Seon Ki Park
Liang Xu *Editors*

Data Assimilation for Atmospheric, Oceanic and Hydrologic Applications (Vol. II)

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Yoshikazu Sasaki (*right*) *and his mentor Shigekata Syono working on hydrodynamic theory of vortex motion during Syono's visit to the University of Oklahoma* (*December 1963*). Drawn by John M. Lewis, using pen, brush, and India ink.

To Yoshi K. SASAKI and Roger W. DALEY

Preface

Since the first session for data assimilation (DA) had been organized at the Asia Oceania Geosciences Society (AOGS) Annual Meeting in 2005, we have conducted several successful sessions under the title of "Yoshi K. Sasaki Symposium on Data Assimilation for Atmospheric, Oceanic and Hydrologic Applications." It was to honor Prof. Yoshi K. Sasaki of the University of Oklahoma for his lifelong contributions to DA in geosciences. Yoshi had introduced the variational method to meteorology as early as the 1950s, and since then DA has developed into an utmost important technique in modern numerical prediction in various disciplines of geosciences.

The first volume of this book, under the same title of the Sasaki Symposium, has been published in March 2009 with a collection of notable invited papers along with those selected from previous symposiums up to 2008. Among them, John M. Lewis, one of Yoshi's students, contributed a chapter titled "Sasaki's Pathway to Deterministic Data Assimilation." I. Michael Navon provided a thorough review of variational DA for numerical weather prediction, while Yoshi himself introduced a new theory based on the entropic balance. Milija and Dusanka Zupanski discussed some issues in ensemble DA, and Zhaoxia Pu overviewed the effect of satellite DA to improve forecasts of tropical cyclones. A coastal application of the ocean DA was reviewed by Xiaodong Hong and colleagues, and the variational approach to hydrologic DA was discussed by Francois-Xavier Le Dimet. Rolf H. Reichle and colleagues addressed recent advances in land data assimilation at the NASA/GMAO, and Nasim Alavi and colleagues surveyed assimilation of soil moisture and temperature into land surface models. As demonstrated, the previous volume covered important topics on DA in meteorology, oceanography, and hydrology, by dealing with both theoretical and practical aspects.

It has been more than 3 years since the first volume has been published. Since then we had three successful symposiums - held at Singapore in August 2009, at Hyderabad in July 2010, and at Taipei in August 2011, each with about 30 presentations. Therefore we decided to publish the second volume under the same title, again by collecting both invited papers and selected papers from the three symposiums. This volume includes excellent overviews of estimation theory, nudging and variational methods, and Markov chain Monte Carlo methods. Most prominently, Yoshi has extended his entropy balance theory for tornado DA from the previous volume.

In this volume, theoretical and methodological aspects encompass estimation and entropic balance theory, variational and ensemble methods, nudging and representer methods, Monte Carlo and ensemble adaptive methods, the maximum likelihood ensemble filter, the local ensemble transform Kalman filter, micro-genetic algorithm, etc., with applications to oceanic, meteorological, and hydrologic DA; radar/lidar/satellite assimilation; parameter estimation; adjoint sensitivity; and adaptive (targeting) observations.

This book will be useful to individual researchers as well as graduate students as a reference to the most recent progresses in the field of data assimilation. We appreciate Boon Chua at Naval Research Laboratory and Francois-Xavier Le Dimet, who have served as the co-conveners of the Sasaki Symposium. We are very honored to dedicate this book to Yoshi Sasaki and the late Roger Daley for their significant contributions in data assimilation.

Ewha Womans University, Seoul — Seon Ki Park
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Chapter 1
A Survey of Observers for Nonlinear Dynamical Systems*

Wei Kang, Arthur J. Krener, Mingqing Xiao, and Liang Xu

Abstract The Kalman filter, invented initially for control systems, has been widely used in science and engineering including data assimilation. For the last several decades, the estimation theory for dynamical systems has been actively developed in control theory. In this paper, we survey several observers, including Kalman filters, for nonlinear systems. We also review some fundamental concepts on the observability of systems defined by either differential equations or a numerical model. The hope is that some of these ideas will inspire research that can benefit the area of data assimilation.

Keywords Observers and estimation • Nonlinear systems • Observability

1.1 Introduction

In modern control theory, the term *Observer* has a technical meaning. An observer is a system defined by differential or difference equations and associated computational algorithms which accepts the measured data from another system as input and

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returns an estimate of the state of the other system. Observers play a critical role in control systems because many feedback controllers depend on the accurate estimate of state variables of the system to be controlled. An accurate estimation of the state in the presence of noise and uncertainties is essential for a controller to achieve high quality performance.

Estimation from data with random noise can be traced to Gauss about 200 years ago who invented the technique of deterministic least-squares for orbit measurements. In the early twentieth century, Fisher introduced maximum likelihood estimation. Then in the middle of the twentieth century Wiener invented his well known optimal filter for stationary processes. Around 1960s, Kalman and Bucy introduced an optimal recursive filter for dynamical systems. This filter, now known as the Kalman filter, is "the very foundation for data mixing in modern multisensor systems (Gelb 1974)." The estimation for systems governed by differential equations has been an active research field in control theory for more than 50 years. In addition to the Kalman filter, which is essentially a recursive solution to the least square problem, estimation processes have been developed for various performance requirements, such as asymptotically stable estimation, H_∞ estimation, and minimum energy estimation. Fundamental theory has been developed to analyze observability, an intrinsic property of systems with sensors that largely determines the invertibility from past measurement to the state of the system.

Data assimilation is an area of estimation theory and an application to systems with extremely high dimensions. Both filtering and smoothing methods are critical to date assimilation. Although we focus on nonlinear filtering methods in this paper, smoothing algorithms can be developed using similar ideas. Approaches such as ensemble Kalman filters and 4D-Var are based on the theory of optimal estimation, especially the Kalman filter and minimum energy estimation. The data assimilation community has done extensive research on these topics for over 30 years. While this book is focused on problems in data assimilation, this article is to provide a survey on some ideas and results that have been actively developed in control theory, but not widely used in data assimilation. The goal is to lay out some related but different concepts and methods. We hope that some of them may inspire different approaches that benefit the area of data assimilation.

1.2 Observability

In this paper, we consider systems defined by differential equations. The sensor measurement is defined by an output function. For example,

$$\begin{aligned} \dot{x} &= Ax \\ y &= Cx \\ x(0) &= x_0 \end{aligned} \tag{1.1}$$

is a linear system in which $x \in \mathbb{R}^n$ is the state variable, $y \in \mathbb{R}^p$ is the output variable whose value can be measured, $A \in \mathbb{R}^{n\times n}$ and $C \in \mathbb{R}^{n\times p}$ are known constant or time varying matrices. Given A, C, and the past sensor information about $y(t)$, the problem is to estimate x or a function of the state variable in the presence of noise and uncertainties. A nonlinear system is defined similarly,

$$\begin{aligned} \dot{x} &= f(x) \\ y &= h(x) \\ x(0) &= x_0 \end{aligned} \tag{1.2}$$

An immediate question to be answered before observer design is whether a system (1.1) or (1.2) admits a convergent estimator. In other words, how to determine that the past values of $y(t)$ contain adequate information to achieve a reliable estimate of $x(t)$. This leads to the concept of observability. Two initial states x_{01} and x_{02} are said to be distinguishable if the outputs $y_1(t)$ and $y_2(t)$ of (1.2) satisfying the initial conditions $x_0 = x_{01}$ and $x_0 = x_{02}$ differ at some time $t \geq 0$. The system is said to be observable if every pair x_{01}, x_{02} are distinguishable. Observability can be easily verified for linear systems. The output of (1.1) and its derivatives at time $t = 0$ are

$$\begin{aligned} y(0) &= Cx_0 \\ \dot{y}(0) &= CAx_0 \\ \ddot{y}(0) &= CA^2x_0 \\ &\vdots \\ y^{(n-1)}(0) &= CA^{n-1}x_0 \end{aligned} \tag{1.3}$$

Obviously, (1.1) is observable if the mapping from x_0 to the derivatives of $y(t)$ is one-to-one. In fact, it can be proved that (1.1) is observable if and only if the following observability matrix has full rank

$$O = \begin{bmatrix} C \\ CA \\ CA^2 \\ \vdots \\ CA^{n-1} \end{bmatrix}$$

For nonlinear systems, the output and its derivatives are given by the iterated Lie derivatives

$$\begin{aligned} y(0) &= y(x_0) \\ \dot{y}(0) &= L_f(h)(x_0) = \frac{\partial h}{\partial x}(x_0)f(x_0) \end{aligned}$$

$$\ddot{y}(0) = L_f^2(h)(x_0) = \frac{\partial L_f(h)}{\partial x}(x_0)f(x_0)$$

$$\vdots$$

$$y^{(k-1)}(0) = L_f^{k-1}(h)(x_0) = \frac{\partial L_f^{k-2}(h)}{\partial x}(x_0)f(x_0)$$

for some integer $k > 0$. If the mapping from x_0 to $h, L_f(h), L_f^2(h), \cdots$ distinguishes points then the system is observable. For a real analytic system this is a necessary and sufficient condition for observability. For simplicity of exposition, suppose $p = 1$. Consider the matrix

$$\begin{bmatrix} \frac{\partial h}{\partial x}(x_0) \\ \frac{\partial L_f(h)}{\partial x}(x_0) \\ \vdots \\ \frac{\partial L_f^{n-1}(h)}{\partial x}(x_0) \end{bmatrix}$$

If this matrix is invertible, then the system is locally observable at x_0. This observability matrix is a topic addressed in almost all textbooks of linear and nonlinear control theory, for instance Kailath (1980) for linear systems and Isidori (1995) for nonlinear systems.

For high dimensional systems, it is important to quantitatively define observability. The observability Gramian is a widely used concept for this purpose (Kailath 1980). Consider a linear system (1.1), an arbitrary initial state x_0 of a trajectory

$$x(t) = e^{At}x_0$$

can be uniquely determined from the known function $y(t) = Cx(t)$ if and only if the columns in the matrix

$$Ce^{At}$$

are linearly independent over $[t_0, t_1]$. This is equivalent to say that

$$G = \int_{t_0}^{t_1} e^{A^T t}C^T Ce^{At}dt$$

is nonsingular. This matrix is called the observability Gramian. In fact, the L^2-norm of the output satisfies

$$\int_{t_0}^{t_1} ||y(t)||^2 dt = x_0^T G x_0$$

Therefore, the eigenvalues of G represent the gain from the initial state to the output. If G has a zero eigenvalue, then its eigenvector results in a zero output. The system is unobservable. If G has a very small eigenvalue, then the system is weakly observable, i.e. a small noise in $y(t)$ can cause a large estimation error. Therefore, the smallest eigenvalue of G is used as a quantitative measure of observability.

For nonlinear systems, an empirical observability Gramian can be numerically computed (Krener and Ide 2009). Consider (1.2) and a nominal trajectory $x(t)$ with initial state $x(0) = x_0$. Define a mapping

$$\begin{array}{l} \delta x_0 \rightarrow h(\hat{x}(t)) - h(x(t)) \\ \text{subject to} \\ \dot{\hat{x}}(t) = f(\hat{x}(t)) \\ \hat{x}(0) = x_0 + \delta x_0 \end{array} \tag{1.4}$$

Let $v_1, v_2, \cdots, v_n$ be an orthonormal basis in $\mathbb{R}^n$. Let $\rho > 0$ be a small number. In the direction of ρv_i, the variation of the output can be estimated empirically by

$$\Delta_i(t) = \frac{1}{2\rho}\left(h(x^+(t)) - h(x^-(t))\right), \tag{1.5}$$

where

$$\begin{array}{l} \dot{x}^{\pm}(t) = f(x^{\pm}(t)) \\ \hat{x}^{\pm}(0) = x_0 \pm \rho v_i, \end{array}$$

The mapping, (1.4), from the initial state to the output space can be locally approximated by a linear function

$$\delta x_0 = \sum_{i=0}^{n} \alpha_i v_i \rightarrow \sum_{i=0}^{n} \alpha_i \Delta_i(t) \tag{1.6}$$

Therefore, the observability Gramian of the nonlinear system can be approximated by the Gramian associated to (1.6)

$$\begin{aligned} G &= (G_{ij})_{i,j=1}^n \\ G_{ij} &= \int_{t_0}^{t_1} \Delta_i^T(t)\Delta_j(t)dt \end{aligned} \tag{1.7}$$

Locally around the nominal trajectory, the eigenvalues of (1.7) measure the gain from the variation of the initial state to the variation of the output. If G has a small eigenvalue, then $x(t)$ is weakly observable. A small noise in $y(t)$ can result in a large estimation error.

The Gramian or empirical Gramian in Kailath (1980) and Krener and Ide (2009) measures the observability of full initial states. However, for systems with very high dimensions, the problem of full observability is, in many cases, ill-posed. Some discussions on the partial observability, or Z-observability, for complex systems were introduced in Kang and Barbot (2007). Meanwhile, quantitatively measure partial observability has been rapidly developed in a sequence of papers (Kang 2011; Kang and Xu 2009a,b, 2011). For PDEs, the observability is defined and computed for the finite dimensional approximations of the original model. In Kang and Xu (2009a,b), dynamic optimization is used as a tool for the definition.

Definition 1.1. Given a trajectory $x(t)$, $t \in [t_0, t_1]$. Let $W \subseteq \mathbb{R}^n$ be a subspace. Let $\rho > 0$ be a constant. Define ϵ as follows

$$
\begin{aligned}
&\epsilon = \min_{\bar{x}(t)} ||h(\bar{x}(t)) - h(x(t))|| \\
&\text{subject to} \\
&\dot{\bar{x}} = f(\bar{x}), \\
&||\bar{x}(0) - x_0|| = \rho \\
&\bar{x}(0) - x_0 \in W
\end{aligned}
$$

Then the ratio ρ/ϵ is a measure of observability for the W-component of $x(0)$.

If $\rho \to 0$, the ratio ρ/ϵ can be considered as an extension of the observability Gramian. Consider a linear system (1.1). Suppose $W = \mathbb{R}^n$. Then the observability Gramian, G, satisfies (Kailath 1980; Krener and Ide 2009)

$$||y||^2_{L^2} = x_0^T P x_0 \tag{1.8}$$

Given $||x_0|| = \rho$, we have

$$\epsilon^2 = \lambda_{min} \rho^2 \tag{1.9}$$

where λ_{min} is the smallest eigenvalue of G. Therefore, the ratio ρ^2/ϵ^2 equals the reciprocal of the smallest eigenvalue of the observability Gramian. In Kang and Xu (2009a,b), the concept of partial observability was applied to more general problems using various types of norms and knowledge of the system. An example of optimal sensor location by maximizing the observability for data assimilations was given in Kang and Xu (2011).

1.3 Asymptotic Observers

Following control theory, asymptotic observers are systems defined by differential or difference equations and associated computational algorithms which accepts the measured data from another system as input and returns an estimate of the state of the other system. In the case of a perfect model without noise and uncertainties, the estimated state should converge to the true state of the system being observed. Also if the initial state of the observer equals the true state, then the estimation error is zero along the entire trajectory. In most observer designs, such as Luenberger observers and Kalman filters, an observer consists of a copy of the original system plus a correction term which is a function of the measured data.

Asymptotic observers are widely used in control systems to achieve stable estimates of state variables. The design emphasizes the stability and simplicity of the estimation process. In general it does not optimize any performance measure. The Luenberger observer for linear systems is a simplest example that illustrates the fundamental idea of asymptotic observers.

1.3.1 Luenberger Observer

Given a dynamical system with an output

$$\begin{aligned} \dot{x} &= Ax \\ y &= Cx \end{aligned} \tag{1.10}$$

where $x \in \mathbb{R}^n$ is the state variable, $y \in \mathbb{R}^p$ is the output which can be measured, $A \in \mathbb{R}^{n\times n}$ and $C \in \mathbb{R}^{p\times n}$ are matrices. We assume that A, C and the output $y(t)$ are known information. The goal is to find an estimate, estimate, denoted by $\hat{x}(t)$, of the state variable so that $\hat{x}(t)$ asymptotically approaches $x(t)$. The observer has the following form

$$\dot{\hat{x}} = A\hat{x} + G(y - C\hat{x}) \tag{1.11}$$

The matrix $G \in \mathbb{R}^{n\times p}$ is called the observer gain, which is used to stabilize the estimation error. Define

$$e = x - \hat{x}$$

then the error dynamics has the following form

$$\begin{aligned} \dot{e} &= Ae - G(y - C\hat{x}) \\ &= (A - GC)e \end{aligned} \tag{1.12}$$

It is obvious that $e(t)$ asymptotically approaches zero if the eigenvalues of $A - GC$ are all located in the left half plane. To estimate $x(t)$, one can use any initial guess $\hat{x}(0)$. Then $\hat{x}(t)$ from (1.11) satisfies

$$\lim_{t\to\infty} e(t) = 0$$

When applying the observer, $y(t)$ is measured online and the (1.11) is numerically propagated in real-time to provide an estimate of $x(t)$.

It can be proved that, for any set of n complex numbers, there always exists an observer gain, G, so that the eigenvalues of the error dynamics (1.12) are placed at these locations, if the pair (A, C) is observable, i.e. the following observability matrix has full rank

$$\begin{bmatrix} C \\ CA \\ CA^2 \\ \vdots \\ CA^{n-1} \end{bmatrix}$$

This result guarantees that one can always find linear observers with stable error dynamics for observable systems. For systems in which (A, C) is not observable, it is still possible to achieve asymptotic stability of (1.12). This depends on the spectrum of A, which can be divided into observable modes and unobservable modes. Details are referred to Kailath (1980). If all the unobservable modes are on the left half plane, then there always exists a G that stabilizes (1.12).

The error dynamics does not include measurement error. If the output is corrupted by noise, the asymptotic stability of the observer guarantees that $\hat{x}(t)$ is stabilized around the true value. There are infinitely many observer gains to stabilize the observer. A high gain observer has fast convergence to the true value of the system, however it is very sensitive to sensor noise. Although asymptotic observers do not guarantee optimal performance in any sense, their advantage lies in the simplicity. For real time applications, each estimate at a given time is simply computed by one step integration of the observer equation, which can be implemented using any numerical algorithm for solving ordinary differential equations (ODEs). Luenberger observers can be found as a standard topic in almost all textbooks on control theory, for instance (Kailath 1980; Khalil 2002).

1.3.2 Observers with Linear Error Dynamics

For nonlinear systems, observer design with a guaranteed asymptotically stable error dynamics is a difficult task (Hermann and Krener 1977). The Luenberger observer works for linear systems because its error dynamics is decoupled from the unknown trajectory being observed. For nonlinear systems, however, this is not true in general. There is a large volume of literature on the construction of nonlinear observers that admit a linear error dynamics. In the pioneering work (Krener and Isidori 1983) a technique called output injection was introduced. In addition, necessary and sufficient conditions are found under which the error dynamics of the nonlinear observer is equivalent to a linear ODE. Consider a nonlinear dynamical system with an output

$$\begin{aligned} \dot{x} &= f(x) \\ y &= h(x) \end{aligned} \tag{1.13}$$

in which $x \in \mathbb{R}^n$ is the state variable, $y \in \mathbb{R}^p$ is the output which can be measured, $f(x)$ and $h(x)$ are vector valued functions with adequate smoothness. In Krener and Isidori (1983), it is propose to find a change of coordinates around a fixed point x_0

$$\begin{aligned} z &= z(x) \\ z(x_0) &= 0 \end{aligned} \tag{1.14}$$

so that (1.13) is transformed into a linear system with a nonlinear output injection

$$\begin{aligned} \dot{z} &= Az + \phi(y) \\ y &= Cz \end{aligned} \tag{1.15}$$

for some matrices $A \in \mathbb{R}^{n\times n}$ and $C \in \mathbb{R}^{p\times n}$. If this is the case, then we can easily construct a Luenberger type of observer as follows.

$$\dot{\hat{z}} = A\hat{z} + \phi(y) + G(y - C\hat{z}) \tag{1.16}$$

Let

$$e = z - \hat{z}$$

then the error dynamics is a linear system decoupled from $z(t)$

$$\dot{e} = (A - GC)e$$

If G, the observer gain, is chosen so that the eigenvalues of $(A - GC)$ are all in the left half plane, then

$$\lim_{t\to\infty} e(t) = 0$$

Not all nonlinear systems can be transformed into a linear system with output injection. The existence of the change of coordinates (1.14) can be determined using Lie differentiation. Given a function $h(x)$, let dh represents the 1-form, or the gradient,

$$dh(x) = \left[\frac{\partial h}{\partial x_1}(x) \; \frac{\partial h}{\partial x_2}(x) \cdots \frac{\partial h}{\partial x_n}(x) \right]$$

The Lie derivative is defined as follows

$$\begin{aligned} L_f(h) &= dh \cdot f \\ L_f(dh) &= f^T \frac{\partial^2 h}{\partial x} + dh \frac{\partial f}{\partial x} \end{aligned}$$

The following theorem was proved in Krener and Isidori (1983).

Theorem 1.1. *There exists a local change of coordinates (1.14) that transforms (1.13) into a linear system with output inject (1.15) if and only if*

$$\begin{aligned} f(x_0) &= 0 \\ h(x_0) &= 0 \end{aligned}$$

and $L_f^n(dh)$ *is a linear combination of* $L_f^k(dh)$ *for* $k = 0, 1, \cdots, n-1$.

Note that the theorem guarantees the existence of a local change of coordinates around an equilibrium. Therefore, the observers are limited in a local neighborhood of an equilibrium point. Among a large number of publications on the observer design by achieving linearized error dynamics, we would like to bring up (Kazantzis and Kravaris 1998). In this work, the formulation of the observer design problem is realized via a system of singular first-order linear partial differential equations (PDE). The theory is applicable to a larger family of systems than that addressed in Krener and Isidori (1983). In fact, after a nonlinear change of coordinates, the resulting system is not required to have a linear output like in (1.15). Another advantage of the work in Kazantzis and Kravaris (1998) is that the solution to the PDEs is locally analytic and this enables the development of a series solution method, that is programmable using symbolic software packages. In the presence of noise, some types of output injection, such as a y^2 term, may result in a biased estimation because $E[(y+n)^2] = E[y^2] + E[n^2]$, where n is a random noise.

Other related work includes Zeitz's extended Luenberger observer based upon a local linearization technique (Zeitz 1987). Nonlinear coordinate transformations have also been employed to transform the nonlinear system to a suitable observer canonical form, where the observer design problem may be solved (Bestle and Zeitz 1983; Ding et al. 1990; Xia and Gao 1989; Zheng et al. 2007).

1.3.3 Observers Based on Lyapunov Functions

For systems that do not admit a linear error dynamics, nonlinear observers can be derived so that its stability is guaranteed by a Lyapunov function. A widely used approach is based on the high gain observer proved in Gauthier et al. (1992). Once again, consider the nonlinear system (1.13). Using a single output case as an example, consider the mapping, $z = z(x) : \mathbb{R}^n \rightarrow \mathbb{R}^n$, defined by

$$z(x) = \begin{bmatrix} h(x) \\ L_f h(x) \\ \vdots \\ L_f^{n-1} h(x) \end{bmatrix} \tag{1.17}$$

We assume that $z = z(x)$ is a diffeomorphism on a region $\Omega \subseteq \mathbb{R}^n$. Under this transformation, the original system is equivalent to the system in the form

$$\begin{aligned} \dot{z} &= \begin{bmatrix} z_2 \\ z_3 \\ \vdots \\ z_n \\ \phi(z) \end{bmatrix} \\ y &= z_1 \end{aligned} \tag{1.18}$$