Z^*) = f(Z^*/\beta) = (2\pi)^{-\frac{1}{2}} det|C_x|^{-\frac{1}{2}} exp\left[\frac{1}{2}(Z^* - Z)^T C_Z^{-1}(Z^* - Z)\right] \tag{19}$$

Here C_x is the covariance matrix of the prior errors

$$C_Z = \begin{bmatrix} C_x & 0 \\ 0 & C_p \end{bmatrix} \tag{20}$$

where C_x and C_p are the covariance matrices of the prior model and model parameter errors ($C_x = \sigma_x^2 V_x$).

In practice maximum likelihood(ML) estimates are generally obtained by minimizing the "log-likelihood"

$$S = -2\ln\left[L(\beta/Z^*)\right] \tag{21}$$

where we can explicitly write S as

$$S = \log detC_z + \frac{1}{2}(Z^* - Z)^T C_z^{-1}(Z^* - Z) \tag{22}$$

This criterion has the desirable property that the log-likelihood of a hypothesis, given all the data, is the sum of the log-likelihood of the same hypothesis, given each separate set of data.

This allows one to introduce prior information about the parameters into the estimation scheme and to analyze data representing conditions created by a variety of initial and boundary conditions. An excellent survey of approximation of the ML method to parameter estimation of aquifer parameter is represented by Carrera and Neuman(1986). Dee(1995) used ML for covariance parameter estimation.

The method was used in oceanography application by ten-Brummelhuis et al. (1990, 1993). Wahba(1990) and more recently Wahba et al. (1994, 1995) used more advanced statistical methods such as Gong et al. (1996) generalized the statistical parameter estimation using generalized cross validation(see also Wahba et al., 1995) as well as unbiased risk methods for adaptive tuning of parameters in one space and one time variables for the equivalent barotropic vorticity equation on a latitude circle, simultaneously tuning some smoothing, weighting and physical parameters.

4. Total variation as an L_1 regularization method for parameters with discontinuities

Using Total Variation (TV) regularization may turn out to be particularly useful to the meteorological community related to the potential of the method to deal with parameter functions which may have jump discontinuities.

This approach bypasses the difficulty of standard regularization techniques that they do not allow discontinuous solutions (Acar and Vogel, 1994).

The method was used by Santosa and Symes (1988) for reconstructing blocky impedance profiles in seismology and for parameter identification by Gutman (1990). Blocky profiles means functions that are piecewise constant and hence have sharply defined edges (Dobson and Santosa, 1994, 1995).

Since 1990 there has been a wide interest in the TV methods for recovering "blocky", possibly discontinuous images, from noisy data. Significant work includes Rudin and Osher (1994), Rudin, Osher and Fatemi (1992), Acar and Vogel (1994), Rudin (1987), Osher and Rudin (1990), Alvarez Lions and Morel (1992) and recent work by Dobson and Santosa (1994), Vogel and Oman (1995) and Vogel and Wade(1995).

Using Total Variation methods can indeed result in a significant contribution to problems in optimal parameter estimation where location and size of discontinuities are important.

The topic of Total Variation regularization was also the subject of 2 articles in SIAM News (December 1993 by Rudin and July 1994 by Santosa) where the work of Rudin et al. (1994) and Osher as well as the work of for denoising and deblurring images was described and illustrated.

Consider solving ill-posed operator equation $AU = Z$ Solving the problem of constrained minimization

$$\min_{U} \; J(\mathbf{U}) \tag{23}$$

Subject to $\|A\mathbf{U} - \mathbf{Z}\|^2 = \sigma^2$ This will achieve stability with the requirement that the solution be of bounded variation rather than smooth.

Here A is a linear operator from $L^p(\Omega)$ into a Hilbert space Z containing data vector $\mathbf{Z}$.

Data $\mathbf{Z}$ and operator A are inexact.

σ^2 is an estimate of the size of the error in the data and $J(\mathbf{U})$ is a Bounded Variation (BV) norm or semi-norm of U.

$$J_\beta(\mathbf{U}) = \int_\Omega \sqrt{|\nabla \mathbf{U}|^2 + \beta}\; dx \tag{24}$$

$$\beta \geq 0 \tag{25}$$

$$\|\mathbf{U}\|_{\beta V} = \|\mathbf{U}\|_{L_1(\Omega)} \tag{26}$$

Another approach is to solve the regularized minimization problem

$$\min_{U} \; \|A\mathbf{U} - \mathbf{Z}\|^2 + \alpha J(\mathbf{U}) \tag{27}$$

This can be viewed as a penalty method approach for solving the constrained optimization problem. The penalty parameter $\alpha > 0$ controls trade off between goodness of fit to data measured by $\|A\mathbf{U} - \mathbf{Z}\|^2$ and variability at jumps in approximate solution as measured by $J(\mathbf{U})$.

The final form of the Total Variational penalized least-squares functional is

$$\frac{1}{2}\|A\mathbf{U} - \mathbf{Z}\| + \alpha \int_{\Omega} \sqrt{|\nabla \mathbf{U}|^2 + \beta} \tag{28}$$

Under mild conditions on the operator A equation (24) has a unique minimizer U^* and U^* depends continuously on the parameters α β and the data Z and on the operator A.

The choice of the penalty parameter α in (24) depends on factors like signal-to-noise ratio.

When the error level is very low, α tends to be very small. A number of standard minimization methods can be applied for an unconstrained minimization of the modified TV penalty functional.

A nonlinear preconditioned conjugate gradient algorithm will perform well or one can use augmented Lagrangian methods.

The application of total variation problems to meteorological parameter estimation problems will address the issue of parameters which have jump discontinuities - allowing us to bypass difficulty of standard regularization technique that do not allow discontinuous solutions.

5. Parameter estimation by Extended Kalman Filter

The Model system is given by

$$W_k^f = \psi_{k-1}\left(W_{k-1}^a\right) \tag{29}$$

W_{k-1}^a - best estimation of model state.

ψ_{k-1} - state transition function.

$$W_k^t = \psi_{k-1}\left(W_{k-1}^t\right) + b_{k-1}^t \tag{30}$$

b_{k-1}^t is a Gaussian white noise sequence.

$$E b_k^t (b_l^t)^T = Q_k \delta_{k,l} \tag{31}$$

Q_k - model error covariance.

Evolution of system is measured by observation contaminated by error b_k^o,

$$W_k^o = h_k\left(W_k^t\right) + b_k^o \tag{32}$$

$$E b_k^o \left(b_l^o\right)^T = R_k \delta_{k,l} \tag{33}$$

superscripts t, a, f denote truth, analysis and forecast. A linear estimation of the model state based on observation (despite the fact that dynamic model ψ_k and observation h_k may be nonlinear) is sought:

$$W_k^a = W_k^f + K_k\left(W_k^o - W_k^f\right) \tag{34}$$

K_k - weight assigned to "observations".

Weights are optimized by minimizing the function

$$J_k = E\left[\left(W_k^a - W_k^t\right)^T \left(W_k^a - W_k^t\right)\right] = trace\left[P_k^a\right] \tag{35}$$

P_k^a being the analysis error covariance.

EKF linearly approximates ψ_k and h_k at each step along the trajectory resulting from a continuous model update with "observations".

The EKF algorithm when "observations" are available at time-step k is:

$$W_k^f = \psi_{k-1}\left(W_{k-1}^a\right) \tag{36}$$

$$P_k^f = \Psi_{k-1}\left(W_{k-1}^a\right) P_{k-1}^a \Psi_{k-1}^T\left(W_{k-1}^a\right) + Q_{k-1} \tag{37}$$

Updating step

$$W_k^a = W_k^f + K_k\left(W_k^o - h_k\left(W_k^f\right)\right) \tag{38}$$

$$P_k^a = \left[I - K_k H_k\left(W_{k-1}^a\right)\right] P_k^f \tag{39}$$

$$K_k = P_k^f H_k^T\left(W_k^f\right)\left[H_k\left(W_k^f\right) P_k^f H_k^T\left(W_k^f\right) + R_k\right]^{-1} \tag{40}$$

where

$$\Psi\left(W_k^a\right) = \frac{\partial \psi_k(W)}{\partial W}\Big|_{W=W_k^a} \tag{41}$$

$$H_k\left(W_k^f\right) = \frac{\partial h_k(W)}{\partial W}\Big|_{W=W_k^f} \tag{42}$$

K_k is called the Kalman gain representing optimal weight given by observations.

Ψ_k is the state transition matrix - a linear propagator of forecast error covariance in time.

Hao(1994b), Hao et al. (1994a) as well as Hao et al. (1996), Hao and Ghil(1995) and Ghil(1996) applied EKF method to estimate model parameters by incorporating the unknown parameter in the scheme such that it is treated as an additional state variable.

$$W_k^f = \psi_{k-1}\left(W_{k-1}^t, \mu_{k-1}^t\right) + b_{k-1}^t \tag{43}$$

$$\mu_k^f = U_{k-1}^t + b_{k-1}^{\mu t} \tag{44}$$

$$W_k^o = h_k\left(W_k^t\right) + b_k^o \tag{45}$$

where W_k and μ_k can be combined into a composite state vector $W_k^{\prime}$.

Issues of identifiability and regularity will require some attention and further research, as well the fact that parameter estimation with EKF is trajectory dependent. The number of observations required for successful optimal parameter estimation is found to be proportional to the size of the errors in the assimilated state fields when the parameter error is left uncorrected, while correct estimation of "important" model parameters, results in improved estimation of model state. Hao and Ghil(1995) addressed the issue of *identifiability* and show that the scheme in Eqs. (43-45) can be extended to a set of parameters - where μ will serve as a vector.

The dimension of the system increase by the number p of parameters to be estimated, which is usually small, i. e., $p << n$. Their research also shows that the number of observations required to estimate a given parameter is proportioned to the sensitivity of the state-estimation errors to the parameter value.

Parameter estimation using Kalman filtering is addressed in a number of textbooks such as Goodwin and Sin (1984), Haykin (1986) and Ljung (1987).

6. Sensitivity Analysis as a Tool in Parameter Estimation.

Sensitivity is a measure of the effect of changes in a given input parameter on a selected response (any forecast aspect). The general definition of sensitivity of a response to variations in system parameters is the *Gâteau* differential.

The G differential $VR(\mathbf{X}^0, \boldsymbol{\alpha}^{\mathbf{o}}, \mathbf{h}_{\boldsymbol{x}}, \mathbf{h}_\alpha)$ of a specific response $R(\mathbf{X}, \boldsymbol{\alpha})$

$$R(\mathbf{x}, \boldsymbol{\alpha}) = \int_{\boldsymbol{t_o}}^{\boldsymbol{t_a}} \boldsymbol{r}(\boldsymbol{t}; \mathbf{x}, \boldsymbol{\alpha}) \boldsymbol{dt} \tag{46}$$

at the nominal values $(\mathbf{X}^0, \boldsymbol{\alpha}^{\mathbf{o}})$, where $\boldsymbol{\alpha}$ is a model parameter vector, for increments $(\mathbf{h}_x, \mathbf{h}_\alpha)$ around $(\mathbf{X}^0, \boldsymbol{\alpha}^{\mathbf{o}})$ is given by

$$VR(\mathbf{x}^0, \boldsymbol{\alpha}^{\mathbf{o}}; \mathbf{h}_{\boldsymbol{x}}, \mathbf{h}_\alpha) = \int_{\boldsymbol{t_o}}^{\boldsymbol{t_R}} \boldsymbol{r'}_{\mathbf{x}} \cdot \mathbf{h}_{\boldsymbol{x}} \boldsymbol{dt} + \int_{\boldsymbol{t_o}}^{\boldsymbol{t_R}} \boldsymbol{r'}_{\boldsymbol{\alpha}} \cdot \mathbf{h}_\alpha \boldsymbol{dt} \tag{47}$$

$$r'_{\mathbf{x}} = \Big[\big(\frac{\partial r}{\partial x_1}, \ldots, \frac{\partial r}{\partial x_P} \big) \Big]_{(\mathbf{x}^0 \boldsymbol{\alpha}^{\mathbf{o}})} \tag{48}$$

$$r'_{\boldsymbol{\alpha}} = \Big[\big(\frac{\partial r}{\partial \alpha_1}, \ldots, \frac{\partial r}{\partial \alpha_N} \big) \Big]_{(\mathbf{x}^0, \boldsymbol{\alpha}^{\mathbf{o}})} \tag{49}$$

N is the dimension of the vector of model parameters and P is the dimension of the model variable.

If a variation occurs solely in the n-th parameter the corresponding variation $h^n_{\boldsymbol{\alpha}}$ of the parameter vector is

$$h^n_{\boldsymbol{\alpha}} = (0, \ \ldots, \ h^n_\alpha, \ \ldots, \quad 0)^T \tag{50}$$

and the corresponding sensitivity is VR^n.

The relative sensitivity S_n is the dimensionless quantity

$$S_n = \frac{VR^n}{R}\left(\frac{\mathbf{h}_\alpha^n}{\boldsymbol{\alpha}_{\boldsymbol{n}}^{\mathbf{o}}}\right)^{-1} \tag{51}$$

The *relative* sensitivity clearly demonstrates the measure of the importance of the input parameter. The higher the relative sensitivity, the more important the input parameter in question. Thus, one of the crucial aspects of sensitivity analysis is to identify the most important input parameters whose changes impact the most the chosen response. The magnitudes of relative sensitivities can serve as a guide to ranking importance of model parameters for use in choosing candidates for optimal parameter estimation.

For models that involve a large number of parameters and comparatively few responses, sensitivity analysis can be performed very efficiently by using deterministic methods based on adjoint functions. It can be shown (Zou *et al.*, 1993a) that the changes in the response function can be expressed in terms of adjoint dynamics $q(t)$, which is an adjoint variable corresponding to the model variable $x(t)$. The use of the adjoint model eliminates the need to calculate, by forward integration, $\delta x(t)$ $(= x(t) - x^0(t))$, a quantity whose dynamics is governed by the so-called linear tangent equations, where $x(t)$ and $x^0(t)$ are the perturbed and the actual model trajectories in phase space. These forward calculations happen to be explicitly dependent on the changes in the initial conditions $\delta x(t_0)$ and the model parameters changes and must be repeated every time these are altered; the formulation using the adjoint solution to the linear tangent dynamics does not suffer from this shortcoming and is therefore extremely economical when dealing with large models possessing several parameters.

Based on work of Cacuci (1981, 1988), Zou et al. (1993a) extended sensitivity analysis to general operator type responses such as time and space dependent functions of the model state variables and parameters. This since the most interesting and revealing meteorological cases involve sensitivity with respect to operator responses that depend on both time and space. We intend to use those methods to carry out extensive sensitivity studies using the NMC model with physics and its adjoint.

Sensitivities amongst other may quantify the extent that uncertainties in parameters contribute to uncertainties in model results. Furthermore the adjoint sensitivity analysis may also provide a quantitative measure of the importance of data or a region in phase space in contributing to an adequately chosen response function. One limitation of such sensitivity study is the restriction of each result to one of the forecast aspects. Therefore, one should carefully select different responses.

Sensitivity studies with the full physics adjoint model will be carried out with the intention of using a stratification based on various meteorological seasons corresponding to different meteorological situations - for instance, seasonally dependent sensitivities (see Errico et al., 1993a, b). In our ranking of model parameters to be used in the parameter estimation, we shall use various response functions and compare resulting parameter rankings. This implies stratification of relative sensitivities both by response and by season - thus implying that the subset of model parameters chosen is of real impact on the model response. It is well known that the adjoint sensitivity approach indicates both geographical areas and meteorological parameters to which a given model function is most sensitive (Rabier et al., 1992, 1993).

7. Summary and Conclusions

Parameter estimation using adjoint of full physics NWP models or oceanographic models will pose serious challenges which were not fully encountered in either meteorology and oceanography when only few parameters were estimated. The issues of identifiability, taken usually for granted in optimal parameter estimation with adjoint method for either atmospheric or ocean general circulation models should be carefully addressed. The mathematical framework for assessing uniqueness and identifiability in optimal parameter estimation using adjoint optimal control methods was outlined. This issue has particular importance since the potential for benefits using variational data assimilation with adjoint methods is highly accrued if one can optimally estimate key parameters in aforesaid oceanic and atmospheric models. Basic research results, using recent advances in issues related to identifiability, regularization stability and total variation regularization were shown to be required to establish robust parameter estimation procedures.

Relative sensitivity analysis will serve as a guide to identify most important parameters whose changes impact most chosen relevant responses for the atmospheric or oceanographic models employed.

The rich experience accumulated by research workers from other fields such as water-resources and seismology as exemplified by the few references provided in this paper can serve as a guide for efforts of reliable optimal parameter estimation in meteorology and oceanography.

Methods of large-scale constrained minimization for the solution of optimal parameter estimation for range-bounded parameters will have to employ sequential quadratic programming and projected gradient minimization methods.

When the optimal parameter estimation is done for a full physics model and his adjoint, as is the case in atmospheric NWP models, methods of stratification of parameters by physical package, seasonality and other considerations (see Louis and Živković, 1994) should be tested.

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Appendix A

Rigorous Mathematical Framework for Identifiability and Regularization

There has been a serious mathematical effort to understand in depth parameter estimation starting with the seminal works of Richard Bellman and collaborators in 1965 (Bellman et al. 1965a, b) while in the last twenty years works closely related to the use of the adjoint method include contributions of Chavent, 1979, Kitamura and Nakarigi, 1977, Kubrusly, 1977 and more recently works of Banks and Rosen (1987), Banks and Kunish, 1989; Omatu and Seinfeld, 1989 and Banks, 1992a, b and references therein. It is therefore incumbent upon the meteorological community at both the operational and university level to acquaint itself with these new results.

Let $\mathcal{A}$, $\cup$ and $\mathcal{F}$ be Banach spaces, where $\mathcal{A}$ represents a space of partial differential operators, $\cup$ represents the space of solutions and $\mathcal{F}$ the space of right hand sides.

Consider a system represented by

$$\Psi(A, U) = f \tag{A.1}$$

where Ψ is a mapping not necessarily linear from $\mathcal{A} \times \cup$ into $\mathcal{F}$.

We assume

(a1) Ψ is of C^k class ($k \geq 1$).

(a2) There is an open subset $\mathcal{A}_c$ of $\mathcal{A}$ and an open subset $\cup_c$ of $\cup$ s. t. $\forall A \in \mathcal{A}_c$.

Eq. (A. 1) admits a unique solution $U \in \cup_c$.

(a3) $\forall A \in \mathcal{A}_c$, $\forall u \in \cup_c$, $\left(\frac{\partial\psi}{\partial u}\right) A(u)$ is a linear homeomorphism of $\cup$ on to $\mathcal{F}$.

Thus one can define an implicit function

$$U = \Phi(A) \tag{A.2}$$

as the solution of Eq. (A. 1). Φ is of C^k class from $\mathcal{A}_c$ into $\cup_c$. Furthermore, consider that A depends on a set of parameters p belonging to the Banach space $\wedge$. The set of physically admissible parameters p is $\wedge_{ad}$. We assume

(a4) A, $\wedge \rightarrow \mathcal{A}$ is of C^k class ($k \geq 1$)

(a5) $\wedge_{ad}$ is a norm-closed convex subset of $\wedge$

(a6) $\mathcal{A}(\wedge_{ad}) \leq \mathcal{A}_c$

The parameter identification problem can be posed as follows:

Knowing mappings Ψ, $\mathcal{A} \times \cup \rightarrow \mathcal{F}$ and $\mathcal{A}$; $\wedge \rightarrow \mathcal{A}$ and the element $f \in \mathcal{F}$ and given an observation Z_d of U, find $p \in \wedge_{ad}$ to satisfy equation (A. 1).

Thus the identification problem can be viewed as solving in $\wedge_{ad}$ the nonlinear operator equation

$$(C \cdot \Phi \cdot A)(p) = Z_d \tag{A.3}$$

If this operator $C \cdot \Phi \cdot A$: $\wedge_{ad} \rightarrow \mathcal{H}$ has an unique inverse - and the inverse is continuous, one can apply the least-squares method (adjoint method).

It consists of minimizing over $\wedge_{ad}$ the functional

$$J_{LS}(p) = \|C(\Phi(A(p))) - Z_d\|^2_{\mathcal{H}} \tag{A.4}$$

Often the problem of solving (A. 3) is ill-posed. Hence minima of $J_{LS}(p)$ over $\wedge_{ad}$ will not depend continuously on the data Z_d.

To regularize parameter p, we introduce a more regular space $\mathcal{R}$ for which we assume,

(b1) $\mathcal{R}$ is a Hilbert space.

(b2) $\mathcal{R}$ is densely imbedded in $\wedge$.

(b3) The embedding operator from $\mathcal{R}$ into $\wedge$ is compact.

Define $\mathcal{R}_{ad} = \mathcal{R} \cap \wedge_{ad}$. It follows that $\mathcal{R}_{ad}$ is a norm-closed convex subset of $\mathcal{R}$. Introduce now stabilizing functional (regularization).

$$J_s(p) = \|p\|^2_{\mathcal{R}} \qquad p \in \mathcal{R}_{ad} \tag{A.5}$$

and smoothing functional

$$J_\beta(p) = J_{LS}(p) + \beta J_s(p)$$

$$= \|C(\Phi(A(p))) - Z_d\|^2_{\mathcal{H}} + \beta \|p\|^2_{\mathcal{R}} \quad p \in \mathcal{R}_{ad} \tag{A.6}$$

Identification of parameters by regularization proceeds as follows (Nakarigi, 1983; Kravaris and Seinfeld, 1986)

Given observation $Z_d \in \mathcal{H}$ find $p_\beta \in \mathcal{R}_{ad}$ so as to minimize cost functional $J_\beta(p)$.

Upon modification of the algorithms by regularization and by using appropriate constraints- the estimated parameters improve significantly.

When *'a priori'* knowledge about constraints for certain problem is available a constrained optimization algorithm may be an efficient choice for solving the parameter estimation problem (Chavent, 1991; Kunish and Sachs, 1992) otherwise the use of penalty-regularization terms in the cost function may be preferable.

Several key issues need to be examined:

(1) Whether equation (A. 3) admits a unique solution (identifiability). This means that there is a chance for the optimally estimated parameter to be close to the true unknown parameter.

(2) Whether solution of equation (A. 3) depends continuously on the observations Z_d (stability). The stability of the estimated parameter is with respect to perturbations on the observations. (See Kravaris and Seinfeld, 1985, 1986; Chavent, 1979)

(3) Relationship between dimensionality of state space, observation space and parameter space.