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Particle Filters for State Estimation of Confined Aquifers

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Particle Filters for State Estimation of Confined Aquifers

by
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ABSTRACT

Mathematical models are used in engineering and the sciences to estimate properties of systems of interest, increasing our understanding of the surrounding world and driving technological innovation. Unfortunately, as the systems of interest grow in complexity, so to do the models necessary to accurately describe them. Analytic solutions for problems with such models are provably intractable, motivating the use of approximate yet still accurate estimation techniques. Particle filtering methods have emerged as a popular tool in the presence of such models, spreading from its origins in signal processing to a diverse set of fields throughout engineering and the sciences including medical research, economics, robotics, and geophysics.

In groundwater hydrology, a key component of aquifer assessment is the determination of the properties which permit water resource managers to estimate aquifer drawdown and safe yield. Presented is a particle filtering approach to estimate aquifer properties from transient data sets, leveraging recently published analytically-derived models for confined aquifers. The approach is examined experimentally through validation against three common aquifer testing problems: determination of (i) transmissivity and storage coefficient from non-leaky confined aquifer performance tests, (ii) transmissivity, storage coefficient, and vertical hydraulic conductivity of a confining unit from leaky confined aquifer performance tests, and (iii) transmissivity and storage coefficient from non-leaky confined aquifer performance tests with noisy data and boundary effects. The first two problems are well-addressed and the presented approach compares favorably to the results obtained from other published methods. The third problem, which the presented method can tackle more naturally than previously-published methods, underscores the flexibility of particle filtering and, in turn, the promise such methods offer for a myriad of other geoscience problems.

Chapter 1

Introduction

Engineering and the sciences, both physical and social, are replete with mathematical models which relate the relevant entities of a system of interest and their rates of change. Inferences drawn from these models enable a variety of human achievements. Orbital models are used by astrophysicists to ensure efficient space flight of craft both manned and unmanned [Mashiku et al., 2012]. Meteorological models enable the accurate forecasting of weather patterns, aiding individuals with short-term predictions as well as food-suppliers with seasonal outlooks [van Leeuwen, 2009]. Health epidemics are simulated and planned for through the use of infectious disease models by various national and international health organizations [Hofmannand, 2007]. Economists and financial mathematicians utilize volatility models to predict and evaluate the underlying trust that markets have in the valuations of financial products [Stroud et al., 2004]. In engineering, models are used to simulate, track, and estimate a wide variety of complex systems e.g., wireless communication [Huber and Haykin, 2003], global positioning/navigation [Gustafsson et al., 2002], and automation [de Freitas, 2002].

1.1 Filtering and State Estimation

Performing inference on such models involves estimating quantities of interest given measured data. When the estimate is of a future event or quantity, as in the case of forecasting weather

patterns or market conditions, the inference problem is one of prediction and undertaken with measurement data that are historical with respect to the quantities of interest. Other applications require estimates of the current value of quantities of interest. Navigation, for example, relies upon heading, velocity, and position estimates which are successively predicted and then updated, or *filtered*, with each arrival of new information. The celebrated Kalman filter [Kalman, 1960] provides an on-line solution to the recursive computation of the predict/update cycle necessary in these types of inference problems so long as the models being dealt with are of a special type. Within these models, the functions describing both the underlying system of interest, as well as the measurement process responsible for the observations on that system, are *linear* and any disturbances to these processes are accounted for by random variables drawn from Gaussian distributions. For the case of linear-Gaussian models, the Kalman filter provides an optimal estimate.

As systems of interest grow in complexity, so to do the models used to accurately describe them. Analytic solutions to inference problems become computationally intractable in the absence of specific, and often restrictive, model properties. This necessitates the use of approximation strategies in cases where the use of non-linearity or non-Gaussianity is required to better represent the system of interest.

Particle filters have emerged as a computationally efficient framework with which to preform approximate Bayesian inference in the presence of such modeling conditions. The technique is a simulation based approach whereby a set of hypotheses are evolved in accordance with their ability to produce simulated results which are in agreeance with actual measurement data collected from the system under observation.

1.2 Thesis Contributions

Investigated herein is the application of this technique to the set of models describing the groundwater aquifer performance test, whereby the response of an aquifer system to a controlled excitation is used to estimate parameters which are key to the management of the aquifer. This estimation problem is canonical within the domain of hydrology and, as such, was utilized by [Field et al., 2016] in an introduction to particle filtering targeted towards that community. This thesis compliments that work by

(i) providing a mathematical primer to particle filtering which was not achievable within the submission restrictions;

(ii) and presenting new results, from within the same problem space, leveraging algorithmic innovations.

1.3 Thesis Organization

Presented is an extension of [Field et al., 2016], focusing on the standard particle filtering algorithm and its underlying mathematical concepts. Chapter 2 presents optimal Bayesian filtering, its intractability in the absence of restrictive modeling assumptions, and the requisite techniques for its approximation. After providing the necessary mathematical primer, the standard particle filtering algorithm is presented. Chapter 3 reproduces a previous publication, [Field et al., 2016], which examines the efficacy of the particle filtering algorithm when applied to the hydrogeological problem of estimating groundwater aquifer parameters from transient monitoring data. Chapter 4 presents recommendations for future research by briefly introducing algorithmic improvements of interest and the initial findings of their application to the aquifer parameter estimation problem prior to the concluding remarks.

Chapter 2

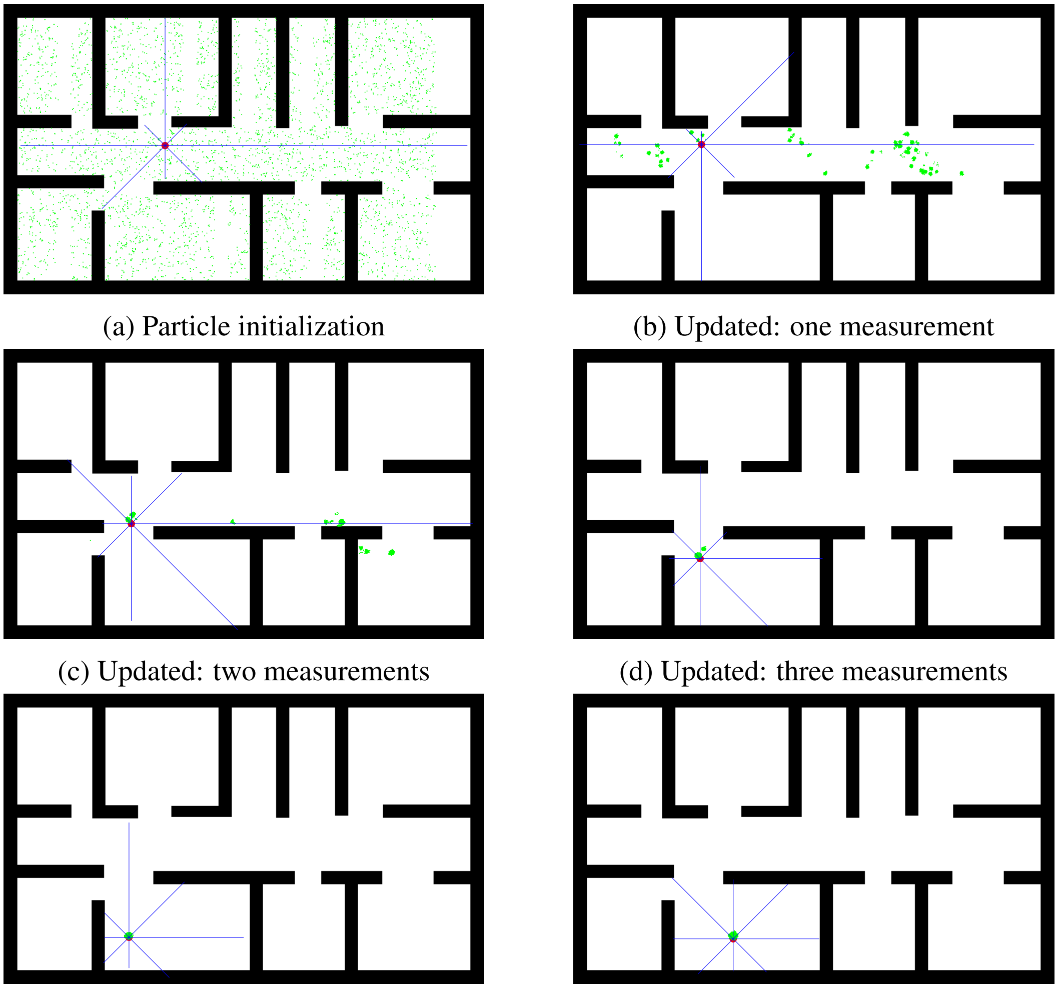
Background

Particle filtering provides an approximation to the often computationally intractable optimal Bayesian filter, or the recursive probabilistic framework whereby inference on some latent state process is made on-line through a sequence of noisy observations, providing an "up to the minute" estimate for a dynamical system of interest. This chapter provides an introductory example to the particle filtering algorithm, the relevant mathematical preliminaries which underpin it, and the rationale for its application to the groundwater hydrology problem of estimating aquifer parameters.

2.1 Motivation: A Robot Localization Scenario

The particle filtering algorithm works by simulating measurements from a set of sampled hypothetical values for quantities of interest, then evaluating those hypotheses against actual observations. Samples within this set, called particles, propagate through time in accordance with the assumed model describing the system of interest. Particles are either discarded or replicated based, in essence, upon their ability to produce simulated measurements which agree with the actual measurements collected.

As an motivating example, consider the challenge in localizing a robot within a building whose map is known. The robot's sensor package is made up of laser rangefinders which provide noisy



(a) Particle initialization
(b) Updated: one measurement
(c) Updated: two measurements
(d) Updated: three measurements
(e) Updated: four measurements
(f) Updated: five measurements

Figure 2.1: Visualization of particle filtering applied to the problem of robot localization.

distance measurements to the robot's nearest obstacles. Given no prior knowledge, the initial hypotheses (particles) pertaining to the robot's location are distributed uniformly throughout the map (Figure 2.1a). After the robot receives its first sensor report, these particles are evaluated and subjected to a 'survival of the fittest' process which discards particles situated over unlikely locations on the map and replicates those whose positions produce simulated measurements which more closely resemble the current observation (Figure 2.1b). Particle locations are moved in accordance with the actions taken by the robot and subjected to the same fitness evaluation at each time step (Figures 2.1c, 2.1d, 2.1e, 2.1f), eventually resulting in the collapse of the particle cloud about the robot's true location.

This example, and its accompanying visualization, should make clear the general methodology of creating a set of hypotheses and evolving them based on the simulated measurements which they produce. The following section presents the mathematics upon which the this process is based.

2.2 Preliminary Mathematics

Prior to describing general Bayesian estimation, a descriptive language of the system under investigation must first be introduced. Used throughout is the characterization of the quantities of interest and the accessible observations within a generic discrete-time stochastic dynamic system model in state-space form. This model enables the creation of a space whose axes are the set of state variables (the quantities of interest), thereby allowing the system state to be fully described by a vector within this space.

Following that is a brief introduction to the recursive Bayesian framework whereby inference on some latent state vector is made on-line through a sequence of noisy measurements. In the absence of specific and restrictive model assumptions, the computation of the optimal state estimate is often intractable, necessitating the use of approximation strategies.

Finally, Monte Carlo integration and importance sampling techniques are presented which seek to approximate the difficult multi-dimensional integrals encountered in recursive Bayesian estimation.

2.2.1 State-Space Representation

Let the discrete time sequence be indexed by the variable n. Given a state vector of interest $\mathbf{x}_n \in \mathbb{R}^m$ and an observation vector $\mathbf{y}_n \in \mathbb{R}^p$, the general state space model used throughout is as follows,

$$\mathbf{x}_{n+1} = f(\mathbf{x}_n, \mathbf{d}_n) \quad \Leftrightarrow \quad p(\mathbf{x}_{n+1}|\mathbf{x}_n) \tag{2.1}$$

$$\mathbf{y}_n = h(\mathbf{x}_n, \mathbf{v}_n) \quad \Leftrightarrow \quad p(\mathbf{y}_n|\mathbf{x}_n) \tag{2.2}$$

where Equations 2.1 and 2.2 will be referred to as the process and measurement equations respectively. The process model describes the evolution of the state vector over time and its dependence on some user-defined noise process $\mathbf{d}_n$. Similarly, the measurement model describes the observations made on the system in each time period as a function of the current state value and some corrupting noise process $\mathbf{v}_n$. Equations 2.1 and 2.2 also characterize the state transition probability $p(\mathbf{x}_n|\mathbf{x}_{n-1})$ and measurement likelihood $p(\mathbf{y}_n|\mathbf{x}_n)$ with the process model assuming first-order Markovianity i.e., $p(\mathbf{x}_n|\mathbf{x}_{0:n-1}) = p(\mathbf{x}_n|\mathbf{x}_{n-1})$, and the measurement model asserting the conditional independence of the measurements given the state. These models are assumed to be either known in advance or already designed with prior domain knowledge of the problem. Both f and h can themselves be time-varying, and in turn indexed by n, but there are no such models at the heart of the estimation problems presented in this thesis.

The above setup is analogous to that which underlies the Kalman filter with the exceptions that the process and measurement models need not be linear and their associated noise distributions need not be Gaussian. It should be noted that the non-stochastic control variables have been omitted from the above, as well as from the rest of this document, as a matter of notational convenience.

2.2.2 Recursive Bayesian Estimation

What follows is a brief introduction to the recursive Bayesian framework whereby inference on some latent state vector is made on-line through a sequence of noisy measurements.

Restated, the goal is to recursively compute the posterior distribution $p(\mathbf{x}_n|\mathbf{y}_{0:n})$. The application of Bayes rule and the Law of Total Probability,

$$\begin{aligned} p(\mathbf{x}_n|\mathbf{y}_{0:n}) &= \frac{p(\mathbf{y}_n|\mathbf{x}_n)p(\mathbf{x}_n|\mathbf{y}_{0:n-1})}{p(\mathbf{y}_n|\mathbf{y}_{0:n-1})} \\ &= \frac{p(\mathbf{y}_n|\mathbf{x}_n)\int_{\mathbf{x}_{n-1}} p(\mathbf{x}_n|\mathbf{x}_{n-1})p(\mathbf{x}_{n-1}|\mathbf{y}_{0:n-1})d\mathbf{x}_{n-1}}{\int_{\mathbf{x}_n} p(\mathbf{y}_n|\mathbf{x}_n)p(\mathbf{x}_n|\mathbf{y}_{0:n-1})d\mathbf{x}_n} \end{aligned}$$

yields a recursive predict-update framework whereby a state prediction is made from the previous posterior,

$$p(\mathbf{x}_n|\mathbf{y}_{0:n-1}) = \int_{\mathbf{x}_{n-1}} p(\mathbf{x}_n|\mathbf{x}_{n-1})p(\mathbf{x}_{n-1}|\mathbf{y}_{0:n-1})d\mathbf{x}_{n-1} \tag{2.3}$$

and is updated by the likelihood of receiving the most recent observation

$$p(\mathbf{x}_n|\mathbf{y}_{0:n}) = \frac{p(\mathbf{y}_n|\mathbf{x}_n)p(\mathbf{x}_n|\mathbf{y}_{0:n-1})}{p(\mathbf{y}_n|\mathbf{y}_{0:n-1})}. \tag{2.4}$$

This general framework enables the recursive computation of the posterior $p(\mathbf{x}_n|\mathbf{y}_{0:n})$, however it is numerically intractable in the absence of model linearity and Gaussianity. Given linear models with normally distributed noise variables, the Kalman filter provides the optimal estimator.

2.2.3 Monte Carlo Integration and Importance Sampling

Monte Carlo (MC) integration techniques offer an approximate evaluation of the intractable integrals presented in the previous section. The premise is that an expectation can be approximated by an average given that the underlying distribution can be sampled from and that

these samples are independent and identically distributed.

Let F be some intractable integral, over a domain $\mathscr{D}$, of some function f.

$$F = \int_{\mathscr{D}} f(\mathbf{x}) d\mathbf{x}$$

Decompose $f(x)$ into a function $g(x)$ multiplied by the underlying probability density $p(x)$,

$$f(x) = g(x)p(x)$$

then

$$F = \int_{\mathscr{D}} f(\mathbf{x}) d\mathbf{x} = \int_{\mathscr{D}} g(\mathbf{x}) p(\mathbf{x}) d\mathbf{x} = \mathbb{E}[g(x)]$$

for the chosen density p. Given a sufficient number of i.i.d random samples, $x_{1:N} \sim p(x), N \gg 1$,

$$\widehat{F}_N = \frac{1}{N} \sum_{i=1}^{N} g(x^i) \tag{2.5}$$

which approaches F as N approaches infinity.

Importance sampling extends the MC integration technique by enabling the estimation of intractable integrals whose underlying distributions cannot be easily or efficiently sampled from. Samples are instead taken from a *proposal* distribution whose support covers that of $p(\mathbf{x})$. The integral is estimated from these samples as follows:

$$\mathbb{E}[g(\mathbf{x})] = \int g(\mathbf{x}) \frac{p(\mathbf{x})}{q(\mathbf{x})} q(\mathbf{x}) d\mathbf{x} = \int g(\mathbf{x}) w(\mathbf{x}) q(\mathbf{x}) d\mathbf{x} \tag{2.6}$$

where $w(\mathbf{x}) \triangleq \frac{p(\mathbf{x})}{q(\mathbf{x})}$ is known as the *importance weight*. Equation 2.6 is approximated in the same manner as 2.5,

$$F \approx \frac{1}{N} \sum_{i=0}^{N} w^i g(\mathbf{x}^i) = \widehat{F} \tag{2.7}$$

where samples $\mathbf{x}^i \sim q(\mathbf{x})$.

2.3 Particle Filters

Particle filters are simulation based algorithms designed for approximate recursive Bayesian inference. They make the assumption that the posterior can be approximated as a finitely parameterized sum of weighted samples,

$$p(\mathbf{x}_n|\mathbf{y}_{0:n}) \approx \sum_{i=1}^{N} w_n^i \delta(\mathbf{x}_n - \mathbf{x}_n^i) \triangleq \hat{p}(\mathbf{x}_n|\mathbf{y}_{0:n}) \tag{2.8}$$

where $\sum_{i=1}^{N} w_n^i = 1$. The family of particle filtering algorithms provide a computationally efficient means with which to determine $\{\mathbf{x}_n^i, w_n^i\}_i^N$.

2.3.1 Sequential Importance Sampling

The Sequential Importance Sampling (SIS) algorithm, presented in Algorithm 1, represents particle filtering in its most rudimentary form.

Revisiting the proposal from subsection 2.2.3, if the proposal factors as such,

$$q(\mathbf{x}_{0:n}|\mathbf{y}_{0:n}) = q(\mathbf{x}_{0:n-1}|\mathbf{y}_{0:n})q(\mathbf{x}_n|\mathbf{x}_{0:n-1}\mathbf{y}_{0:n}) \tag{2.9}$$

then combining Equation 2.4 with the importance weight definition yields the following weight update recursion,

$$\begin{aligned}
w_n^i &\propto \frac{p(\mathbf{x}_{0:n-1}^i|\mathbf{y}_{0:n-1})p(\mathbf{y}_n|\mathbf{x}_n^i)p(\mathbf{x}_n^i|\mathbf{x}_{n-1}^i)}{q(\mathbf{x}_{0:n-1}^i|\mathbf{y}_{0:n-1})q(\mathbf{x}_n^i|\mathbf{x}_{0:n-1}^i,\mathbf{y}_{0:n-1})} && (2.10)\\
&= \frac{p(\mathbf{x}_{0:n-1}^i|\mathbf{y}_{0:n-1})}{q(\mathbf{x}_{0:n-1}^i|\mathbf{y}_{0:n-1})}\frac{p(\mathbf{y}_n|\mathbf{x}_n^i)p(\mathbf{x}_n^i|\mathbf{x}_{n-1}^i)}{q(\mathbf{x}_n^i|\mathbf{x}_{0:n-1}^i,\mathbf{y}_{0:n-1})} && (2.11)\\
&= w_{n-1}^i \frac{p(\mathbf{y}_n|\mathbf{x}_n^i)p(\mathbf{x}_n^i|\mathbf{x}_{n-1}^i)}{q(\mathbf{x}_n^i|\mathbf{x}_{0:n-1}^i,\mathbf{y}_{0:n-1})} && (2.12)
\end{aligned}$$

thus enabling the sequential computation of Equation 2.8. Selecting the transitive prior $p(\mathbf{x}_n|\mathbf{x}_{n-1})$ for the proposal distribution further simplifies the weight update recursion to

$$w_n^i \propto w_{n-1}^i p(\mathbf{y}_n|\mathbf{x}_n^i). \tag{2.13}$$

Algorithm 1: Sequential Importance Sampling

Data: $\{\mathbf{x}_{0:n-1}^i, w_{n-1}^i\}_{i=1}^N, \mathbf{y}_{0:n}$
Result: $\{\mathbf{x}_{0:n}^i, w_n^i\}_{i=1}^N$
for $i = 1 : N$ **do**
  Predict:
  Draw $\mathbf{x}_n^i \sim q(\mathbf{x}_n|\mathbf{x}_{0:n-1}^i, \mathbf{y}_{0:n})$
  Update:
  Assign weights $\tilde{w}_n^i \propto w_{n-1}^i \frac{p(\mathbf{y}_n|\mathbf{x}_n^i)p(\mathbf{x}_n^i|\mathbf{x}_{n-1}^i)}{q(\mathbf{x}_n^i|\mathbf{x}_{0:n-1}^i, \mathbf{y}_{0:n})}$
for $i = 1 : N$ **do**
  Normalize weights $w_n^i = \frac{\tilde{w}_n^i}{\sum_{i=1}^N \tilde{w}_n^i}$

2.3.2 Degeneracy and Resampling

The chief deficiency of the SIS algorithm is the inevitable accumulation of weight by a fraction of the N particles. In order to quantify this phenomenon, [Kong et al., 1994] proposed a measure of degeneracy, N_{eff}, or the *effective sample size* which is used in the modified SIS algorithm to trigger a resampling procedure in the event that significant particle weight degeneracy is detected. An efficient approximation of the measure is provided below,

$$N_{eff} \approx \frac{1}{\sum_{i=1}^N (w_n^i)^2} = \widehat{N}_{eff}. \tag{2.14}$$

In the event that $\widehat{N}_{eff}$ falls below a user defined threshold, usually $\frac{N}{2}$, the current particle set is resampled in accordance to the importance weights. This new set of samples are then equally weighted. That is, $\{x_n^i, w_n^i\}_{i=1}^N \rightarrow \{\bar{x}_n^i, \frac{1}{N}\}_{i=1}^N$.

The incorporation of this degeneracy prevention measure leads to what is known as the sequential importance resampling algorithm and is presented in Algorithm 2.

Algorithm 2: Sequential Importance Resampling

Data: $\{\mathbf{x}^i_{0:n-1}, w^i_{n-1}\}^N_{i=1}, \mathbf{y}_{0:n}$
Result: $\{\mathbf{x}^i_{0:n}, w^i_n\}^N_{i=1}$
for $i = 1 : N$ **do**
  Predict:
  Draw $\mathbf{x}^i_n \sim q(\mathbf{x}_n|\mathbf{x}^i_{0:n-1}, \mathbf{y}_{0:n})$
  Update:
  Assign weights $\tilde{w}^i_n \propto w^i_{n-1} \frac{p(\mathbf{y}_n|\mathbf{x}^i_n)p(\mathbf{x}^i_n|\mathbf{x}^i_{n-1})}{q(\mathbf{x}^i_n|\mathbf{x}^i_{0:n-1}, \mathbf{y}_{0:n})}$
for $i = 1 : N$ **do**
  Normalize weights $w^i_n = \frac{\tilde{w}^i_n}{\sum^N_{i=1} \tilde{w}^i_n}$
if $\widehat{N}_{eff} < \frac{N}{2}$ **then**
  Sample $\bar{\mathbf{x}}^{1:N}_n$ from $\mathbf{x}^{1:N}_n$ according to w_n
  $\{\mathbf{x}^i_n, w^i_n\}^N_{i=1} \rightarrow \{\bar{\mathbf{x}}^i_n, \frac{1}{N}\}^N_{i=1}$

2.4 Aquifer Pump Test Modeling

Applying the particle filtering methodology to the models describing aquifer performance testing is the primary topic of the remainder of this thesis. The investigations presented herein are restricted to aquifer parameter estimation from transient monitoring data obtained through well tests on unsteady non-leaky and unsteady leaky confined aquifers. In both scenarios, water is extracted from the aquifer by a pump well at a rate great enough to cause a measurable change in pressure levels within the aquifer. The subsequent change in water level (drawdown) is measured at one or more observation wells. Figure 2.2 provides a graphical representation of this process.

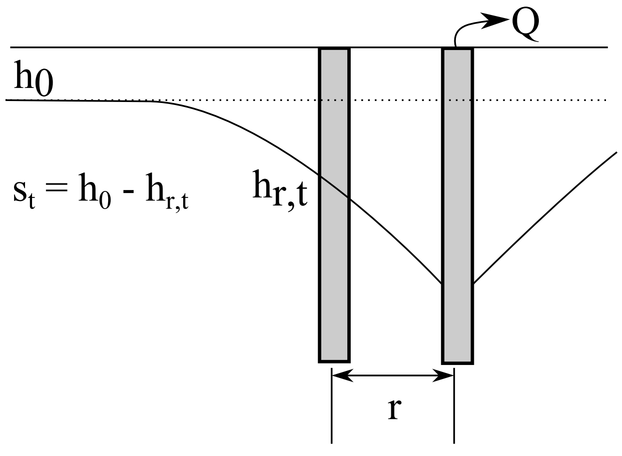


Figure 2.2: Aquifer performance test diagram where s_t is the drawdown observed within the observation well at time t and Q is the rate at which the pump well is operating.

In the case of unsteady non-leaky confined aquifers, the parameters of interest, specific storage (S) and transmissivity (T), are related to the drawdown (s) measurements obtained from the observation well(s) through the Theis equation [Theis, 1935],

$$s = \left(\frac{Q}{4\pi T}\right)\left[-0.5772 - \ln(u) + u - \frac{u^2}{2\times 2!} + \frac{u^3}{3\times 3!} - ...\right] \tag{2.15}$$

$$u = \frac{r^2 S}{4Tt} \tag{2.16}$$

where Q is the rate at which the pump well is operating, r is the radius between pump and observation wells, and t is the elapsed time between the start of the test and the time at which measurement s was taken. In the case of the unsteady leaky confined aquifer scenario, a third quantity of interest is introduced, vertical hydraulic conductivity K_v of the confining unit through which vertical leakage occurs. The Hantush well function [Hantush, 1997] describes the

relationship between drawdown measurement (s) and the three quantities of interest,

$$
\begin{aligned}
u &= \frac{r^2 S}{4Tt} \\
B &= \sqrt{\frac{Tb'}{K_v}} \\
s &= \frac{Q}{4\pi T}\int_u^\infty \frac{\exp\left(-y - r^2/4B^2 y\right)}{y} dy
\end{aligned}
\tag{2.17}
$$

where b' is the thickness of the permeable confining unit.

As the parameters of interest are assumed to be static in nature, the system equation describing their evolution through time is simply $\mathbf{x}_n = \mathbf{x}_{n-1}$. Paradoxically, the simplicity of this system presents a challenge to the particle filtering methodology as it removes the mechanism by which exploration of the state space occurs. Our approach follows [Liu and West, 2001] by introducing "artificial dynamics" to the system, thereby slightly perturbing the state vectors at each iteration e.g,

$$
\mathbf{x}_n = \mathbf{x}_{n-1} + \mathbf{d}_{n-1}, \quad n = 0, 1, 2, \ldots, \tag{2.18}
$$

where $\mathbf{d} \sim \mathcal{N}(0, \Sigma_d)$.

The generalized state space representation of the system is then:

$$
\text{System Equation:} \qquad \mathbf{x}_{n+1} = f(\mathbf{x}_n, \mathbf{d}_n) \tag{2.19}
$$

$$
\text{Measurement Equation:} \qquad \mathbf{y}_n = h(\mathbf{x}_n, \mathbf{v}_n) \tag{2.20}
$$

where f and h come from 2.18 and either 2.15 or 2.17 accordingly.

Chapter 3

Previous Publication

This chapter is a reproduction of [Field et al., 2016] published in the journal of *Water Resources Management*. The article's authors are Graeme Field, German Tavrisov, Christopher Brown, Alan Harris, and O. Patrick Kreidl.

3.1 Introduction

Groundwater is a key component of the worldwide water supply. In the USA, the National Groundwater Association estimates that up to 33% of all water used is from a groundwater source. Similar uses occur in many countries around the globe. Unfortunately, groundwater aquifers are being depleted worldwide at an alarming rate [Qiu, 2010, Konikow, 2013]. Therefore, the assessment of remaining groundwater resources is of critical importance. Groundwater aquifers used for water supply or irrigation purposes are primarily either unconfined, water-table aquifers or deeper confined aquifers. Confined aquifers are typically preferred by water resource managers, owing to their isolation from possible pollution sources due their protective confining layers. Ongoing assessment of shrinking groundwater resources usually includes the determination of aquifer properties and the development of yield estimates from the studied aquifer based upon acquired field data.

Using transient monitoring data for the purposes of determining aquifer properties is a common

technique in the groundwater industry. The most common method is the aquifer performance test, where a pumping well is used to stress the aquifer by removing water at a high rate and causing drawdown of pressure levels in the aquifer. The drawdown is measured at one or more observation wells placed at different radii from the pumping well. The aquifer test itself results in a transient condition within the aquifer, where drawdown is a function of time and space as well as various boundary conditions. In the most basic model for this process, water is pumped from a homogeneous and isotropic confined aquifer of infinite extent with no effect from boundary conditions: this so-called unsteady non-leaky confined aquifer test [Theis, 1935] has been studied extensively by a host of researchers with the intent being to estimate the two primary aquifer parameters, the transmissivity (T) and the storage coefficient (S). Another well-studied model, the so-called unsteady leaky confined aquifer test, assumes that the well derives its pumped groundwater laterally from within the primary confined aquifer and from leakage either above or below the primary aquifer through a semi-pervious confining unit [Hantush and Jacob, 1955]. In addition to parameters T and S, estimating the vertical hydraulic conductivity of the confining unit (K_v) is also of concern.

Numerous extensions to the two confined aquifer tests have been proposed and studied. [Walton, 1962] generalized the Theis solution and found graphical methods to estimate transmissivity and storativity using a ”type curve” approach. [Dagan, 1985] and [Dagan and Rubin, 1988] have looked at flow in confined aquifers using a stochastic approach. [Lebbe and Breuck, 1995] used inverse numerical modeling to estimate aquifer parameters along with factors that materially affect the accuracy of the estimates themselves. [Tumlinson et al., 2006] used numerical evaluations to develop estimates of aquifer parameters in laterally heterogeneous confined aquifers. [Trinchero et al., 2008] have studied pumping tests in leaky-confined aquifers, where the solution reverts to a confined aquifer curve if leakance of the confining unit is very small. [Veling and Maas, 2010] re-evaluated the Theis and Hantush well functions used in type curve matching mentioned earlier. [Singh, 2010b] proposed an alternate approximate analytical solution to the unsteady leaky confined aquifer case. [Yeh and Chang, 2013] recently examined research

advances regarding the modeling of well hydraulics including those for confined aquifers. [Yang and Yeh, 2012] developed a general semi-analytical solution for partially penetrating aquifer test wells in a confined aquifer. [Brown, 2013] used optimization routines in Microsoft Excel and Solver to estimate aquifer properties in both non-leaky and leaky confined models.

While these unsteady (non-leaky and leaky) confined aquifer tests lend themselves to well-developed methods for estimating aquifer properties from data, it is also well-known that they neglect many real-world issues. Thus, richer models and techniques for deriving estimates from such models remain of interest. For example, aquifer performance tests in the field are often subject to "signal noise" from another nearby well or from boundary effects, which can result in an erratic drawdown at the primary monitoring well that may be difficult to interpret within existing solution approaches. This paper describes a relatively new computational technique called "particle filtering" in combination with previously-published analytical solutions to efficiently estimate confined aquifer parameters from field drawdown data measured at one or more observation wells. To our knowledge, this technique has not been used to solve these problems previously, yet we find when applied properly that it is no less accurate than previously published methods but also more flexible in the sense that it readily extends to richer models not easily solved otherwise. The technique is demonstrated and validated using three aquifer testing scenarios, namely the aforementioned canonical non-leaky and leaky confined aquifer tests as well as a third test in which signal noise is introduced into the data. The results provide strong evidence that the particle filtering method provides accurate estimates in all cases, including the third case in which previously-published methods are not as applicable. Further uses of particle filtering in groundwater hydrology are suggested for future research.

3.2 Particle Filtering Approach

3.2.1 Technical Rationale

The use of particle filters in the geosciences is fairly new, but the related Kalman filter has been used to study various groundwater problems since the 1990s. The Kalman filter equations are derived assuming that the measurement model is linear and all noise sources are Gaussian, neither of which is necessarily the case in aquifer drawdown tests. Thus, its application to groundwater problems introduces numerous additional considerations, such as how to approximate the models before processing each measurement or how to correct the Kalman filter equations to maintain acceptable performance when involving a nonlinear model. In one of the first geoscience applications of the Kalman filter, [Ferraresi et al., 1996] estimated hydrogeological parameters for aquifers in Libya. [Hantush, 1997] looked at spatially varying aquifer parameters using a Kalman filtering approach. [Yeh and Huang, 2005] use a modified Kalman filtering approach to develop estimates for leaky-confined aquifer pumping tests. [Yeh et al., 2007] compared global optimization methods to extended Kalman filter solutions for leaky-confined aquifer parameter problems. [Singh, 2010a] developed diagnostic curves for identifying leaky confined aquifer parameters using a Kalman filter among other techniques. [Nan and Wu, 2011] used an ensemble Kalman filter with localization to estimate hydrogeologic parameter fields in two dimensions and three dimensions. Zhou et al. (2011) proposed new approaches of handling limitations inherent in the ensemble Kalman filter. Xu et al. (2013) used an ensemble Kalman filter to evaluate hydraulic conductivity, using parallel computing to increase computational power and decrease computational time.

As the limitations regarding the linear assumptions underlying the Kalman filter were being characterized, other researchers were investigating alternate approaches to study groundwater hydrology problems. [Shigidi and Garcia, 2003] used artificial neural networks to estimate aquifer parameters. [Camp and Walraevens, 2009] used a sampling approach employing Latin

hypercube parameter sampling to develop estimates of key aquifer parameters during field testing. They used numerical inversion of LaPlace space solutions using the well-known Stehfest algorithm to develop analytical solutions that were linked to the parameter sampling approach. [Wang and Huang, 2011] used a Monte-Carlo approach to study the effect of aquifer heterogeneity on flow and solute transport in two-dimensional isotropic porous media. Recently, new data assimilation techniques have been used to improve hydrologic and hydrogeologic predictions. Included in these new techniques are "Sequential Monte Carlo (SMC)" methods in statistics, which are closely related to particle filtering methods in the sense that both employ sampled-based approximations for the probability distributions from which estimates are derived. A particle filter, however, organizes its computations more akin to the Kalman filter for linear-Gaussian models, while placing no restriction on the underlying models as long as they can be efficiently implemented as a computer program to be invoked repeatedly within each step of the filter. Recent work along these lines in the geoscience literature includes [Noh et al., 2011], studying surface water hydrologic problems, and [Pasetto et al., 2012], comparing the performance of the ensemble Kalman filter and a particle filter for a synthetic hydrogeologic case. Particle filtering is especially popular for object tracking and robotic navigation problems in electrical engineering and computer science, where numerous survey papers are now available [Arulampalam et al., 2002, Doucet and Johansen, 2011]

3.2.2 General Solution Methodology

Estimating parameters using a particle filter depends upon characterizing the unknown parameters and the available data within a general stochastic dynamic system model in state-space form. In such models, each stage $k = 0, 1, \ldots$ is comprised of two equations that together characterize the evolution of a (latent) state vector $\mathbf{x}_k$ (representing the unknown values in stage k) as well as how the (observed) measurement vector $\mathbf{y}_k$ (representing the data received in stage k) depends upon that

state:

$$\text{System Equation:} \qquad \mathbf{x}_{k+1} = f(\mathbf{x}_k, \mathbf{d}_k) \tag{3.1}$$

$$\text{Measurement Equation:} \qquad \mathbf{y}_k = h(\mathbf{x}_k, \mathbf{v}_k) \tag{3.2}$$

This is analogous to the setup underlying the Kalman filter except that (i) the functions f and h need not be linear and (ii) the random vectors $\mathbf{d}_k$ and $\mathbf{v}_k$, which model uncertainty in the state evolution and in the measurement process, respectively, need not be described by Gaussian distributions. Another component of such models is a given distribution for the initial state vector $\mathbf{x}_0$, which also need not be Gaussian as is assumed by the Kalman filter.

A particle filter begins with using the given initial state distribution to generate N equally-weighted samples, or *particles*, denoted by the collection $\{\mathbf{x}_0^i\}_{i=1}^N$. Then, upon receiving the initial measurement $\mathbf{y}_0$, the weights of all particles are reassigned by comparing their simulated measurements $\mathbf{y}_0^i = h(\mathbf{x}_0^i, \mathbf{v}_0)$ to the observed measurement $\mathbf{y}_0$, where particles in areas of the state space that produce simulated measurements close to what is actually observed become more highly weighted. These updated weights are then normalized so that they sum to unity and the collection of weighted particles $\{(\mathbf{x}_0^i, w_0^i)\}_{i=1}^N$ approximate the state distribution conditioned on the observed measurement. Specifically, the associated minimum-mean-square-error estimate $\hat{\mathbf{x}}_0$ is approximated by the weighted average of all the particles i.e.,

$$\hat{\mathbf{x}}_0 \approx \sum_{i=1}^{N} w_0^i \mathbf{x}_0^i \tag{3.3}$$

and, denoting by $\mathbf{A}'$ the as the transpose operation of a matrix $\mathbf{A}$, the associated error covariance is approximated by

$$\hat{\Sigma}_0 \approx \sum_{i=1}^{N} w_0^i \left(\mathbf{x}_0^i - \hat{\mathbf{x}}_0\right) \left(\mathbf{x}_0^i - \hat{\mathbf{x}}_0\right)'. \tag{3.4}$$

The particle filter then proceeds to the so-called resampling step, in which a new collection of N particles is generated in a manner that allows for the deletion of lowly-weighted particles in favor

of the replication of highly-weighted particles. These resampled particles are then simulated through the system equation $\mathbf{x}_1^i = f(\mathbf{x}_0^i, \mathbf{d}_0)$, predicting the next state by a new collection of equally-weighted particles $\{\mathbf{x}_1^i\}$ in preparation for another reweighting by the subsequent measurement $\mathbf{y}_1$. This procedure continues for $k = 1, 2, 3, \ldots$ until the final measurement is processed, the sequence of estimates $\hat{\mathbf{x}}_1, \hat{\mathbf{x}}_2, \hat{\mathbf{x}}_3, \ldots$ and the associated error covariances computed analogously to equations (3.3) and (3.4) for the initial stage. In short, the algorithm sequentially evolves its solution according to a "survival of the fittest" process in which particles with unlikely parameter estimates are discarded and those whose estimates produce simulated measurements resembling the observations are retained. Key algorithmic considerations in the implementation of a particle filter include how many particles to use and what type of sampling/resampling procedures to invoke in each iteration, design choices which are application-dependent to the extent that they are entwined with properties of the model's functions f and h as well as the distributions characterizing the system disturbances $\mathbf{d}_k$, measurement noises $\mathbf{v}_k$ and initial state $\mathbf{x}_0$. The reader interested in more details is encouraged to consult available tutorial papers and texts [Arulampalam et al., 2002, Doucet and Johansen, 2011]. The following sections present a particle filter that solves the parameter estimation problems for both non-leaky and leaky unsteady aquifer cases.

3.3 Methodology Applied to Aquifer Parameter Estimation

In this section, the general particle filtering methodology described in Section 3.2 is specialized to the problem of aquifer parameter estimation. We start with the well-studied unsteady non-leaky confined aquifer scenario of [Theis, 1935], where the unknown aquifer parameters of interest are its transmissivity T and storativity S, while the observations are a sequence $y_0, y_1, y_2, \ldots$ of (scalar) drawdown measurements taken during an aquifer performance test. Our state-space model utilizes the well function defined by [Theis, 1935], which relates the transmissivity T and storativity S to

synthetic drawdown s via the series approximation

$$s = \left(\frac{Q}{4\pi T}\right)\left[-0.5772 - \ln(u) + u - \frac{u^2}{2\times 2!} + \frac{u^3}{3\times 3!} - ...\right] \tag{3.5}$$

$$u = \frac{r^2 S}{4Tt} \tag{3.6}$$

where Q denotes the known pumping rate, r denotes the known radius from the pump to the observation well and t denotes the known observation time. It should be noted that Equation 3.5 is not the only way to approximate Theis' well function; for example, [Abramowitz and Stegun, 1964] provide efficient polynomial approximations instead of the series solution. While the results in this paper are based on using the series approximation, the particle filtering methodology applies equally well when using other approximations for the governing well function.

Armed with a well function, let the state vector $\mathbf{x}_k = [S\ T]'$ contain the unknown aquifer parameters of interest. Then, the measurement equation h of our state space model in successive stages $k = 0, 1, 2, \ldots$, in correspondence with a sequence of observation times $t_0 < t_1 < t_2 < \ldots$ with which to evaluate equations (3.5) and (3.6), can be expressed as

$$y_k = h(\mathbf{x}_k, v_k) = s_k + v_k, \quad k = 0, 1, 2, \ldots.$$

Here, random variable v_k captures drawdown measurement error as well as modeling errors arising within Theis' approximation, which we assume is described by a zero-mean Gaussian distribution with known standard deviation σ_v. This measurement equation is linear in synthetic drawdown s_k and measurement noise v_k, but it is worth noting that the former is a highly nonlinear function of the state vector $\mathbf{x_k}$, or the aquifer parameters S and T to be estimated.

It remains to specify the system equation f of our state-space model. Because the unknown parameters are assumed to have fixed values during the aquifer performance test, the static model $\mathbf{x}_{k+1} = \mathbf{x}_k$ is appropriate in principle. However, static models are problematic for a particle

filtering approach because the dynamics of the system equation are the mechanism by which a particle filer judiciously explores the state space; that is, in the case of static state dynamics, the candidate state values are entirely determined by the stage-0 samples from the initial state distribution—only their weights, not their locations, are revised as observations are processed. Satisfactory performance with static models depends on luck that at least one initial particle location takes its value near the correct one, the chance of which can be increased only by increasing the number of particles used (and incurring the associated computational overhead). This phenomenon for static models is referred to as "particle impoverishment" and is a known limitation of the approach. The use of "artificial dynamics," introduced by [Liu and West, 2001], overcomes this limitation of static models by rather perturbing the state vector in each iteration e.g.,

$$\mathbf{x}_{k+1} = f(\mathbf{x}_k, \mathbf{d}_k) = \mathbf{x}_k + \mathbf{d}_k, \quad k = 0, 1, 2, \ldots,$$

where we assume that the disturbance $\mathbf{d}_k$ is a zero-mean Gaussian random vector with known covariance matrix Σ_d. The initial state distribution is taken to be jointly uniform over given lower and upper bounds on the two parameters, storativity S and tranmissivity T, based on knowledge of the region under test.

Algorithm 3 summarizes the particle filter implementation specified above for the described unsteady non-leaky confined aquifer scenario, while Figure 3.1 visualizes its behavior at seven selected iterations after initialization. The figure shows eight scatter plots of all particle locations in the state space, the horizontal and vertical axes in each plot corresponding to storativity S and transmissivity T, respectively. Specifically, Subfigure 3.1a visualizes the $N = 2000$ samples drawn from a given uniform initial state distribution across the entire state space $[10^{-5}, 10^{-2}] \times [50, 10000]$, each such initial particle assigned equal weight and thus the initial parameter estimate (the blue triangle marker) is simply the central value. Subfigures 3.1b-3.1h visualize the collection of weighted particles $\{\mathbf{x}_k^i, w_k^i\}_{i=1}^N$ as drawdown observations are sequentially processed, each subfigure showing (i) the particle locations occupying smaller and

smaller portions of the state space, (ii) the particle weights coded relatively by color (with red and blue indicating high and low, respectively) and (iii) the implied parameter estimate (i.e., the sample mean and sample covariance via equations (3.3) and (3.4), respectively) evolving to the upper-left region of the state space. This dataset has thirteen stages and the final state estimate $\hat{\mathbf{x}}_{12}$ after the thirteenth iteration is $[1.09 \times 10^{-3}\ 708]'$, which compares well with previously-published answers of $[1.06 \times 10^{-3}\ 712]'$ derived from graphical curve fitting methods (the black square marker).

Algorithm 3: Particle Filter for Estimating Aquifer Parameters

Step 0: Initialization

Iteration $k := 0$

for $i = 1 : N$ **do**

  Generate sample $\mathbf{x}_0^i$ drawn uniformly from the entire state space $[0, S_{\max}] \times [0, T_{\max}]$;

  Set initial weight $w_0^i := 1/N$

end

Step 1: Prediction Step

Upon receiving observation y_k (associated to time t_k of the aquifer performance test),

if $k > 0$ **then**

  for $i = 1 : N$ **do**

    Draw sample $\mathbf{d}_{k-1}$ from a zero-mean Gaussian distribution with covariance matrix Σ_d;

    Update particle location $\mathbf{x}_k^i := \mathbf{x}_{k-1}^i + \mathbf{d}_{k-1}$

  end

end

Step 2: Correction Step

for $i = 1 : N$ **do**

  Compute synthetic drawdown s_k^i via (3.5) and (3.6) with S and T taken from particle $\mathbf{x}_k^i$;

  Update particle weight $\tilde{w}_k^i := w_{k-1}^i \cdot \exp\left(-\frac{1}{2}(y_k - s_k^i)^2/\sigma_v^2\right)$

end

Upon computing total wieght $W_k := \sum_{i=1}^N \tilde{w}_k^i$,

for $i = 1 : N$ **do**

  Normalize weight $w_k^i := \tilde{w}_i^k / W_k$

end

Update second-order statistics via (3.3) and (3.4)

Step 3: Resample Decision

Upon quantifying degeneracy by calculating the effective sample size $N_{eff} = \left(\sum_{i=1}^N (w_k^i)^2\right)^{-1}$,

if $N_{eff} < \frac{N}{2}$ **then**

  Resample N particles form the current weighted set

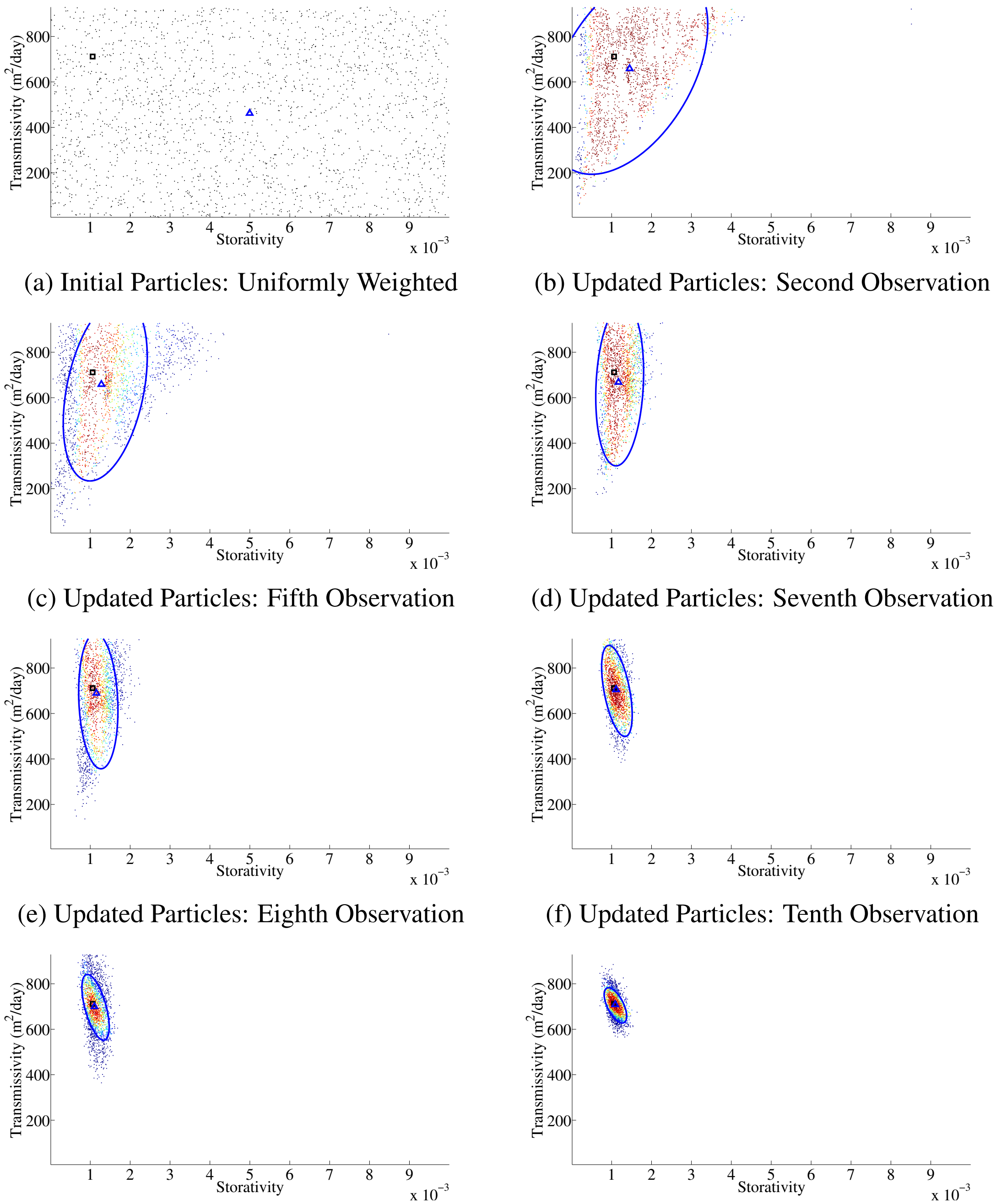
  for $i = 1 : N$ **do**

    Re-initialize weight $w_k^i := 1/N$

  end

end

Iteration $k := k + 1$ and return to **Step 1**



(a) Initial Particles: Uniformly Weighted

(b) Updated Particles: Second Observation

(c) Updated Particles: Fifth Observation

(d) Updated Particles: Seventh Observation

(e) Updated Particles: Eighth Observation

(f) Updated Particles: Tenth Observation

(g) Updated Particles: Eleventh Observation

(h) Updated Particles: Thirteenth Observation

Figure 3.1: Visualization of seven selected iterations after initialization of our particle filtering solution for the unsteady non-leaky confined aquifer scenario of [Mays, 2011]. Each subfigure shows a collection of weighted particles (with red and blue indicating high and low weights, respectively) over the two-dimensional state space, the horizontal and vertical axes corresponding to storativity S and transmissivity T, respectively. Each subfigure also indicates the minimum-mean-square parameter estimate and its error covariance (the blue triangle and two-sigma ellipse) implied by the shown set of particles, which clearly converges to a previously-published answer (the black square) derived from graphical curve-fitting methods on the entire dataset.

Observe in Figure 3.1 how the initial set of particles sparsely cover the entirety of the state space. After several observations, particle locations are updated such that coverage density about the likely area of the state space is increased. This desirable property occurs because of the artificial dynamics—the particle filter with a static state equation would not alter the initial locations and thus the density of particles in likely regions of the state space would never increase from that implied by Subfigure 3.1a. This behavior, namely the concentration of computational resources to the most likely areas of the state space, is an important feature of particle filters, especially for models having higher dimensional state vectors. For example, the leaky confined aquifer scenario assumes flow during a performance test can also arise from vertical leakage through confining units from aquifers above or below the zone of interest, and thus introduces vertical hydraulic conductivity K_v as a third state variable. The above particle filter extends readily to this scenario, modifying the measurement equation h with formulas to efficiently estimate the Hantush well function ([Hantush and Jacob, 1955]). Specifically, letting drawdown s, rate Q, radius r and time t be defined as in the Theis model and defining m' as the thickness of the confining bed through which leakage occurs, [Veling and Maas, 2010] propose a computationally efficient approximation in terms of the exponential integral E_1 and the modified Bessel Function K_0,

$$s = \left(\frac{Q}{4\pi T}\right) F(\rho,\tau) \tag{3.7}$$

where,

$$F(\rho,\tau) = \begin{cases} 2K_0(\rho) - J(\rho,\tau) & \tau > 0 \\ J(\rho,-\tau) & \tau \leq 0 \end{cases}$$

and

$$J(\rho,\tau) = \omega(\rho)E_1\left(\frac{\rho}{2}\exp(-\tau)\right) + (1-\omega(\rho))E_1(\rho\cosh(\tau)),$$

$$\omega(\rho) = \frac{E_1(\rho) - K_0(\rho)}{E_1(\rho) - E_1(\frac{\rho}{2})}, \qquad \rho = \frac{r}{\sqrt{Tc}}, \qquad \tau = \ln\left(\frac{2}{\rho}\frac{t}{Sc}\right), \qquad c = \frac{m'}{K_v}.$$

In turn, augmenting the state to $\mathbf{x}_k = [S\ T\ K_v]'$ and employing (3.7) in Step 2 of Algorithm 1 extends the particle filter solution to the leaky confined problem.

3.4 Results

3.4.1 Unsteady Non-Leaky Confined Aquifers

The solution methodology presented herein is first validated via two well known and previously published benchmark non-leaky confined aquifer parameter estimation problems. In the first, from [Mays, 2011], a test well screened in a confined aquifer is pumped at a rate of $31.5 \times 10^{-3}\ m^3/sec$ for 4,000 minutes. Time-drawdown data was collected at an observation well located 61 m from the test well. After 4,000 minutes the maximum drawdown measured at the observation well was 2.13 m. Mays' graphical curve fitting solution provides an estimate of the aquifer properties as 1.06×10^{-3} and 712 m^2/day for S and T respectively.

When provided the input parameters collected in Table 3.1, the particle filter estimates an S of 1.08×10^{-3} and a T of 714 m^2/day. A visual representation of the output of Algorithm 1, after having sequentially processed all observations in the data set, is provided in Subfigure 3.1h and reproduced in Figure 3.2.

Table 3.1: Mays Particle Filter Parameters

$Q[m^3/min]$	$r[m]$	N	range	Σ	σ
1.89	61	2000	$\begin{bmatrix} 10^{-5} & 10^{-2} \\ 50 & 10000 \end{bmatrix}$	$\begin{bmatrix} 10^{-9} & 0 \\ 0 & 10^{5} \end{bmatrix}$	0.1

The time-drawdown data for this aquifer test, accompanied by synthetic drawdown curves produced by the parameter estimates of both the published Mays solution and the particle filtering solution, is presented in Figure 3.3 with the sum of squared error metric for both sets of parameter

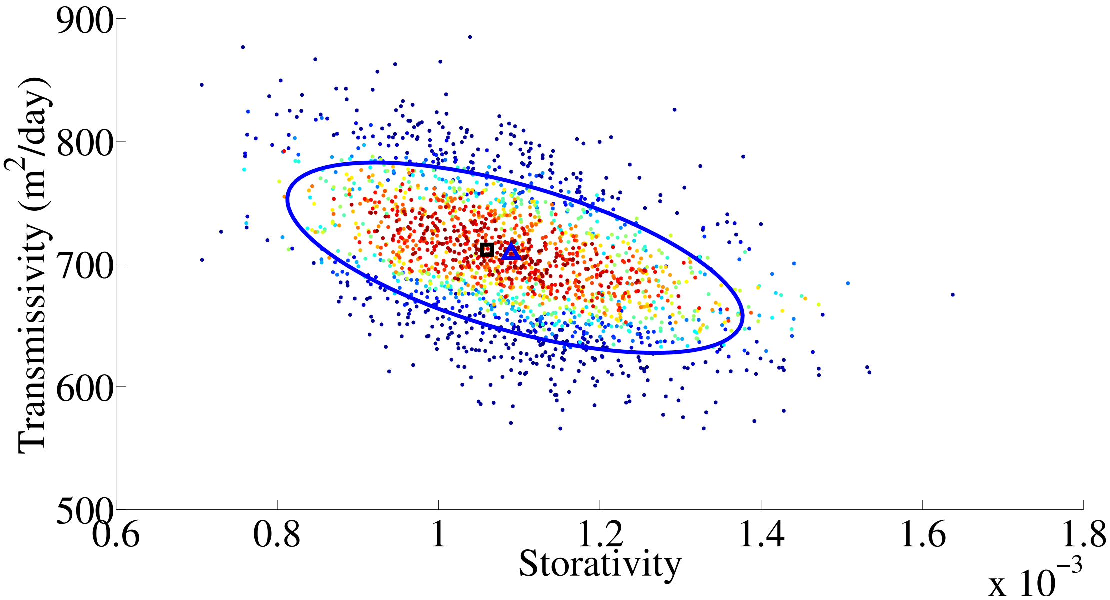


Figure 3.2: Final particle cloud for the [Mays, 2011] aquifer test. Particles, colored in accordance to their respective likelihoods where red is more likely than blue, are presented relative to the previously published solution (black square) as well as the particle filter's estimate and error covariance (blue triangle and ellipse).

estimates.

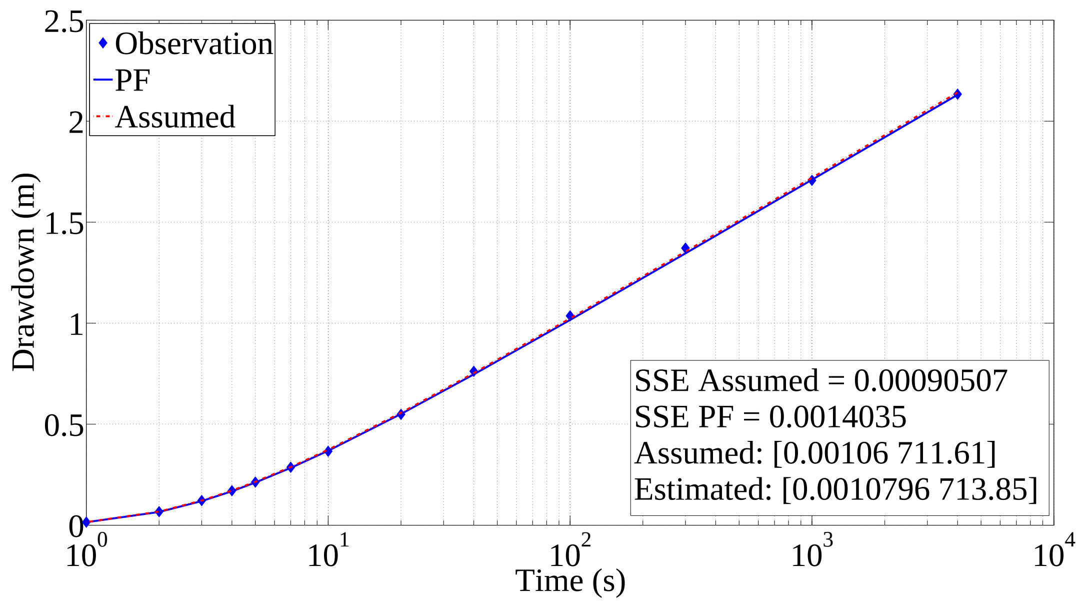


Figure 3.3: Drawdown vs time plot of the [Mays, 2011] data set with the synthetic drawdown curves produced by the parameter estimates from both the observed results (red) and the particle filter estimator (blue) overlain.

In the second problem, a data set collected from an aquifer test carried out in 1953 on a village well in Gridley, Illinois, in which the effects of a constant-rate excitation of $13.879 \times 10^{-3} m^3/sec$ located 251m from the observation well were recorded. [Walton, 1962] presents transmissivity and storativity parameter estimates for this dataset computed from the superposition of time-drawdown field data onto the non-leaky artesian type curve, arriving at S and T estimates of 2.2×10^{-5} and 125.45 m^2/day respectively. Additional parameter estimates were generated by the AQTESOLV pumping test software (Hydrosolve, 2013), producing 2.095×10^{-5} and 123 m^2/day.

When provided the input parameters collected in Table 3.2, the particle filtering methodology presented herein produces estimates of 2.12×10^{-5} and 122.6 m^2/day for S and T respectively.

Table 3.2: Walton - Gridley Particle Filter Parameters

$Q[m^3/min]$	$r[m]$	N	range	Σ	σ
0.833	251	2000	$\begin{bmatrix} 10^{-5} & 10^{-2} \\ 50 & 10000 \end{bmatrix}$	$\begin{bmatrix} 10^{-9} & 0 \\ 0 & 10^{5} \end{bmatrix}$	0.1

Figure 3.4 presents the time-drawdown field data from the 1953 Gridley aquifer test. Superimposed are synthetic drawdown curves produced by the Theis well function, Equation 3.5, utilizing both the Aqtesolve and particle filter parameter estimates.

3.4.2 Unsteady Leaky Confined Aquifers

Validation of the proposed solution methodology is continued through the use of two previously published benchmark leaky confined aquifer tests. The two necessary adaptations to Algorithm 1 are (i) an increase in the dimension of the latent state variable $\mathbf{x}$ in order to accommodate the vertical hydraulic conductivity term k_v, and (ii) the substitution of the measurement function in Step 2 of Algorithm 1 with that which is presented in equation (3.7).

First, a dataset presented by [Walton, 1962] originating from a controlled pump test made under

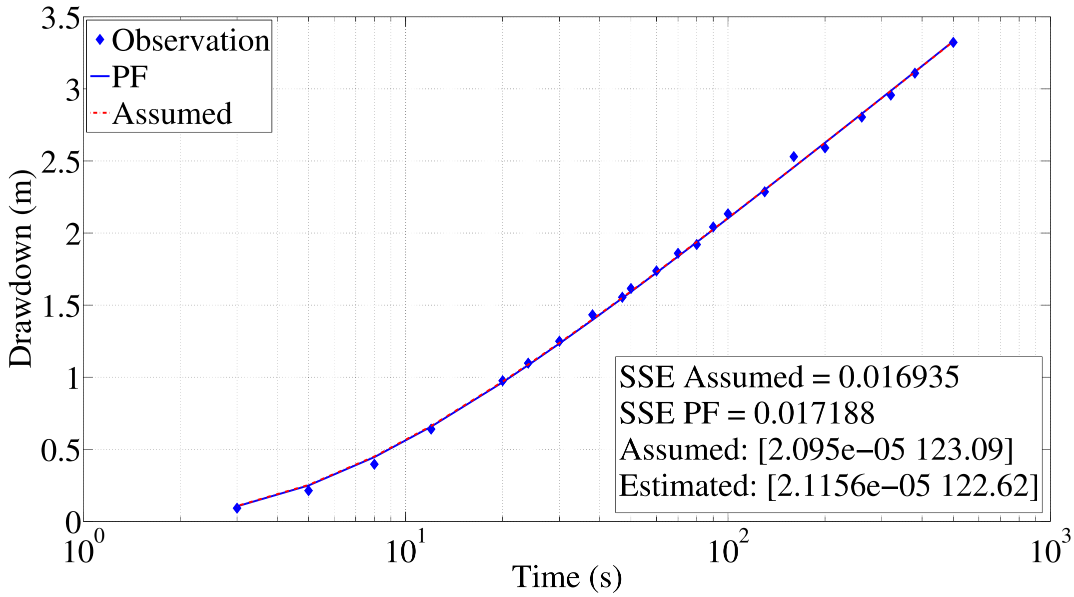


Figure 3.4: Walton - Gridley time-drawdown data set with the synthetic drawdown curves produced by the parameter estimates from both AQTESOLV (red) and the particle filter estimator (blue) overlain.

leaky artesian conditions in glacial drift aquifers near Dieterich, Illinois. The test well was pumped at a constant rate of 135.9 m^3/day for $1,185$ minutes while the effect of said excitation was observed in a well located 29.3 m from the test well. The thickness of the overlying confining unit was 4.27 m. After 1,185 minutes the maximum drawdown measured at the observation well was 1.96 m. Walton reports aquifer parameter estimates of 2.0×10^{-4} for S, a T of 18.754 m^2/day, and a K_v value of 4.482×10^{-3} m/day.

Parameter estimates found by the methodology presented in this paper are 1.74×10^{-4}, 21.54 m^2/day, and 3.28×10^{-3} m/day for S, T, and K_v, respectively. Input parameters to the modified Algorithm 1 are collected in Table 3.3 and a comparison of synthetic drawdown curves produced by the previously published estimation results and those found by the particle filter are presented in Figure 3.5.

For the second benchmark estimation problem under leaky artesian conditions, a test well screened in a leaky confined aquifer [Cooper, 1963] is pumped at a rate of $5,451$ m^3/day for

Table 3.3: Walton - Dieterich Particle Filter Parameters

$Q[m^3/min]$	$r[m]$	$m'[m]$	N	range	Σ	σ
0.0944	96	4.27	2000	$\begin{bmatrix} 10^{-5} & 10^{-2} \\ 50 & 10000 \\ 10^{-4} & 1 \end{bmatrix}$	$\begin{bmatrix} 10^{-9} & 0 & 0 \\ 0 & 10^{5} & 0 \\ 0 & 0 & 10^{-4} \end{bmatrix}$	0.1

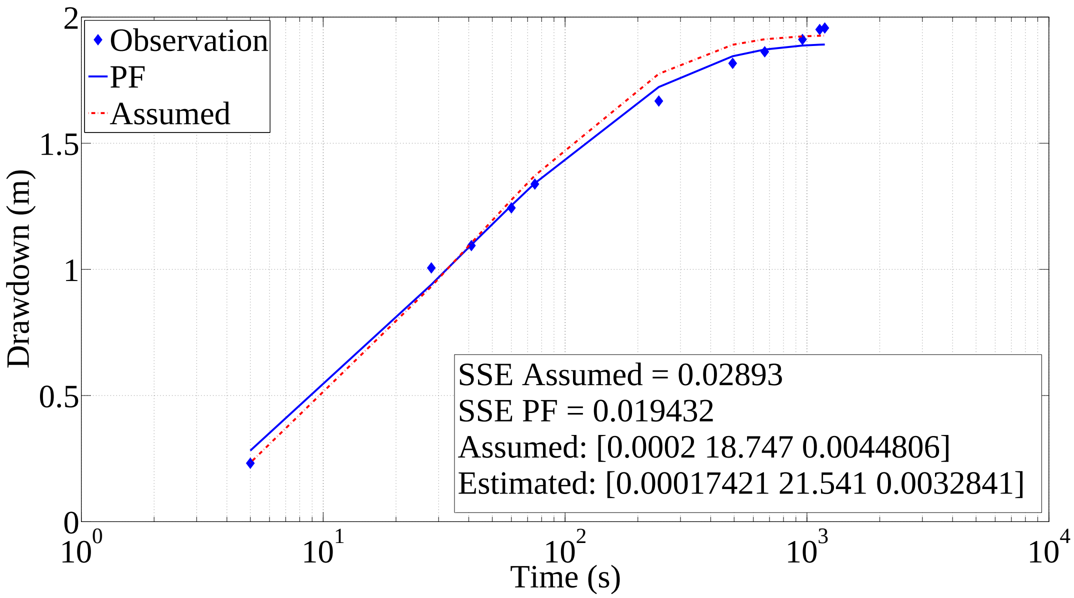


Figure 3.5: Drawdown vs time plot of the Walton - Dieterich data set with the synthetic drawdown curves produced by the parameter estimates from both the previously published (red) and particle filter solutions (blue) overlain.

1,000 minutes. The thickness of the overlying confining unit was 30.48 m. Time-drawdown data was collected at an observation well located 30.48 m from the test well. After 1,000 minutes the maximum drawdown measured at the observation well was 2.2 m. [Lohman, 1972] reports the aquifer properties as an S of 9.95×10^{-5}, a T of $1,236\ m^2/day$, and a K_v value of 0.1 m/day. The estimate using the methodology presented in this paper using particle filtering gives values of 1.08×10^{-4}, $1,193\ m^2/day$, and $0.124\ m/day$ for S, T, and Kv, respectively. Figure 5 presents the time-drawdown data as well as the synthetic drawdown curves produced by Lohman's previously published parameter estimates and those arrived at by the particle filter solution methodology initialized with the parameters collected in Table 3.4.

Table 3.4: Cooper Particle Filter Parameters

$Q[m^3/min]$	$r[m]$	$m'[m]$	N	range	Σ	σ
3.785	30.48	30.48	2000	$\begin{bmatrix} 10^{-5} & 10^{-2} \\ 50 & 10000 \\ 10^{-4} & 1 \end{bmatrix}$	$\begin{bmatrix} 10^{-9} & 0 & 0 \\ 0 & 10^5 & 0 \\ 0 & 0 & 10^{-4} \end{bmatrix}$	0.1

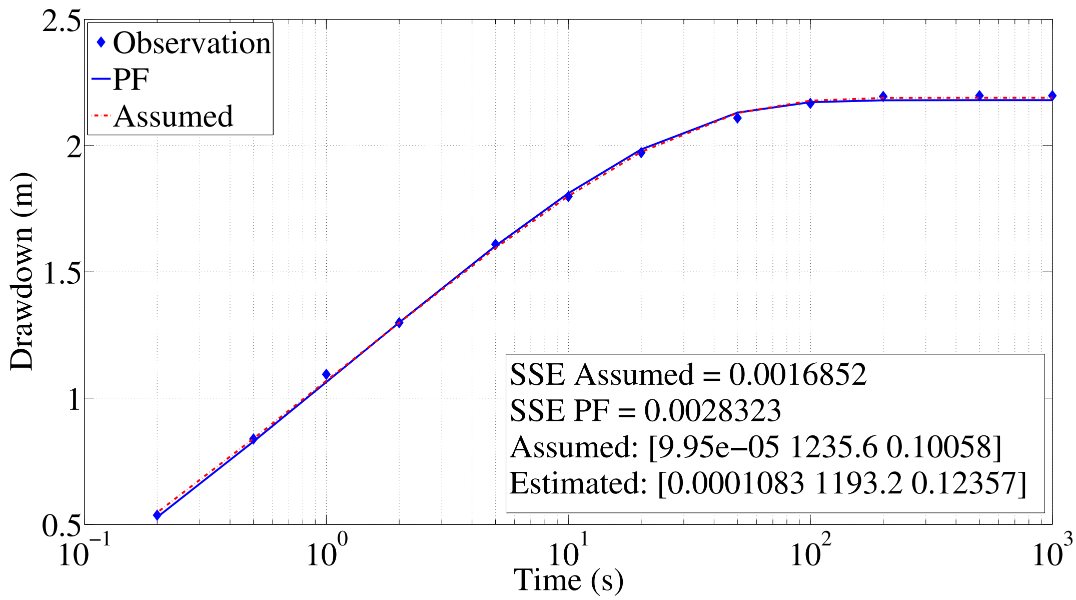


Figure 3.6: Time-drawdown plot of the Cooper (1963) data set with the synthetic drawdown curves produced by the parameter estimates from [Lohman, 1972] (red) and the particle filter estimator (blue).

3.4.3 Unsteady Confined Aquifer with Noise and Boundary Effects

Synthetic validation data was developed using the three dimensional finite-difference groundwater modeling code MODFLOW [McDonald and Harbaugh, 1988]. This validation experiment includes a pumping well withdrawing water from a non-leaky confined aquifer at a rate of $1,136$ m^3/day. The aquifer is 30 m thick with T value of 850 m^2/day and an S value of 5×10^{-4}. Aquifer drawdown is monitored in an observation well located 45.72 m directly east of the pumping well. For the sake of computational efficiency, the model grid is one quadrant with

the pumping well located at the origin. The model grid size is unimodal with grid cells at 7.62 $m \times 7.62$ m. The MODFLOW model was validated against the Theis analytical solution discussed above and matched the exact solution closely underestimating the exact drawdown by 0.015m on average. Once the initial validation was completed, the base model was modified to include a second pumping well located 140.5 m northeast from the model observation well. This well withdraws water from the non-leaky confined aquifer at a rate of 70.8 m^3/day, however, due to the model boundaries on the quadrant model, the effective drawdown is about double what an actual field drawdown would be in an infinite aquifer. This well also only pumps every 12 hours versus continuously for the first pumping well. Therefore, this second pumping well imparts a sinusoidal noise factor to the observation well.

In order to make this validation test totally blind, the solution methodology presented herein utilizes neither the "noise" well's position nor pumping rate. This simulation is comparable to real-world aquifer tests when a local irrigation well is known to exist nearby but the exact location cannot be established due to access restrictions. Therefore, in order to estimate the S and T values, the methodology contends with observation well data subject to three different types of noise simulating real-world issues including unidirectional low bias from the actual numerical model results; no-flow boundary effects that multiply the assigned model pumping rate; and, sinusoidal drawdowns due to temporal pumping rate without an exact location. Accuracy of the presented methodology largely depends on the ability to classify those data points which are corrupted by the secondary excitations and increase accordingly the parameter which encapsulates the filter's measurement uncertainty, σ_v, for those filter iterations.

Figure 3.7 presents the time-drawdown data for this problem as well as the drawdown curves produced by the known parameter values and particle filtering estimate when initialized with the input parameters collected in Table 3.5.

Table 3.5: Noise/Boundary Effects Particle Filter Parameters

$Q[m^3/min]$	$r[m]$	N	range	Σ	σ
1136	45.72	2000	$\begin{bmatrix} 10^{-5} & 10^{-2} \\ 50 & 20000 \end{bmatrix}$	$\begin{bmatrix} 10^{-9} & 0 \\ 0 & 10^{5} \end{bmatrix}$	0.1,1

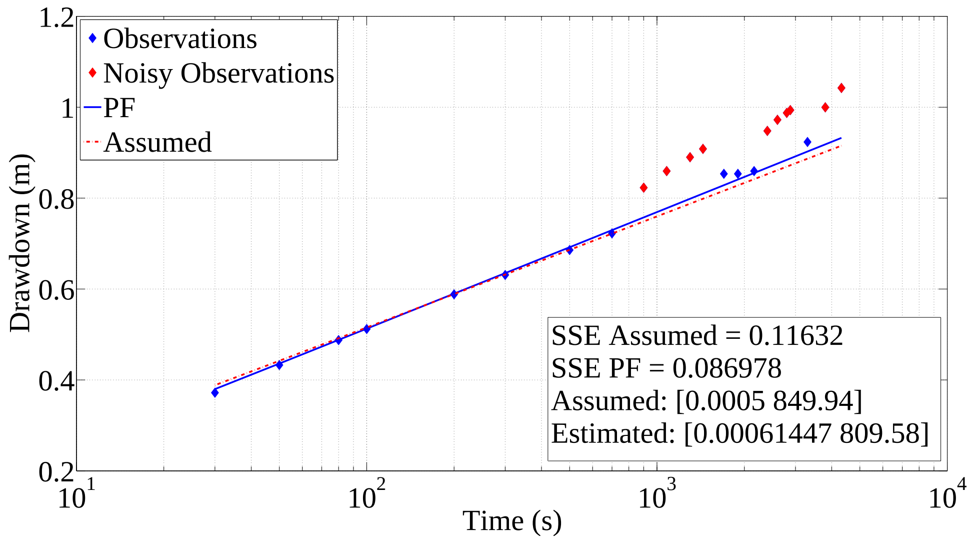


Figure 3.7: An original time-drawdown data set with significant sinusoidal signal corruption due to a periodic secondary well with an unknown pump rate and at an unknown location. The known model parameters provide the (red) drawdown curve in the absence of the corrupting well, while the (blue) drawdown curve is produced by the particle filter's parameter estimates derived from the entire data set.

3.5 Conclusion and Future Work

This paper has applied the particle filtering methodology to estimate properties of confined aquifers using transient data from aquifer performance tests. Experimental results demonstrate (i) an accuracy that matches that of previously-published solution methods in numerous well-studied scenarios and (ii) an ability to generalize to scenarios not as easily addressed by previously-published methods. Particle filtering as a means to address measurement uncertainty is common practice in the sub-disciplines of electrical engineering and applied mathematics, but it is only beginning to find application in the water research community. The widespread familiarity of the first four data sets that we considered, two under non-leaky assumptions using the Theis

well function and two under leaky assumptions using the Hantush well function, affords an accessible introduction of the particle filtering approach. Its true usefulness, however, becomes evident in the fifth data set that we considered, which injects noise into the drawdown data in a manner that challenges previously-published solution methods but is readily addressed by the particle filtering approach.

An interesting extension of the work presented here is to estimate properties of tidally responsive aquifers, as first described by [Jacob, 1950]. The effect of earth tides on aquifer response at groundwater monitoring wells was further studied by [Bredehoeft, 1967], who introduced specific storage and porosity estimates. Of particular interest are the recent adaptations of Jacob's original models for coastal confined aquifers presented by [Dong et al., 2012].

Recall the results in Figure 2.1, which illustrate a particle filters ability to provide estimates (and the associated error intervals) sequentially during the performance test (in contrast with solutions that operate on the drawdown data in-batch after the test). A sequential algorithm presents the opportunity to avoid unnecessarily long performance tests if diminishing marginal improvement in estimation accuracy is observed or if it can otherwise be inferred that neither surface water bodies nor impervious boundaries will likely be reached by continuing the test. Quantifying the extent to which a particle filter can adequately inform an online decision process for when to terminate a performance test, potentially avoiding unnecessary expense, is another interesting direction for future work.

Finally, the particle filtering approach taken in this paper should be applicable to parameter estimation problems that arise within other hydrogeology applications. Solutions based on classical approaches (e.g., the Kalman filter, least-squares) carry the risk of oversimplifying the underlying models to satisfy the needed linear-Gaussian assumptions. That said, there are examples in the hydrogeology literature that address nonlinear estimation problems using the so-called extended Kalman filter and its variations. Thus, a related line of inquiry could be to compare (both in estimation accuracy and in computational overhead) a particle filtering solution

to previously-published nonlinear estimation techniques in the hydrogeology literature.

Chapter 4

Recommendations and Conclusion

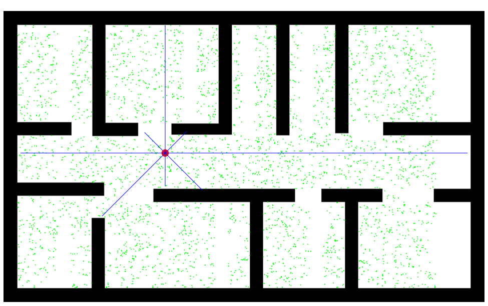
The recommendations for future work of [Field et al., 2016] are expanded upon by presenting an area of algorithmic improvement to the standard particle filtering algorithm (Algorithm 3). Addressed is the computational burden incurred by fixing the number of hypotheses evaluated at each iteration. A mechanism is introduced which allows the algorithm to self-select the size of this set in accordance with its ability to approximate the underlying distribution, thereby inversely coupling computational expenditure to estimator performance. Background on the rationale for the improvement, initial findings on its application to the aquifer parameter estimation problem, and concluding remarks are presented in the following sections.

4.1 Set-Size Tuning

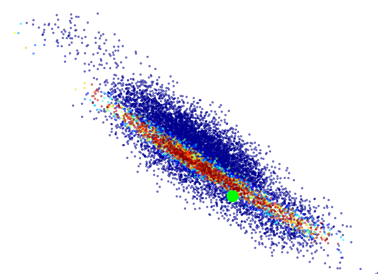
The particle filtering algorithm's efficiency and estimation accuracy are largely governed by the number of particles used. Decreasing the size of this set reduces the amount of computations required during each iteration; however, having too-few particles introduces the risk of an irrecoverable position in which the initial distribution fails to capture probable regions in the state space. Recall the robot localization example of Chapter 2. Using Figure 2.1 as an example, this equates to the initial uniform distribution, reproduced below in Figure 4.1a, being absent of particles near the robot's actual position. The number of particles to utilize is therefore selected to

avoid this outcome.

What results is the situation where the number of particles required to accurately estimate the state of the system after the cloud has collapsed is much smaller than the number required in the initial iterations. This situation, for a two-dimensional state vector, is depicted in Figure 4.1b. It shows a cloud of particles, colored in accordance to their respective likelihoods where red is more likely than blue, relative to the actual target location represented in green. Clearly, many of the blue dots could be omitted and the weighted average of the remaining particles would be negligibly changed. During each iteration, computational resources are spent on evaluating a large number of these already determined unlikely positions due to the number of particles being a fixed parameter. An algorithm which self-tunes the number of particles used based upon the statistics of the current estimate would show increased computational efficiency over one with a fixed sample size by discarding particles when they are found to be unnecessary.



(a) Particle initialization



(b) Eventual particle distribution

Figure 4.1: Motivational visualization of the set-size problem where (a) presents the required and sensible uniform distribution of hypotheses throughout the application's bounded state space and (b) presents an eventual particle cloud whose colors are drawn from a heat map in accordance with their likelihood surrounds the actual (hidden) state of interest.

4.1.1 KLD-Sampling

The canonical algorithmic mechanism for set-size tuning was introduced by Dieter Fox [Fox, 2003]. Fox's technique utilizes the Kullback-Leibler divergence, which essentially quantifies the penalty for using one distribution to approximate another, between the current approximation of the posterior and that of the previous iteration's. He derives an equation which yields the number of samples necessary for achieving a target divergence between these two distributions by supposing a multi-dimensional histogram over the state-space and tracking the number of bins which have been sampled from. This equation is,

$$n_X = \frac{k-1}{2\varepsilon}\left\{1 - \frac{2}{9(k-1)} + \sqrt{\frac{2}{9(k-1)}}z_{1-\delta}\right\}^3, \tag{4.1}$$

where n_X is the number of prescribed samples, ε is the user-defined K-L divergence between the distributions, k is the number of bins with support, and $z_{1-\delta}$ is the $1-\delta$ upper quantile of the standard normal distribution. Algorithm 4 presents Fox's KLD-sampling particle filtering algorithm.

Algorithm 4: Fox's KLD-Sampling Algorithm

Data: $\{x_{t-1}^i, w_{t-1}^i\}_{i=1}^N, y_t$, bounds ε and δ, bins size Δ

Result: $\{x_t^i, w_t^i\}_{i=1}^N$

$N = n_X = k = 0$;

do

  $N++$;

  Sample an index j from the discrete distribution given by w_{t-1};

  Sample x_t^N from $p(x_t|x_{t-1})$ using x_{t-1}^j;

  $\tilde{w}_t^N = p(y_t|x_t^N)$;

  if x_t^N *falls into an empty bin b* **then**

    $k++$;

    b =non-empty;

    $n_X = \frac{k-1}{2\varepsilon}\left\{1 - \frac{2}{9(k-1)} + \sqrt{\frac{2}{9(k-1)}}z_{1-\delta}\right\}^3$;

  end

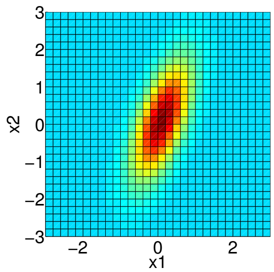
while $N < n_X$;

for $i = 1 : N$ **do**

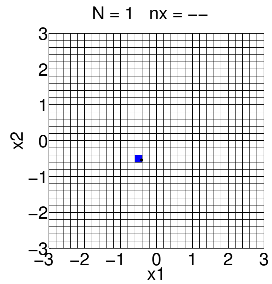
  $w_t^i = \tilde{w}_t^i / \sum \tilde{w}_t$;

end

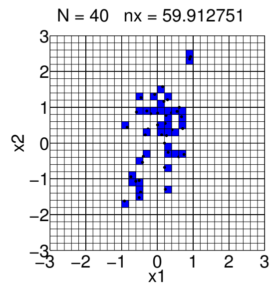
The predict and update operations are identical to the standard SIR particle filter (Algorithm 2, 3), however within this algorithm, samples are drawn each iteration until the sample set size reaches the number prescribed by Equation 4.1. Figure 4.2 presents a visual representation of the algorithm's binning process.



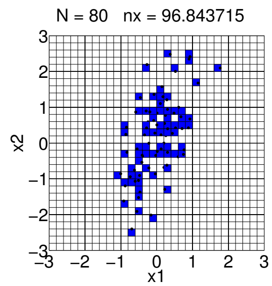
(a) Underlying distribution



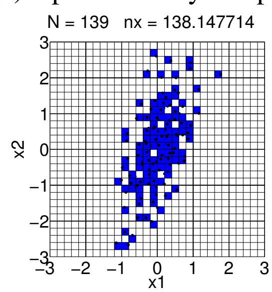
(b) Updated: one sample



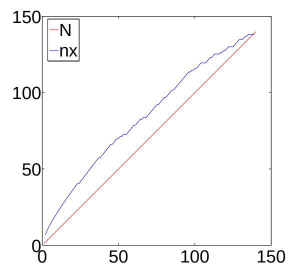
(c) Updated: forty samples



(d) Updated: eighty samples



(e) Updated: final sample



(f) Relation between n_X and N

Figure 4.2: A visual representation of the binning process within the KLD-sampling algorithm. (a) presents the underlying (hidden) multivariate normal distribution being sampled from with (b)-(e) showing the bins with support after 1, 40, 80, and 139 samples respectively. (f) presents the number of prescribed samples for each draw iteration.

When a new particle is sampled from an unsupported bin, that bin is marked as supported and the number of necessary samples n_X is recalculated (Figures 4.2b - 4.2d). At the beginning of each filtering iteration, n_X is increased often as each newly sampled particle is likely to fill an unsupported bin. As the approximated distribution becomes more defined however, n_X is updated less frequently and the exit condition $N > n_X$ becomes more likely to be met, resulting in the end of the sample generation phase of the filtering iteration (Figure 4.2e, 4.2f).

4.1.2 Estimator Performance - Aquifer Parameter Estimation

Following [Fox, 2003], it is assumed that the implementation of the self-tuning algorithmic mechanism does not significantly increase computational costs per sample, and that the average number of samples used during an estimation task is a valid basis of comparison between static and adaptive algorithms. Therefore, it suffices to compare estimators by their ability to minimize an error statistic per number of samples utilized. Figure 4.3 presents such a comparison, in which both the static particle filtering algorithm and Fox's KLD-sampling algorithm are brought to bear on the aquifer transient monitoring data from [Cooper, 1963].

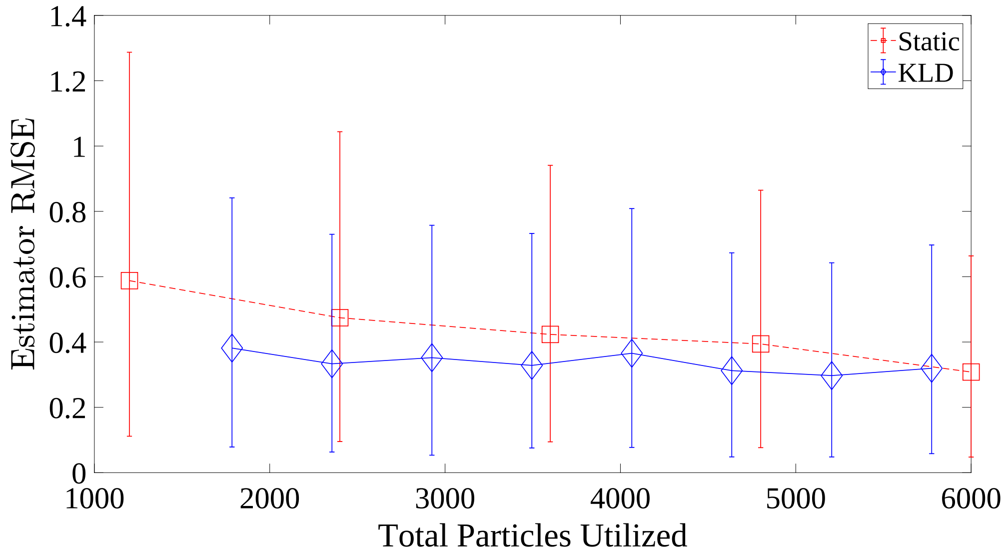


Figure 4.3: Comparison between Fox's KLD sampling algorithm and the standard SIR particle filter tasked with the estimation of aquifer parameters given the [Cooper, 1963] data set. The x- and y-axes are the total number of hypotheses evaluated by a given estimator and its estimation error statistic with 95% confidence intervals, respectively.

Each data point in Figure 4.3 represents the average RMSE of 50 Monte Carlo trials of the estimation task for a given total particle set size. It is clear that the KLD-sampling algorithm outperforms the static particle filter when computational resources are constrained. The main source of this increased performance is the self-tuning algorithm's ability to spend computational resources aggressively in times of filter uncertainty, as is the case during the "localization" phase

of the estimation task. During these initial filtering iterations, the static algorithm exhibits poor performance when less than 5000 total samples are used due to an initial estimate which lacks sufficient hypotheses near the true state, whereas the self-tuning algorithm can saturate the state space during localization and reduce the size of the set after a measurement history has been established. The need for these enhanced algorithms, most often referred to as *adaptive particle filters*, which seek to maximize computational efficiency grows with the dimensionality of the state vector being estimated. As such, their study represents the logical next step in applying this methodology to a greater array of geoscience problems.

4.2 Conclusion

The domain of this thesis has been the estimation of latent state variables from dynamic systems through noisy observations, the long-standing filtering problem. As the models relating these noisy observations to hidden quantities of interest have increased in complexity, the need for methods which perform the filtering operation in the absence of restrictive model conditions has arisen. Particle filters have emerged as a computationally efficient means by which to approximate the latent state vectors of dynamic models which may be non-linear and whose corrupting noise processes may be non-Gaussian.

The first publication to come out of this work, [Field et al., 2016], (*i*) introduced the particle filtering approach to a community through its application to one of their own canonical problems and (*ii*) demonstrated the approach's value by successfully applying it to a subproblem with which traditional methods struggle. This thesis has augmented that publication by providing it a more rigorous mathematical primer than what was achievable within the journal's submission restrictions.

Additionally, initial empirical results utilizing algorithmic mechanisms which self-tune the number

of propagated hypotheses were shown to outperform the previously published methodology when the set size is constrained.

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