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STOCHASTIC INVERSION OF 3-D ERT DATA

by

Xianjin Yang

A Dissertation Submitted to the Faculty of the

DEPARTMENT OF MINING AND GEOLOGICAL ENGINEERING

**In Partial Fulfillment of the Requirements
For the Degree of**

**DOCTOR OF PHILOSOPHY
WITH A MAJOR IN GEOLOGICAL AND GEOPHYSICAL ENGINEERING**

In the Graduate College

THE UNIVERSITY OF ARIZONA

1999

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read the dissertation prepared by Xianjin Yang
entitled Stochastic Inversion of 3-D ERT Data

and recommend that it be accepted as fulfilling the dissertation
requirement for the Degree of Doctor of Philosophy

Mary M. Poulton
Mary M. Poulton

12 Nov 99
Date

Douglas Labrecque
Douglas Labrecque

17 Nov 99
Date

Charles E. Glass
Charles E. Glass

12 Nov 1999
Date

Randall Richardson
Randall Richardson

12 Nov 1999
Date

Tian-Chyi Jim Yen
Tian-Chyi Jim Yen

12 Nov 1999
Date

Final approval and acceptance of this dissertation is contingent upon
the candidate's submission of the final copy of the dissertation to the
Graduate College.

I hereby certify that I have read this dissertation prepared under my
direction and recommend that it be accepted as fulfilling the dissertation
requirement.

Mary M. Poulton
Dissertation Director

11/12/99
Date

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ACKNOWLEDGMENTS

I am very grateful to Dr. Doug LaBrecque, my dissertation supervisor, for his guidance and invaluable assistance. He walked me step by step from a graduate student to a professional geophysicist. What impressed me most is Doug's profound knowledge in all aspects of electrical and electromagnetic geophysics. It is really fortunate that I can proceed my career under his guidance for years to come.

I am grateful to Dr. Mary Poulton, my dissertation committee chair, who extended her warm heart and generous hands helping me out of an awkward situation. I really appreciate her time and patience in arrangements of my oral comprehensive exam and oral defense. It is a great loss that I did not learn enough from her about the unique neural network technology.

Dr. Randall M. Richardson introduced me into the field of geophysical inversion in his Inverse Problems in Geophysics class. The thorough understanding of fundamental inverse problems I gained from his class has proved effective in solving this complicated stochastic inverse problem. It is also worth mentioning that the numerical methods taught by Dr. Shlomo P. Neuman in Hydrology department provided me with implementation details and hands-on experiences in numerical algorithm development. From Dr. Jim Yeh I learned that a large group of hydrologists have been attacking stochastic inverse problems using some innovative approaches for years. Many discussions with him greatly improved my understanding of stochastic inverse problems. Equipped with such knowledge, I did not panic when I began this project.

I thank all committee members of mine, Drs. Douglas LaBrecque, Mary Poulton, Charles Glass, Jim Yeh and Randall Richardson, for their suggestions and comments on this dissertation. I would like to thank Elsie Nonaka for her kind help with all paperwork and contacts with my committee members while I did not live in Tucson.

I particularly appreciate my dear wife, Lihong, and my lovely daughters, Kate and Sophia, for their understanding, patience, love, support and encouragement. Without them I do not know how I can put up with these years of bitter life. I am indebted to my parents who have been waiting for me home for a decade. I also thank all bothers and sisters in Tucson Chinese Christian Fellowship where I saw the light of life.

At this moment, I miss all fellow students, Gianfranco Morelli, Ralf Birken, Lin Zhang, Jun Wang, Emily Sullivan, and Melissa Stubben, to name a few, in the then-LASI lab for their friendship and encouragement. They made my life easier while I stayed in Tucson. I particularly thank Melissa Stubben for her careful review of this dissertation. Lee Paprocki in New Mexico Institute of Technology was in charge of ERT data collection at the STVZ site. Her responsibility in this project really impressed me.

This work was performed at Sandia National Laboratories, SteamTech Environmental Services, the University of Arizona, and New Mexico Tech with funding provided by the U.S. Department of Energy's Office of Energy Research, Environmental Science Management Program under Contract #DE-AC04-94AL85000. I am grateful to SteamTech that generously offered me both a full-time position and an opportunity for completion of this dissertation when I was on the verge of giving-up this dissertation.

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ABSTRACT

A new stochastic inverse algorithm for the inversion of three-dimensional (3-D) electrical resistivity tomography (ERT) data has been developed and tested using both synthetic and field data. My stochastic inverse algorithm produced satisfactory inverse solutions that were very similar to those of the commonly used Occam's inversion. The ill-posed 3-D stochastic inverse problems were stabilized by incorporating *a-priori* information in the algorithm in the form of an *a-priori* model, and data and model covariance matrices. There were several novel features in my algorithm. First, a very fast successive over-relaxation (SSOR) preconditioner was implemented in the conjugate-gradient forward solver. Second, a trade-off factor adapted from the Occam's inversion was employed in the algorithm for better control of convergence. Third, the QMRCGSTAB inverse solver, a quasi-minimal residual (QMR) variant of the stabilized bi-conjugate gradient method (Bi-CGSTAB), was used to solve an asymmetric linearized iterative system, so the inversion of a large model covariance matrix was sidestepped. Therefore my algorithm can handle a variable scale of model correlation. Fourth, much better convergence was achieved by using the data standard deviation instead of the data variance as the entries of data covariance matrix. Fifth, a model covariance weighting scheme using the diagonal of the transposed sensitivity matrix times the sensitivity matrix improved the model resolution greatly in the region where is usually poorly resolved.

The run-time of stochastic inversion with a biconjugate-gradient inverse solver doubled that of the Occam's inversion with a conjugate-gradient solver. To speed up the stochastic inversion in in-situ monitoring applications, I developed an efficient difference inversion algorithm to invert the difference between the background and subsequent data sets. The new difference inversion can be two to three times faster than the stochastic inversion.

I also developed a unique cokriging approach to estimate a 3-D moisture content distribution quantitatively from 3-D ERT data and a limited number of neutron-derived moisture content data for an infiltration experiment in Socorro, New Mexico. I found that one neutron well in the center of ERT mesh, where model parameters are usually poorly resolved in ERT inversion, played an indispensable role in cokriging.

1. STOCHASTIC INVERSION

1.1 Introduction

Detailed and accurate knowledge of electrical properties is extremely valuable in characterizing waste sites and monitoring the migration of wastes, remediation processes, and water movement in the vadose zone. The subsurface geological structure is three-dimensional (3-D) in nature. One-dimensional (1-D) or two-dimensional (2-D) approximations often fail to accurately recover features of earth's 3-D structure. The electrical resistivity tomography (ERT) method is a promising 3-D characterization and monitoring technology for environmental applications (Daily and Ramirez, 1993; LaBrecque et al., 1995; LaBrecque et al., 1996a and 1996b; LaBrecque et al., 1998).

The 3-D inversion of a large number of ERT measurements is the core of the ERT method. The number of unknown model parameters in 3-D inverse problems is generally much greater than the number of measurements. This underdetermined nature makes the inverse solution inherently non-unique, meaning that an infinite number of models may generate the same response which best-fits the observed data. Additional constraints, or regularization, must be imposed on the model to single out one optimal solution (Tikhonov and Arsenin, 1977). There are two common approaches to attack this problem: the regularization method and stochastic inversion.

For the regularization method, physical constraints, such as damping and smoothing, are employed as extra information. The most inexpensive way to add constraints is the Marquardt method (Marquardt, 1963; Lines and Treitel, 1984), also known as the damped least squares method. A constant is added to every diagonal term of the inverse operator of a least squares system. The effect of this constant is to prevent unbounded oscillations and to single out one solution which has minimum length (Menke, 1989). The well-accepted regularization method, known as Occam's inversion (Constable et al., 1987; deGroot-Hedlin and Constable, 1990; LaBrecque et al., 1995; Zhang et al., 1996), finds the smoothest possible model whose response best-fits the data to an *a-priori* Chi-squared statistic. The amount of smoothing, however, depends on the interpreter's belief. The true model must be at least as complex as, but never less complex than, the smooth model obtained through Occam's inversion.

Franklin (1970) laid a theoretical foundation for the stochastic inversion, also known as the maximum likelihood inverse method (Mackie and Madden, 1993; Zhang et al., 1995). Franklin's algorithm was later expanded by Jackson (1979), Aki and Richards (1980) and Tarantola (1987). A lack of information and an inability to obtain accurate data result in uncertainties in the description of real-world problems. One may use statistical tools to characterize these uncertainties. The objective of stochastic inversion is to find the solution that maximizes an *a-posteriori* probability density function of model parameters.

In the stochastic framework, data and model parameters are regarded as random fields. Instead of dealing with subjective damping and smoothing factors, as in the regularized inversion, the stochastic inversion algorithm employs less subjective *a-priori* statistical information about measurements and model parameters in the form of an *a-priori* data covariance matrix, *a-priori* model parameter, and an *a-priori* model covariance matrix, etc.. The *a-priori* knowledge is considered true information obtained independently from the measurements. It is expected that the observed data, together with added *a-priori* information, are adequate to stabilize the inversion process and to resolve the model. A statistical tool, such as the maximum-likelihood method, is employed to characterize the stochastic inverse problems.

The application of stochastic inversion was hindered by the difficulty in handling the model covariance matrix. It is a common practice to incorporate a diagonal data covariance matrix into geophysical inversions with the assumption of uncorrelated data errors. The unrealistic assumption of uncorrelated parameters is often made either for mathematical simplicity or because there is little or no information about parameter variability (Bloxham, 1987; Zelt and Smith, 1992; Lutter et al., 1990). The maximum-likelihood inverse algorithm described by Park and Van (1991) could solve only a relatively small inverse problem, with a mesh size of $20 \times 20 \times 10$, due to limited computing capability. Though they realized that the off-diagonal terms of a model covariance matrix could be employed to smooth the model, they sidestepped the difficulties in handling the non-diagonal model covariance matrix. Instead they added a

Marquardt-type damping term in their algorithm for stabilizing the inversion. The diagonal model covariance matrix may be appropriate for small 1-D and 2-D inverse problems. Pilkington and Todoeschuck (1990, 1991, and 1992) introduced scaling noise covariances to approximate the realistic correlation structures of the model. Unfortunately, their studies were also limited to the small-scale 1-D and 2-D problems. The three-dimensional stochastic inverse problem was attacked by Mackie and Madden (1993) for solving magnetotelluric inverse problems and by Zhang et al. (1995) in resistivity tomography. However, they did not give any explicit method for building the model covariance matrix except for a few empirical guidelines.

It is worth mentioning that the stochastic inversion method was favored by hydrologists (Ginn and Cushman, 1990; Gelhar, 1993). Hydrologists and geophysicists have different understandings of the stochastic inversion method due to their different data sampling strategies. Generally speaking, hydrological data sampling is sparse due to its high cost. In hydrological inverse problems, it is difficult to distinguish between the unknown model parameters and observations since all parameters are, more or less, sampled. This makes hydrological inverse problems largely rely on statistical techniques, like kriging and cokriging (Gutjahr and Wilson, 1989; Ahmed and Marsily, 1993), to cope with the limited availability of field measurements and to take advantage of all available data. The kriging method, known as the best linear unbiased estimator, is used to estimate the unknown variables at unsampled locations using weighted linear combinations of the observed values. Cokriging takes advantage of the spatial cross-correlation of two or

more secondary variables, in addition to the auto-correlation of the primary variable itself, to estimate the primary variable at unsampled locations. When parameters estimated using classical cokriging are employed to solve the governing equation (forward modeling), the numerical solutions are generally inconsistent with their observed data at sampling locations (Zhang, 1996). Yeh et al. (1995), Yeh et al. (1996), and Zhang (1996) introduced an iterative stochastic inverse approach to solve the problem of inconsistency.

Compared with hydrological data sampling, geophysical data acquisition is inexpensive. Geophysical-type stochastic inverse algorithms did not follow kriging and cokriging approaches since manipulating auto-covariance and cross-covariance matrices in the 3-D inverse problems is very expensive. Geophysicists generally use a better regularization method such as weighting, damping and smoothing to alleviate the nonuniqueness in an underdetermined inverse problem.

In the stochastic inverse algorithm, there are two occasions where I will use the terminology Gaussian. First, the fundamental assumption of my stochastic inversion is the Gaussian probability density function of observation errors, modelisation (theoretical) errors, and *a-priori* information on model parameters. Second, when model parameters are assumed a second-order stationary stochastic field, the model covariance matrix may be estimated using either a exponential or a Gaussian function. Such

covariance structures are also called the exponential or Gaussian covariance model respectively.

This dissertation consists of three chapters. The first chapter described a novel stochastic inverse algorithm. In chapter two, I compared and contrasted the new stochastic inverse algorithm with the most commonly used Occam's inverse method. In the last chapter, The newly-developed stochastic inverse method was applied to monitor an infiltration experiment in Socorro, New Mexico. A fast difference inversion algorithm based on my stochastic inverse method was developed for in-situ monitoring applications. The electrical conductivity data was converted into 3-D moisture content distribution using a cokriging technique.

In this chapter, I presented a modified 3-D stochastic inverse algorithm. The novel features of my algorithm include: (1) the introduction of a stabilizing factor adapted from Occam's inversion; (2) the use of a bi-conjugate gradient solver to sidestep the difficulty in the inversion of the model covariance matrix; (3) weighting of the model covariance matrix to improve the model sensitivity in the center of 3-D mesh; and (4) kriging of apparent resistivities estimated from raw data for a better a-priori model. The new algorithm was tested using synthetic ERT data in this chapter.

A finite difference forward solution with an SSOR preconditioner was briefly described first. A modified stochastic inverse algorithm was described in Section 1.3. An explicit

definition of data and model covariance matrices was presented in Section 1.4. Some measures to improve the model sensitivity of stochastic inversion and to obtain a better *a-priori* model were discussed in Sections 1.5 and 1.6. The chapter ended with synthetic data tests and some conclusions.

1.2 Forward Solution

The forward modeling solution used in my inverse algorithm was described by LaBrecque et al. (1995). The forward solution can be obtained by solving the partial differential equation:

$$\frac{\partial}{\partial x} \left(\sigma \frac{\partial V}{\partial x} \right) + \frac{\partial}{\partial y} \left(\sigma \frac{\partial V}{\partial y} \right) + \frac{\partial}{\partial z} \left(\sigma \frac{\partial V}{\partial z} \right) = I(x, y, z), \quad (1.1)$$

where V is the scalar electrical potential, and $I(x,y,z)$ is the electric current source term. The finite difference method with an elemental volume (Dey and Morrison, 1979) was used to discretize the partial differential equation (1.1). A mixed boundary condition (Dey and Morrison, 1979) was implemented. The matrix system was iteratively solved by a conjugate gradient method. The implementation details of such an algorithm can be found in Zhang et al. (1995), Spitzer (1995) and Weller et al. (1996).

The major upgrade to the algorithm in LaBrecque et al. (1995) is a symmetric successive over-relaxation (SSOR) preconditioner instead of a diagonal preconditioner

in the conjugate gradient solver. Among the common preconditioners such as diagonal, incomplete Cholesky decomposition and SSOR preconditioners etc., the SSOR preconditioner has proved to be the best choice as far as storage and speed are concerned. The SSOR preconditioner performs especially well for large meshes (Weller et al., 1996, Barrett et al., 1994). The new forward solver with the SSOR preconditioner cuts down the CPU time by a factor of at least 2 comparing with the solver with a diagonal preconditioner.

1.3 Stochastic Inversion Algorithm

1.3.1 Objective function

My stochastic inverse algorithm was an adapted version of Tarantola (1987). For a nonlinear inverse problem, the data vector, $\mathbf{d}$, is a nonlinear function of model parameter vector, $\mathbf{m}$,

$$\mathbf{d} = \mathbf{g}(\mathbf{m}). \quad (1.2)$$

In the stochastic framework, both data and model parameter are regarded as random fields. Based on the assumptions of Gaussian observation errors, Gaussian modelisation (theoretical) errors, and Gaussian *a-priori* information in the model space, the *a-posteriori* probability density function is given by (Tarantola, 1987)

$$\sigma_M(\mathbf{m}) = \text{const} \cdot \exp \left[-\frac{1}{2} \left((\mathbf{d}_{\text{obs}} - \mathbf{g}(\mathbf{m}))^T \mathbf{C}_D^{-1} (\mathbf{d}_{\text{obs}} - \mathbf{g}(\mathbf{m})) + (\mathbf{m} - \mathbf{m}_{\text{prior}})^T \mathbf{C}_M^{-1} (\mathbf{m} - \mathbf{m}_{\text{prior}}) \right) \right] \quad (1.3)$$

where $\mathbf{d}_{\text{obs}}$ is observed data; $\mathbf{m}_{\text{prior}}$ is the *a-priori* information of model parameters; $\mathbf{C}_M$ is the model covariance matrix; and $\mathbf{C}_D = \mathbf{C}_T + \mathbf{C}_d$, which combines the forward modeling (theoretical) uncertainties ($\mathbf{C}_T$) and observational errors ($\mathbf{C}_d$).

Maximizing the modified *a-posteriori* probability density (1.3) is equivalent to minimizing an objective function

$$S(\mathbf{m}) = (\mathbf{d}_{\text{obs}} - \mathbf{g}(\mathbf{m}))^T \mathbf{C}_D^{-1} (\mathbf{d}_{\text{obs}} - \mathbf{g}(\mathbf{m})) + \alpha (\mathbf{m} - \mathbf{m}_{\text{prior}})^T \mathbf{C}_M^{-1} (\mathbf{m} - \mathbf{m}_{\text{prior}}). \quad (1.4)$$

The objective of stochastic inversion is to minimize a weighted data misfit and a weighted solution deviation from the *a-priori* model. My algorithm differs from the conventional stochastic inversion (Tarantola, 1987) in the addition of α as a stabilizing factor that was used to trade off between the data misfit and model deviation. This factor is equivalent to the roughness factor in the Occam's inversion (LaBrecque et al., 1995; Constable et al., 1987; deGroot-Hedlin and Constable, 1990). The factor α should be reduced from iteration to iteration using an empirical expression (LaBrecque et al., 1995).

Though it improves the convergence, the introduction of a varying stabilizing factor α opposes our expectation for the stochastic inversion. The stochastic inversion one expects should have a realistic model covariance matrix, which is extremely difficult to obtain. A second-order stationarity assumption about model parameters, which will be discussed later, greatly simplifies handling with a large model covariance matrix.

When the two covariance matrices above are diagonal, i.e., assuming uncorrelated data errors and uncorrelated model parameters, then the stochastic inversion algorithm is reduced to the weighted damped least squares method (Aki and Richards, 1980), which does not work well with severely-underdetermined 3-D inverse problems.

I use Newton's method (Tarantola, 1987) to minimize the objective function (1.4). Thus I ended up with the following iterative linearized system.

$$(G_n^T C_D^{-1} G_n + \alpha C_M^{-1}) \Delta m_{n+1} = G_n^T C_D^{-1} (g(m_n) - d_{\text{obs}}) + \alpha C_M^{-1} (m_{\text{prior}} - m_n). \quad (1.5)$$

where the sensitivity matrix is $G_n^{\text{ij}} = \left. \frac{\partial g^i(m)}{\partial m^j} \right|_{m_n}$.

This algorithm does not require $\Delta m_{n+1} = (m_{n+1} - m_n)$ to be as small as possible. The inherent requirement is for the total correction $(m_{n+1} - m_{\text{prior}})$ to be as small as possible

(Tarantola and Valette, 1982). This makes the stochastic inversion prior-model dependent.

1.3.2. QMRCGSTAB inverse solver

Since the Hessian matrix $(\mathbf{G}_n^T \mathbf{C}_D^{-1} \mathbf{G}_n + \alpha \cdot \mathbf{C}_M^{-1})$ in equation (1.5) is a symmetric positive definite (SPD) system, one may solve the linearized system (1.5) using a fast iterative solver, such as the conjugate gradient (CG) method (Golub and van Loan, 1996). In a CG iteration, the inverse of model covariance matrix $\mathbf{C}_M$ times a vector can be solved using another CG loop. Thus, finding the inversion of the model covariance matrix can be avoided. However, I observed erratic convergence behaviors with this method. A preconditioner is supposed to stabilize the solution and speed up the convergence, but it is extremely expensive to obtain since it involves the inversion of a large model covariance matrix.

An alternative to avoid calculating the inversion of the model covariance matrix is to solve an asymmetric system using a Bi-CG method after premultiplying $\mathbf{C}_M$ on both sides of the equation (1.5). Thus one arrives at

$$(\mathbf{C}_M \mathbf{G}_n^T \mathbf{C}_D^{-1} \mathbf{G}_n + \alpha \mathbf{I}) \Delta \mathbf{m}_{n+1} = \mathbf{C}_M \mathbf{G}_n^T \mathbf{C}_D^{-1} (\mathbf{d}_{\text{obs}} - \mathbf{g}(\mathbf{m}_n)) + \alpha (\mathbf{m}_{\text{prior}} - \mathbf{m}_n). \quad (1.6)$$

Unlike the conjugate gradient (CG) method in which minimization of a residual norm may be achieved, a Bi-CG method takes another approach, replacing the orthogonal

sequence of residuals by two mutually orthogonal sequences, at the price of no longer providing a minimization. This implies that the algorithm can exhibit a rather irregular convergence behavior with wild oscillations in the residual norm. Freund and Nachtigal (1991) proposed a Bi-CG-like approach, the quasi-minimal residual (QMR) method, which remedies this problem. The QMR iterates are defined by quasi minimization of the residual norm, which leads to smooth convergence curves. Unfortunately, both Bi-CG and QMR methods require computing a transpose matrix-vector product, which is extremely difficult to obtain.

Chan et al. (1994) described an alternative approach QMRCGSTAB, the quasi-minimal residual extension to Bi-CGSTAB (van der Vorst, 1992) with a smooth convergence behavior. Bi-CGSTAB is a fast stable variant of the Bi-CG algorithm with a somewhat irregular convergence behavior. QMRCGSTAB combines the local minimization in Bi-CGSTAB with a global quasi-minimization of the residual norm. QMRCGSTAB was implemented as the inverse solver for the asymmetric linearized system (1.6). Both QMRCGSTAB and Bi-CGSTAB solvers do not require computing a transpose matrix-vector product.

In a bi-conjugate gradient iteration, two mutually orthogonal sequences need to be updated instead of one orthogonal sequence in a CG iteration. Thus, stochastic inversion with a QMRCGSTAB solver approximately doubles the running time required for the widely-used Occam's inversion, which uses a CG solver.

1.4 Data and Model Covariance Matrices

1.4.1 Introduction

The stochastic inversion differs from other regularized methods in how its data and model covariance matrices are defined. For mathematical convenience, both the *a-priori* data and model covariance matrices were often defined as a diagonal matrix (Bloxham, 1987; Lutter et al., 1990; Zelt and Smith, 1992). In this case, the stochastic inversion was reduced to the weighted damped least squares method (Aki and Richards, 1980; Menke, 1989). The assumption of uncorrelated data errors has been a common practice in the geophysical community. The assumption of uncorrelated models may be appropriate for small-scale 1-D and 2-D inverse problems, but it is unacceptable for severely-underdetermined 3-D inverse problems with tens of thousands of unknowns (Jacobsen, 1993).

An alternative to defining the model covariance using scaling noise was described by Pilkington and Todoeschuck (1990, 1991, and 1992). The diagonal covariance matrix corresponds to a white noise model with a flat power spectrum. Scaling noises have the property that if they are resampled at two different intervals, the samples will look alike when their amplitudes are properly rescaled. Scaling noises have a power spectrum S proportional to some power α of the frequency ω , that is, $S = \epsilon^2 |\omega|^\alpha$. If a scaling noise is Gaussian, it can be fully described by just three parameters: the scaling exponent α , mean and variance (ϵ^2) of scaling noise. The *a-priori* model covariance matrix was then

obtained by doing an inverse Fourier transform on the scaling noise spectrum. This approach was tested on a 2-D seismic tomographic problem with a few hundred unknown model parameters only. Broyles (1994) put forward a fractal covariance model to characterize the spatial continuity of a basin's lower surface in handling stochastic inversion of gravity data. No tests on the large grid were reported using this fractal covariance model.

Hydrologists favor the exponential and Gaussian auto-covariance model to characterize the hydraulic conductivity in hydrological stochastic modeling (Gelhar and Axness, 1983; Sun and Yeh, 1992; Dietrich and Newsam, 1993). This has become a routine assumption for most hydrological stochastic modeling algorithms, since *a-priori* data are rarely available.

When I implemented my covariance matrices, I considered the ease of implementation and flexibility in handling various subsurface geoelectrical structures. I followed the approaches in Journel and Huijbregts (1978) and Tarantola (1987) to define my model covariances.

1.4.2 Data covariance matrix

The data covariance matrix, C_D , combines theoretical and observational uncertainties (Tarantola, 1987). Generally, it is assumed that the forward modelization is exact. Then the data covariance represents the observation errors only. The uncorrelated

measurement error assumption has become well-accepted in the geophysical community, which leads to the diagonal data covariance matrix (Park and Van, 1991; Zelt and Smith, 1992; Zhang et al. 1995)

I have two approaches to estimate the standard deviation of data. First, our experience showed that ERT reciprocal measurements provided fairly accurate estimates of data standard deviation. Second, variance of ERT data may be obtained using

$$C_D^i = A^2 + B^2 \cdot d_i^2, \quad (1.7)$$

where C_D^i is the i-th diagonal term of data covariance matrix; d_i is i-th data value; and A and B are the coefficients for the first two even terms of a Taylor's series about d_i (LaBrecque et al., 1996b). A is usually given by a few percent of the smallest data value and may be around the hardware resolution. B is the average percentage of measurement errors and may range from 1% to 10%. Forward modelization uncertainties are neglected in this definition, which may introduce some errors in the inverse process for an inaccurate forward model.

I found that replacing C_D^{-1} with $C_D^{-1/2}$ in equation (1.6) gave a better resolution for stochastic inversion. With this change, the stochastic inversion converges slower than the original version with C_D^{-1} and tends to fit the larger data better than the smaller ones.

1.4.3 Model covariance matrix

The general form of model covariance between two model parameters, X and Y , can be expressed as

$$\text{Cov}(X, Y) = \sigma_X \cdot \sigma_Y \cdot \rho_{XY}, \quad (1.8)$$

where σ_X and σ_Y are the standard deviations of parameters X and Y respectively, and ρ_{XY} is the correlation coefficient between X and Y . This general definition of covariance requires many realizations (or samples) for model parameters X and Y . In reality, only a single realization for some part of model parameters is available. To obtain covariance using (1.8) is realistically impossible. An assumption of the second-order stationarity for model parameters greatly simplifies the definition and manipulation of the model covariance matrix. Under this assumption, the expectation, or mean, of the model parameter exists and does not vary with the location; and for each pair of the model parameters, the covariance exists and depends on the separation distance between two parameters only (Journel and Huijbregts, 1978, p. 32). Therefore, one may use a simple function to estimate the model covariance. I regard the covariance model and covariance function as synonyms below.

Commonly-used stationary covariance models can be found in Tarantola (1987), Journel and Huijbregts (1978), Deutsch and Journel (1998), and Wang (1993). Gaussian,

exponential, and spherical covariance models were implemented in my algorithm. I then define the correlation length as the number of parameters in each direction. The locations of two elements are $m_1(x_1, y_1, z_1)$ and $m_2(x_2, y_2, z_2)$ respectively. σ_{m1} , and σ_{m2} are the corresponding standard deviations of parameters m_1 and m_2 . The normalized separation distance h is given as

$$h = \sqrt{\frac{(x_2 - x_1)^2}{L_x^2} + \frac{(y_2 - y_1)^2}{L_y^2} + \frac{(z_2 - z_1)^2}{L_z^2}}. \quad (1.9)$$

where L_x , L_y , and L_z are the correlation lengths of model parameter fields in x , y , and z directions respectively. The exponential covariance model is described by an exponential function like

$$C(h) = \sigma_{m1} \cdot \sigma_{m2} \cdot \exp(-k \cdot h), \quad (1.10)$$

the Gaussian covariance model is given by

$$C(h) = \sigma_{m1} \cdot \sigma_{m2} \cdot \exp(-k \cdot h^2), \quad (1.11)$$

and the spherical covariance model is given by

$$C(h) = \sigma_{m1} \cdot \sigma_{m2} \left[1 - \frac{3 \cdot h}{2} + \frac{h^3}{2} \right]. \quad (1.12)$$

Figure 1.1 shows how these covariance functions decay. The constant factor, k in equations (1.10) and (1.11), was chosen to be 3, so the covariance, $C(h)$, will approach 0 when the parameter separation in either direction reaches the correlation distance. Note that the exponential function decays faster than the Gaussian function, and the spherical function lies between the exponential and Gaussian functions (Figure 1.1).

The vertical correlation length is usually defined as smaller than the horizontal ones because layering structures are common and ERT has a better resolution in the vertical direction in which ERT wells are oriented. The correlation scales in two horizontal directions are often set equal due to lack of information.

One may obtain the empirical resistivity covariance model and correlation lengths for a site based on any *a-priori* knowledge such as outcrops, geophysical well logs and hydrological data. For an unknown site, the exponential covariance model is always an acceptable assumption. One may also assume that parameters will correlate with its immediate neighbor vertically and with its nearest two or three parameters horizontally.

1.5 Weighting Of Model Covariances

The model sensitivity of 3-D ERT surveys is not uniform in the 3-D volume. The model sensitivity decreases with increasing distance away from the electrodes (Sasaki, 1994). Zhang et al. (1995) showed some similar results. They all noticed that the near-electrode model blocks have a larger sensitivity. Without additional constraints, the inversion of surface resistivity survey data tends to make larger resistivity changes for the near-surface layers, especially for the near-electrode model blocks. The same phenomenon was also observed by Spies and Ellis (1996). They applied a Gaussian-type distance weighting function to accentuate conductivity variations in the center of the interborehole region. Their weighting function tends to suppress conductivity changes near the boreholes and enhance the structure in the central region where the target of the survey is located. I implemented a non-uniform spatial weighting to obtain uniform model sensitivity in a whole 3-D volume by weighting model variances.

1.5.1 Model sensitivity analysis

The diagonals of the transposed sensitivity matrix times the sensitivity matrix weighted by the square root of data covariance, $\text{Diag}(\mathbf{G}^T \mathbf{C}_D^{-1/2} \mathbf{G})$, can be utilized as a model sensitivity measure of ERT surveys. The dipole-dipole array configuration has become a better choice for ERT surveys, since handling pole-pole data is complicated by the introduction of infinity electrodes. The model sensitivity analysis was carried out using a skip-one dipole-dipole array. The skip-one here indicates that the dipole length equals two times the electrode spacing.

The test model is a 10 $\Omega\cdot\text{m}$ rectangular body embedded in a 100 $\Omega\cdot\text{m}$ homogeneous half-space. This model is a simplified version of Figure 1.2, where the four-layered earth is replaced by a 100 $\Omega\cdot\text{m}$ homogeneous half-space without any other alterations in the mesh. Four wells were installed with a well separation of 5.25 meters. There are 13 electrodes in each well with an electrode spacing of 0.762 meters. Four surface electrodes were added to improve the model sensitivity of the near-surface layer. The 3-D volume to be imaged was discretized into $14 \times 14 \times 24$ cells without considering the additional boundary cells.

As high as six orders of dynamic range in $\text{Diag}(\mathbf{G}^T \mathbf{C}_D^{-1/2} \mathbf{G})$ can be observed in Figure 1.3. It is clear that the model blocks near electrodes had a higher model sensitivity. The surface electrodes improved the model sensitivity in the near-surface region. The lower central part of the 3-D volume, where it is farthest away from the electrodes, showed the worst model sensitivity in a 3-D ERT survey. These results reflect the reality of ERT surveys.

1.5.2 Weighting of model covariances

The poor model sensitivity in the center of the imaging volume can be improved by weighting model covariances using the model sensitivity measure, $\text{Diag}\{ \mathbf{G}^T \mathbf{C}_D^{-1/2} \mathbf{G} \}$. I gave more freedom to change to those model parameters that have a poorer model sensitivity by increasing their variances. Following Morelli and LaBrecque (1996) on

the roughness weighting, I used $\text{Diag}\{ \mathbf{G}^T \mathbf{C}_D^{-1/2} \mathbf{G} \}$ as weights on the model parameter standard deviation. Thus:

$$\sigma'_{mi} = \sigma_{mi} \cdot \{ \text{Diag}(\mathbf{G}^T \mathbf{C}_D^{-1/2} \mathbf{G})_i \}^{-n}, \quad i = 1, 2, \dots, M. \quad (1.13)$$

where σ_{mi} is the original standard deviation of i -th model parameter; σ'_{mi} is the model standard deviation after weighting; $\mathbf{G}$ is the sensitivity matrix; $\mathbf{C}_D$ is the diagonal data covariance matrix; Operator $\text{Diag}\{\}$ extracts the diagonal elements of the matrix $\mathbf{G}^T \mathbf{C}_D^{-1/2} \mathbf{G}$; and M is the total number of model parameters. Also, n is an empirical weighting factor that ranges from 0.05 to 0.25.

Figure 1.4 shows the effect of weighting factor n on the ERT inverse solutions with a skip-one dipole-dipole array. The test model was the modified version of Figure 1.2 mentioned in the last section. Note that 3% Gaussian noises were added to the data. An exponential covariance model with correlation lengths of 3, 3, and 1 in x , y , and z directions respectively was assumed. The initial roughness was set to 1000. The 3-D target was recovered better as the weighting factor n was increased from 0.0 to 0.30. Without weights ($n = 0.0$), the 3-D target was barely detectable. A weighting factor, n , larger than 0.25 tends to produce erratic images when noise is present in the data.

1.6 *A-priori* Information

Since stochastic inversion reconstructs the model whose response best fits the observed data and which deviates from an *a-priori* model as little as possible, a poor *a-priori* model may ruin the inversion. A crude estimate of the resistivity of a homogeneous half space based on the regional geology may give a better prior model than a random guess. There are, however, better ways to obtain a more accurate *a-priori* model.

1.6.1 Kriging of apparent resistivities

Generally speaking, one rarely has complete resistivity information throughout the volume, which is the goal of an ERT survey. However, by taking advantage of ERT measurements, one may calculate the apparent resistivity for those model blocks around wells using electrode configurations in the same well with a small separation. Then, the *a-priori* resistivity distribution in the 3-D volume can be estimated by kriging the near-well apparent resistivities using a 3-D kriging method (Deutsch and Journel, 1998). This kriging procedure tends to build a layered *a-priori* model since no apparent resistivity estimates are available inside the volume.

A pole-pole array can usually provide more apparent resistivity data than a dipole-dipole array, so it is preferred by this kriging scheme. For the dipole-dipole array, a good homogeneous *a-priori* model may be obtained by averaging the limited apparent resistivity data.

1.6.2 Hydrological data

The resistivity of soils and rocks is a function of hydraulic properties such as moisture content, porosity, saturation, fluid salinity, etc.. It is possible to convert hydrological data into an *a-priori* resistivity model. The well-accepted empirical relationship that correlates the electrical conductivity of a water-bearing and clay-free rock to its hydraulic properties is Archie's law (1942). The modified general Archie's equation can be represented as

$$\rho_t = \frac{a \cdot \rho_w}{\phi^{-m}} \quad (1.14)$$

where ρ_t is the bulk resistivity of saturated rocks;

ρ_w is the pore fluid resistivity;

ϕ is porosity;

a and m are constants. $a = 0.81$ and $m = 2$ for the Schlumberger equation.

The resistivity of partially-saturated, clay-free sediments in the vadose zone can be estimated from the saturation or moisture content (Doveton, 1982).

$$\rho_t = F \cdot \rho_w \cdot \frac{n^2}{\theta^2} \quad (1.15)$$

where ρ_t is the resistivity of partially-saturated clay-free sediments;

F is the formation factor which is the function of porosity;

ρ_w is the pore fluid resistivity;

n is porosity;

θ is moisture content.

Waxman and Smith (1968) gave a more complicated expression for describing the bulk conductivity of clay-bearing sediments.

$$\sigma_T = \frac{\left[\sigma_w + \left(\frac{Q_v \cdot B}{S} \right) \right]}{F \cdot S^m} \quad (1.16)$$

where

σ_T is the bulk conductivity of the rock,

σ_w is the conductivity of the water,

F is the formation factor,

S is the saturation, the fraction of the pore space saturated with water,

m is the saturation coefficient which is usually assumed to be 2,

Q_v is the number of exchangeable cations in equivalents per liter and

B is the Waxman and Smith factor which is the function of water conductivity.

Hydrological data can be converted into an a-priori resistivity model using an appropriate equation above. One may also calibrate his/her own empirical equation based on the relation above.

1.7 Synthetic Data Test

1.7.1 Test model and inversion settings

A widely used model for testing a 3-D inverse algorithm is a single rectangular body in a homogeneous half-space (Shi et al., 1996; Shi et al., 1998; Zhang et al., 1995; Zhang et al., 1996). In Section 1.5.2, stochastic inversion demonstrated its capability in resolving this type of model. In this section, stochastic inversion will be tested over a more complex geoelectrical model adapted from the Socorro Infiltration Test Site in New Mexico.

The test model consists of a $10\ \Omega\cdot\text{m}$ rectangular body embedded in the second layer of a four-layered earth (Figure 1.2), an adapted version of the Socorro Infiltration Test Site in New Mexico. The top layer of $1000\ \Omega\cdot\text{m}$ corresponds to the near-surface dry sands. The third layer of $10\ \Omega\cdot\text{m}$ is used to simulate a thin clay layer. The rest of two layers with $100\ \Omega\cdot\text{m}$ and $200\ \Omega\cdot\text{m}$ respectively correspond to sandstone at various grain sizes. Four wells were installed with a well separation of 5.25 meters. There are 13 electrodes in each well with an electrode spacing of 0.762 meters. Four surface electrodes were added to improve the model sensitivity of the near-surface layer. The inter-well region

to be imaged was discretized into $14 \times 14 \times 24$ cells, not including the cells outside this region created to satisfy the boundary conditions. The element dimension was $0.375\text{m} \times 0.375\text{m}$ horizontally and 0.381m vertically. The mesh size with boundary elements is $26 \times 26 \times 30 = 20280$ elements. 1484 synthetic data were generated over this model with a skip-one dipole-dipole ERT schedule. 3% Gaussian noise was added into the data.

Several empirical factors must be decided before the stochastic inversion starts. An exponential covariance model with a horizontal correlation scale of 3 elements and a vertical correlation scale of one element was assumed. The model standard deviation was set to unity for all parameters since the stabilizing factor, α , with the initial value of 100, will take over the role of trading-off the data misfit and model deviation. The factor, n , for the model covariance weighting was 0.2. The starting model, also the *a-priori* model, was chosen to be a two-layered model with the top layer being the same as the true model ($1000 \Omega\cdot\text{m}$) and the lower half-space having the resistivity of the second layer ($100 \Omega\cdot\text{m}$) in the true model. The inversion was intended to recover the 3-D conductive body, the thin conductive layer, and the bottom layer. A correct 3% noise estimate was chosen in the inversion. The number of iterations was 10 for the inner QMRCGSTAB loop, and 30 for the outer, nonlinear iteration. The data standard deviation was used as the entries of the data covariance matrix. No data reweighting for data outlier removal was applied. These were the general settings for the synthetic data tests below, unless specified otherwise.

1.7.2 Effects of the data covariance matrix

My experiences revealed that the algorithm using the standard deviations as the entries in the data covariance matrix C_D in equation (1.6) performed better than that using the data variances. However, the data covariance matrix in the objective function always had the data variances in its diagonal entries. Figure 1.5 shows the comparison of these two strategies. The standard deviation algorithm recovered the 3-D conductive body more clearly than that with data variances, but did a poorer job of resolving the thin conductive layer. The variance algorithm converged faster than the standard deviation one, though their squared errors intersected at the 13th iteration (Figure 1.6). Unfortunately, both algorithms failed to resolve the bottom layer where ERT usually has a poor model sensitivity.

The inverse algorithm using the data standard deviation in the data covariance matrix fit the large data better, while the algorithm using the data variance in the data covariance matrix fit the small data better.

1.7.3 Effects of the covariance model

Three covariance models, under the assumption of second-order stationarity, were implemented in the stochastic inverse algorithm. They are the exponential, Gaussian, and spherical covariance models (Figure 1.1). As far as the reconstructed image (Figure 1.7) and convergence (Figure 1.8) were concerned, the exponential model performed best and the spherical model did the worst. The spherical model gave a solution with

more artifacts and demonstrated an oscillating behavior at the early stage. For an unknown site, the exponential covariance model is recommended.

1.7.4 Effects of the *a-priori* model

This test will demonstrate the importance of a-priori knowledge about the model. The assumption of second-order stationarity requires good *a-priori* knowledge about the model. Figure 1.9 shows the inverse solutions from different *a-priori* models that were also used as starting models. An accurate *a-priori* knowledge about the top and second layer was assumed in Figure 1.9a, in which the best reconstruction of the original model was shown. With a fairly resistive *a-priori* model of 500 $\Omega\cdot\text{m}$ (Figures 1.9b), nothing but the top resistive layer was recovered well. The thin conductive layer was reconstructed fairly well with a conductive *a-priori* model of 10 $\Omega\cdot\text{m}$ (Figures 1.9c) or an averaged apparent resistivity of about 91 $\Omega\cdot\text{m}$ (Figure 1.9d). The 3-D conductive rectangular body, however, was shifted upward, and strong artifacts can be seen in the top and bottom layers. The bottom layer was not resolved with either *a-priori* model described above. The convergence of the stochastic inversion with different *a-priori* models was variable from case to case (Figure 1.10). There is no doubt that stochastic inversion is prior model dependent.

1.7.5 Effects of model correlation lengths

The flexible choice of correlation lengths enables the stochastic inversion to handle various geoelectrical structures. The vertical correlation length plays an important role

in the stochastic inversion. No vertical correlation (0 correlation distance) or correlating with the immediate neighbors (one element correlation length) seemed an appropriate choice to recover small 3-D features and thin conductive layers (Figure 1.11). The inversion with a vertical correlation length of 2 elements or larger tends to have a poor model sensitivity in the center of the mesh. The reconstructed conductive layer had a discontinuity in the middle. Horizontal correlation lengths of 2 or 3 elements seemed to perform quite well. Large horizontal correlation lengths tend to introduce more artifacts into the reconstructed image, since the model covariance matrix may become singular (Wang, 1993).

If no *a-priori* knowledge is available, a conservative initial guess about the correlation scale would be the horizontal correlation lengths of 2 or 3 elements for both X and Y directions and a vertical correlation length of 1 element.

1.7.6 Effects of data noises

The real-world data are more or less contaminated by various noises. Inaccurate estimates of the amount of noise in the data will have dramatic effects on the inverse solution (LaBrecque et. al., 1996a). In this synthetic data test, I assumed a perfect knowledge of the percentage of noise in the data. I intend to study how much noise one may add into the data without much distortion of the image.

Smaller than 3% data noise had barely any negative effect on the reconstructed image. With 5% data noise, the recovered 3-D body became smaller, the conductive layer was blurry and less continuous, and more artifacts were shown in the bottom layer (Figure 1.12). The conductive body could not be resolved with 10% noise. Figure 1.13 shows the comparison of convergence with different amounts of noise added into the data.

1.8 Conclusions

Stochastic inversion has proved to be a successful inverse algorithm for 3-D ERT data. Compared with the recently-published maximum likelihood method or stochastic inverse method, my stochastic inverse algorithm had a more general and well-defined covariance model. The inversion of a large model covariance matrix was avoided by using a quasi minimal residual variant of the stabilized biconjugate gradient solvers, QMRCGSTAB. The prior-model dependent feature was alleviated by averaging or kriging the near-well apparent resistivities. The introduction of a stabilizing factor, α , greatly improved the convergence of stochastic inversion. The weighting of model covariance matrix using a model sensitivity measure improved the ERT resolution in the center of 3-D mesh.

The stochastic inversion was supposed to guarantee an appropriate level of regularization independent of the interpreter's judgment and thereby avoid the choice of an arbitrary degree of damping and smoothing. This may remain a dream of geophysicists. The stochastic inversion described in this Chapter was based on the

assumption of second-order stationarity. Empirical factors like covariance model and correlation scale will depend on the interpreter's belief because a-priori data are usually unavailable. For a better convergence I also introduced a stabilizing factor to trade off between the data misfit and model deviation.

The run-time of stochastic inversion approximately doubles that of most commonly used Occam's inversion due to the use of a bi-conjugate gradient inverse solver. This is the major disadvantage of the stochastic inversion method. Major improvements in the future should focus on reducing the run-time of stochastic inversion and investigating model covariance models. The conjugate gradient method may be employed to replace the slow QMRCGSTAB inverse solver. The inversion of the model covariance matrix times a vector may be obtained using an additional conjugate gradient loop with little cost, since model correlation lengths are usually chosen to be not too large. This has already been implemented in my code. Unfortunately, the conjugate gradient solver without any preconditioner tends to diverge. The bottleneck for obtaining a diagonal preconditioner was to approximate the diagonal of the inverse of the model covariance matrix. Simply using the reciprocal of the diagonal of the model covariance matrix did not work.

By the way, the stochastic inversion can be as fast as Occam's inversion if one can develop an explicit statistical measure that is equivalent to the roughness matrix in the

Occam's inverse method and does not involve the matrix inversion like model covariance matrix.

In chapter three, I developed an efficient difference inversion algorithm based on my stochastic inverse method for in-situ monitoring applications. The difference inversion can be much faster than Occam's inversion in some cases.

Figure 1.1. The curve of model covariance functions.

Figure 1.2. A 3-D synthetic model – a 10 ohm-m rectangular body embedded in the second layer of a four-layer earth. The 3-D volume to be imaged was discretized into $14 \times 14 \times 24$ elements. Four surface electrodes were employed for a better near-surface resolution. 13 electrodes were installed in each well.

Figure 1.3. 3-D image of $\text{LOG}_{10} \{ \text{diag} (\mathbf{G}^T \mathbf{C}_D^{-1/2} \mathbf{G}) \}$. The test model is a $10 \Omega \cdot \text{m}$ body in a $100 \Omega \cdot \text{m}$ homogeneous half-space, a modified version of Figure 1.2 without any other changes in the mesh.

Figure 1.4. Effect of weighting factor n on stochastic inverse solution. Plotted are $\log_{10}(\text{resistivity})$ images. The model is a $10 \Omega\cdot\text{m}$ body in a $100 \Omega\cdot\text{m}$ homogeneous half-space. Refer to Figure 1.2 for more details about the model and mesh.

Figure 1.5. Effect of data covariance on stochastic inverse solution. Plotted are $\log_{10}(\text{resistivity})$ images. The stochastic inverse solutions were obtained using (a) data standard deviation and (b) data variance as the entries of data covariance respectively. (c) is the true model.

Figure 1.6. Effect of data covariance on the convergence of stochastic inversion. Comparison was made using data standard deviation and data variance as the entries of data covariance in the stochastic inverse algorithm respectively.

Figure 1.7. Effect of covariance models on stochastic inverse solution. Plotted are $\log_{10}(\text{resistivity})$ images.

Figure 1.8. Effect of covariance model on the convergence of stochastic inversion

Figure 1.9. Effect of *a priori* model on stochastic inverse solution. Plotted are $\log_{10}(\text{resistivity})$ images. The *a priori* models are: (a) a two-layer model with a top layer of $1000 \Omega\cdot\text{m}$ and a bottom layer of $100 \Omega\cdot\text{m}$; (b) a homogeneous model of $500 \Omega\cdot\text{m}$; (c) a homogeneous model of $10 \Omega\cdot\text{m}$; and (d) a homogeneous model of $91 \Omega\cdot\text{m}$ obtained by averaging the apparent resistivities near wells.

Figure 1.10. Effect of *a-priori* model on the convergence of stochastic inversion. The captions in the figure represent the *a priori* model. The average of apparent resistivities is about $91 \Omega \cdot m$.

Figure 1.11. Effect of the correlation length on stochastic inverse solution. Plotted are $\log_{10}(\text{resistivity})$ images. The captions represent the correlation lengths in the unit of number of elements in X, Y, and Z directions respectively.

Figure 1.12. Effect of data noises on stochastic inverse solution. Plotted are $\log_{10}(\text{resistivity})$ images. The captions are the percentage of Gaussian noises added in the data.

Figure 1.13. Effect of data noises on the convergence of stochastic inversion.

2. COMPARISON OF OCCAM'S AND STOCHASTIC INVERSION

2.1 Introduction

The underdetermined nature of 3-D inverse problems makes the inverse solution inherently nonunique. Additional constraints, or regularization, must be imposed on the model to single out one optimal solution (Tikhonov and Arsenin, 1977). Occam's inversion and stochastic inversion are two different strategies to attack the nonuniqueness of the underdetermined inverse problems.

Occam's inversion (Constable et al., 1987; deGroot-Hedlin and Constable, 1990) finds the smoothest possible model whose response best fits the data to an *a-priori* Chi-squared statistic. Occam's inversion, with the conjugate gradient solver, is easy to implement on a PC platform without constructing and storing the sensitivity matrix. Occam's inversion has been widely used in the solution of electromagnetic inversion (Newman and Alumbaugh, 1997), magnetotelluric inversion (deGroot-Hedlin and Constable, 1990), DC resistivity inversion (Zhang et al., 1996), and electrical resistivity tomography (ERT) inversion (LaBrecque et al., 1995).

The stochastic inversion, also called maximum likelihood inversion (Zhang et al., 1995; Mackie and Madden, 1993), was implemented in the stochastic framework (Aki and Richards, 1980; Tarantola, 1987). The *a-priori* information is incorporated into the inversion by defining the *a-priori* model and *a-priori* data and model covariance

matrices. The objective of stochastic inversion is to find the solution that maximizes an *a-posteriori* probability density function of model parameters, which is equivalent to minimizing the weighted data misfit and weighted model deviation from the *a-priori* model.

The early stochastic inverse algorithms were limited to solving simple, small-scale problems, due to the difficulty in handling the model covariance matrix. The assumption of uncorrelated parameters was often made either for mathematical convenience or because little or no information about model variability was available (Bloxham, 1987; Zelt and Smith, 1992; Lutter et al., 1990). Though Park and Van (1991) realized that off-diagonal terms of the model covariance matrix could be employed to smooth the model, they sidestepped the difficulty in handling the non-diagonal model covariance matrix. Pilkington and Todoeschuck (1990, 1991, and 1992) introduced scaling noise covariances for representing the realistic correlation structures of the model. Unfortunately, their studies were also limited to the small-scale 1-D and 2-D problems. The three-dimensional stochastic inverse problem was attacked by Mackie and Madden (1993) for solving magnetotelluric inverse problems and by Zhang et al. (1995) in resistivity tomography. However, they did not give any explicit method for building the model covariance matrix except for a few purely empirical guidelines. No hint was found in the paper about how to avoid inverting the model covariance matrix.

My stochastic inversion method described in Chapter 1 provided an explicit definition of the model covariance matrix. It also adapted a stabilizing factor from Occam's inversion into the algorithm in order to achieve better convergence. The inversion of the model covariance matrix was avoided by using a bi-conjugate gradient solver.

In this chapter I compared and contrasted Occam's inversion with the stochastic inversion developed in Chapter 1. ERT data was used for demonstrations and tests. I began with a summary of the two inverse methods and then proceeded with a comparison of the two inverse algorithms. Numerical checks on both methods were performed. ERT data collected at the Socorro-Tech vadose zone (STVZ) facility in Socorro, New Mexico were used to compare the capability of the two inverse methods in resolving a real-world problem. The chapter ended with some conclusions.

2.2 Occam's Inversion

The Occam's inversion finds the smoothest possible model, which may be geologically unreasonable, whose response fits the data to an *a-priori* Chi-squared statistic. The amount of smoothing, however, depends on the interpreter's belief. The true model must be at least as, but never less complex than, the smooth model obtained through Occam's inversion.

The algorithm listed below was described by LaBrecque et al. (1995) and Morelli and LaBrecque (1996). For a nonlinear inverse problem, the data vector $\mathbf{d}$ is a nonlinear

function of model parameter vector $\mathbf{m}$: $\mathbf{d} = \mathbf{g}(\mathbf{m})$. The objective function of Occam's inversion was given by

$$\mathbf{S}(\mathbf{m}) = (\mathbf{d}_{\text{obs}} - \mathbf{g}(\mathbf{m}))^T \mathbf{C}_D^{-1} (\mathbf{d}_{\text{obs}} - \mathbf{g}(\mathbf{m})) + \alpha \cdot (\mathbf{m} - \mathbf{m}_{\text{prior}})^T \mathbf{R} (\mathbf{m} - \mathbf{m}_{\text{prior}}). \quad (2.1)$$

$\mathbf{C}_D$ is the diagonal data weight matrix. $\mathbf{R}$ is the roughness matrix that is a roughness operator. α is an empirical stabilizing factor which may be reduced from iteration to iteration. $\mathbf{d}_{\text{obs}}$ is the observed data. $\mathbf{m}_{\text{prior}}$ is the prior model which may be set to 0 for no prior knowledge about the model. The nonlinear iteration can be expressed as $\mathbf{m}_{n+1} = \mathbf{m}_n + \Delta \mathbf{m}_n$. The parameter change $\Delta \mathbf{m}_n$ at n-th iteration was obtained by solving

$$(\mathbf{G}_n^T \mathbf{C}_D^{-1} \mathbf{G}_n + \alpha \mathbf{R}) \Delta \mathbf{m}_n = \mathbf{G}_n^T \mathbf{C}_D^{-1} (\mathbf{d}_{\text{obs}} - \mathbf{g}(\mathbf{m}_n)) + \alpha \mathbf{R} (\mathbf{m}_{\text{prior}} - \mathbf{m}_n). \quad (2.2)$$

where the sensitivity matrix $G_n^{ij} = \left. \frac{\partial g^i(\mathbf{m})}{\partial m^j} \right|_{\mathbf{m}_n}$.

The symmetric positive definite (SPD) system (2.2) was solved using the conjugate gradient method with a diagonal preconditioner (LaBrecque et al., 1995; Zhang et al., 1996). A data error reweighting scheme was implemented to suppress the effects of data outliers (Morelli and LaBrecque, 1996). To improve the resolution in the center of the 3-D volume to be imaged, a roughness weighting scheme was incorporated (Morelli and LaBrecque, 1996).

2.3 Stochastic Inversion

In the stochastic framework, data and model parameters are treated as random fields. Instead of dealing with subjective damping and smoothing factors in the Occam's inversion, the stochastic inversion algorithm employs less subjective *a-priori* statistical information about measurements and model parameters in the form of the *a-priori* data covariance matrix, the *a-priori* model parameter vector, and the *a-priori* model covariance matrix. The stochastic inversion guarantees an appropriate level of regularization independent of the interpreter's judgment and, therefore, avoids the choice of an arbitrary degree of damping and smoothing. This has been the goal of geophysicists. Unfortunately, *a-priori* information is not readily available. The stochastic inversion described in Chapter 1 was based on the assumption of second-order stationarity. Empirical factors, like covariance model and correlation scale, will depend on the interpreter's belief because *a-priori* data are usually unavailable. For a better convergence, I also introduced a stabilizing factor to trade off the data misfit and model deviation. The algorithm is summarized as follows. The objective of stochastic inversion was given by

$$S(\mathbf{m}) = (\mathbf{d}_{\text{obs}} - \mathbf{g}(\mathbf{m}))^T \mathbf{C}_D^{-1} (\mathbf{d}_{\text{obs}} - \mathbf{g}(\mathbf{m})) + \alpha \cdot (\mathbf{m} - \mathbf{m}_{\text{prior}})^T \mathbf{C}_M^{-1} (\mathbf{m} - \mathbf{m}_{\text{prior}}). \quad (2.3)$$

$\mathbf{d}_{\text{obs}}$ is observed data. $\mathbf{m}_{\text{prior}}$ is *a-priori* information of model parameters. $\mathbf{C}_D$ is the data covariance matrix. $\mathbf{C}_M$ is the model covariance matrix. α is an empirical trade-off factor

adapted from Occam's inversion. The parameter change vector $\Delta \mathbf{m}_n$ may be obtained by solving the following linearized iterative system below.

$$(\mathbf{C}_M \mathbf{G}_s^T \mathbf{C}_D^{-1} \mathbf{G}_s + \alpha \cdot \mathbf{I}) \Delta \mathbf{m}_s = \mathbf{C}_M \mathbf{G}_s^T \mathbf{C}_D^{-1} (\mathbf{d}_{obs} - \mathbf{g}(\mathbf{m}_s)) + \alpha \cdot (\mathbf{m}_{prior} - \mathbf{m}_s). \quad (2.4)$$

$\Delta \mathbf{m}_n = \mathbf{m}_{n+1} - \mathbf{m}_n$. The unsymmetric system (2.4) can be solved by QMRCGSTAB (Chan et al., 1994). QMRCGSTAB is the quasi-minimal residual (QMR) extension to a stabilized bi-conjugate gradient method (Bi-CGSTAB) with a smooth convergence behavior (van der Vorst, 1992). QMRCGSTAB combines the local minimization in Bi-CGSTAB with a global quasi-minimization of the quasi-minimal residual method.

2.4 Comparison of Algorithms

Wang (1993) showed the intrinsic equivalence between the regularization methods using damping and smoothing constraints, and the stochastic inversion method using covariance matrices as *a-priori* information. In regularization methods, physical constraints like damping and smoothing are implemented as extra information. In stochastic inversions, the *a-priori* information is incorporated into the inversion by defining an *a-priori* model covariance matrix. He also stated that the damping controls the model variance, and relative weights of damping and smoothing control the correlation length. Combining damping with different kinds of smoothing operators is equivalent to defining different covariance functions.

Comparing equations (2.1), (2.2), (2.3) and (2.4), one may notice some amazing similarities between the stochastic inversion and Occam's inversion. From the objective functions (2.1) and (2.3), one may observe that both Occam's and stochastic inversions attempt to minimize the weighted data misfit and some kind of model norm. They both look for some constrained model whose response fits the data. Both algorithms use an empirical trade-off factor, α , between the data error and model norm.

The two inverse algorithms differ mainly in two aspects. First, Occam's inversion uses the model roughness as a constraint, while stochastic inversion deals with the model covariance. This is the major difference between the two inverse algorithms. For mathematical simplicity, model parameters are assumed to be a second-order stationary field in the stochastic inversion. Thus the covariance between two parameters depends on their separation distance only. The assumption of second-order stationarity requires the parameter field to have a constant mean and variance throughout the region of study. This prerequisite can be satisfied only by removing the trend in the parameter field, which is the role of the *a-priori* model. This is why the stochastic inversion is prior model dependent.

Second, the counterpart of the model roughness matrix is the inverse of the model covariance matrix. It is well-known that the roughness matrix has a very simple structure with a few vectors of storage requirement and can be constructed explicitly with little effort. The inversion of the non-diagonal model covariance matrix, however,

is extremely expensive to obtain and store. Unlike Occam's inversion, where the conjugate gradient method is used as the inverse solver, stochastic inversion solves the linearized system using a biconjugate gradient method, thanks to the fast calculation of the model covariance matrix times a vector. Unfortunately, the bi-conjugate gradient solver needs two matrix-vector products per iteration. This makes the bi-conjugate gradient solver double the run-time of the conjugate gradient solver, which requires only one matrix-vector product per iteration.

2.5 Comparison Using Synthetic Data

The synthetic model described in Section 1.7.1 of chapter 1 was reused here without any change. A summary of the model description is as follows. The test model (Figure 1.2) consists of a 10 Ω -m rectangular body embedded in the second layer of a four-layer earth. Four wells are installed to image the volume within the well bounds. The well separation is 5.25 meters. There are 13 electrodes in each well with an electrode spacing of 0.762 meters. Four surface electrodes were added to improve the resolution of the near-surface region. The mesh size with boundary elements is $26 \times 26 \times 30 = 20280$ elements. 1484 synthetic data were generated over this model with a skip-one dipole-dipole ERT schedule. 3% Gaussian noises were added into the data.

Stochastic inversion control factors were the same as those stated in Section 1.7.1 of chapter 1. An exponential covariance model, with correlation lengths of 3 elements, 3 elements, and 1 element in the X, Y and Z directions respectively, was assumed. The

model standard deviation was set to unity for all parameters. The factor, n , for the model covariance weighting was 0.2. The initial roughness factor was set to 100. The *a-priori* model was chosen to be a two-layer model with a top layer of 1000 $\Omega\cdot\text{m}$ and a second layer of 100 $\Omega\cdot\text{m}$. The inverse process was supposed to recover the 3-D conductive body, the thin conductive layer, and the bottom layer. A 3% known noise estimate was chosen in the inversion. The number of iterations was 10 for the inner, QMRGSTAB loop, and 20 for the outer, nonlinear iteration. The data standard deviation was used for the entries of the data covariance matrix. No data reweighting for data outlier removal was applied to any inversion.

The Occam's inversion settings differ in a few places. In Occam's inversion I manipulated the model roughness instead of the model covariance and correlation in the stochastic inversion. The initial roughness factor was set to 10. The weight factor of roughness in the vertical (Z) direction was 0.03, which imposes no vertical correlation on the model.

Both Occam's inversion and stochastic inversion recovered the conductive body and thin conductive layer very well (Figure 2.1). Both inverse methods did a poor job in reconstructing the bottom layer. Occam's inversion had a better resolution for the thin horizontal conductive layer than the stochastic inversion. Occam's inversion also converged slightly faster than stochastic inversion (Figure 2.2). The stochastic inversion image had more artifacts, especially in the bottom layer.

2.6 Comparison Using Socorro Infiltration Data

The Socorro-Tech vadose zone (STVZ) facility is located on the New Mexico Institute of Technology campus, Socorro, New Mexico. The field test site was built to validate a hybrid hydrological-geophysical inverse technique for recovering in-situ estimates of vadose zone hydraulic properties. The site was installed in relatively unconsolidated heterogeneous fluvial deposits consisting of gravel, sand, and clays of fairly high hydraulic permeability. The near-surface layer, above 2 meters, consists of dry sands and pebbles. There is a clay layer at a depth of 5 to 6 meters. The rest of the site consists of fine sands with variable contents of clay and iron oxides.

Figure 2.3 shows the top view of the ERT survey setup. The dimension of the site is 10.5 meters (between Wells G and B) by 10.5 meters (between Wells B and E) with PVC cased subsurface access tubes emplaced to a maximum depth of 13 meters. The inner square, consisting of four ERT wells (A, D, K and H), is 6 meters by 6 meters. The innermost square of 3 meters by 3 meters is the infiltrometer made of a matrix of medical needles. There are 17 electrodes with a separation of 0.762 meter (30 inches) in each physical well. A total of 36 surface electrodes were installed to improve near surface resolution. All electrodes were grouped into 15 electrodes per cable since the hardware can handle only 15 electrodes per cable (Figure 2.3). ERT data collected using the inner four wells (Wells A, D, H, and K) and four surface electrodes (C3, F3, I3, and L3) were employed to compare Occam's and stochastic inversions.

The infiltration experiment using the Socorro tap water started on March 11, 1999, referred as to Day 0 hereafter. The flux of infiltration was 2.7 cm/day over a surface of 3 meters by 3 meters. An ERT data set collected on February 16, 1999, about four weeks before the infiltration, was used to characterize the background geoelectrical properties of the site. ERT data were collected everyday, except the days when the hardware broke down, starting March 12, 1999, referred as to Day 1 hereafter. The percent difference of electrical conductivity between the pre-infiltration and post-infiltration data can be calculated from inverted images for monitoring the movement of the wetting front.

The background electrical conductivity structures are shown in Figure 2.4. Logarithmic conductivity was plotted in units of milli-Siemens/meter. The value 2.0 in the color scale corresponds to $10 \Omega\cdot\text{m}$, and 0.0 corresponds to $1000 \Omega\cdot\text{m}$. Both inversion technologies revealed that the near surface dry sands are very resistive with a resistivity of greater than $1000 \Omega\cdot\text{m}$, and the resistivity of the lower half-space of sands ranges from $10 \Omega\cdot\text{m}$ to a few hundred $\Omega\cdot\text{m}$ depending on the grain size of the sands. Occam's inversion demonstrated clearer layering structures. Both inverse methods detected a discontinuous clay layer around a depth of 5 to 6 meters. The resistive anomalies in the lower half-space shown in both images may be inversion artifacts.

Six data sets were chosen and plotted in a logarithmic scale based on the availability of data. These data sets were collected on Day 1, Day 2, Day 5, Day 12, Day 28, and Day

51 respectively. For better visual effects, the percent differences of electrical conductivity were plotted. The 3-D images obtained from Occam's inversions are shown in Figure 2.5. Figure 2.6 is the 3-D images reconstructed by stochastic inversions. The downward movement of the wetting front was faster at the early stage. Then water spread horizontally and started ponding when less permeable barriers were encountered. The volume of the percent difference anomaly from Occam's inversion seemed larger than that from stochastic inversion. This resulted from a relatively small weight factor ($n = 0.1$) over the model covariance in the stochastic inversion compared with the weight factor ($n = 0.2$) over the roughness in Occam's inversion. Both inversion techniques had similar artifacts in the images.

2.7 Conclusions

Occam's inversion and stochastic inversion attack the underdetermined inverse problems from somewhat different perspectives and achieved almost the same goal. These two inverse techniques showed to some extent some intrinsic equivalence. Both methods recovered a synthetic model fairly well. Both Occam's and stochastic inversions were effective in in-situ monitoring of the water movement in the vadose zone.

Compared with the well-accepted Occam's inversion, stochastic inversion still leaves some improvements to be desired. Better covariance models may suppress the artifacts in the stochastic inversion. Implementation of a conjugate gradient inverse solver with a

diagonal preconditioner could make stochastic inversion as fast as Occam's inversion. The difference inversion method described in the next chapter produced less artifacts and was 2 to 3 times faster than the stochastic inversion described in chapter one.

Figure 2.1. Comparison of Occam's inversion and stochastic inversion using a synthetic model. Plotted are $\log_{10}(\text{resistivity})$ images.

Figure 2.2. Comparison of convergence between Occam's inversion and stochastic inversion.

Figure 2.3. A plan-view schematic of the ERT setup at the Socorro-Tech Vadose Zone (STVZ) facility.

Figure 2.4. Background electrical conductivity images using four inner wells at the STVZ site. Plotted are $\text{LOG}_{10}(1000\text{-conductivity})$ images from Occam's inversion and stochastic inversion. 2.0 in the color scale corresponds to $10 \Omega\cdot\text{m}$, and 0.0 corresponds to $1000 \Omega\cdot\text{m}$.

Figure 2.5. The percent difference of electrical conductivity showing wetting front movement at the STVZ site obtained using 3-D Occam's inversion.

Figure 2.6. The percent difference of electrical conductivity showing wetting front movement at the STVZ site obtained using 3-D stochastic inversion.

3. INFILTRATION MONITORING USING STOCHASTIC INVERSION OF 3-D ERT DATA

3.1 Introduction

In order to effectively contain or remediate contamination within the vadose zone, images of the 3-D in-situ moisture content distribution and 3-D monitoring techniques are needed. Hydrological instruments like the neutron probe provide detailed vertical measurements within the vicinity of the borehole but provide little lateral information. The flow properties between the probes are often estimated by certain interpolation or extrapolation methods, such as the kriging technique. This often leads to a poor lateral resolution, since hydrological probes are often installed in vertical boreholes. Cross-borehole ground penetrating radar (XBGPR) can provide detailed knowledge about the in-situ moisture content for the cross-borehole region (Paprocki and Alumbaugh, 1999). However, XBGPR is usually limited to the characterization of a two-dimensional (2-D) cross-section, since the technique is labor-intensive. The fast and cost-effective electrical resistivity tomography (ERT) method has been widely used for three-dimensional (3-D) in-situ monitoring (Daily and Ramirez, 1993; LaBrecque et al., 1995; LaBrecque et al., 1996a and 1996b; LaBrecque et al., 1998).

The application of ERT to monitoring water movement in a vadose zone is an important part of an on-going interdisciplinary research project to develop a hybrid hydrologic-geophysical inverse technique (HHGIT) for vadose zone characterization. The Socorro-

Tech vadose zone facility was set up on the New Mexico Institute of Mining and Technology campus, Socorro, New Mexico. ERT was the only tool installed at the site for three-dimensional characterization of the development of the wetted bulb.

The difference between the background and later electrical resistivity data sets in an in-situ monitoring ERT experiment was usually plotted to visualize the change of a target (Bevc and Morrison, 1991; Park, 1998; Stubben and LaBrecque, 1998a and 1998b; LaBrecque et al., 1998). The resistivity difference image may qualitatively demonstrate the temporal changes of moisture content in an infiltration experiment. But, the exact moisture content distribution still remains unknown. LaBrecque et al. (1999) proposed a local and empirical quantitative relationship to estimate the moisture content from electrical resistivity. Two power law relations were presented for pre-infiltration and post-infiltration conversions from electrical conductivity to moisture content. The converted moisture content from ERT data was not guaranteed to agree with any in-situ moisture content measurements. In this chapter, I propose an innovative approach to estimating 3-D moisture content distribution by cokriging 3-D electrical conductivity and a limited number of neutron-derived moisture content measurements.

Stochastic inversion, described in chapter 1, took more than 80 hours on a Pentium II 400MHz PC for the inversion of a complete dipole-dipole ERT data set collected at the STVZ site. Occam's inversion took about 45 hours for an inversion with the same setup. Both inverse methods are not efficient for a model with more than 60,000 unknowns

and 20,000 data points. In this chapter, I presented a fast difference inverse algorithm for use of ERT data for in-situ monitoring applications. Instead of doing an inversion of electric potential data, my difference inversion algorithm inverts the difference between the background data and the subsequent data sets with the background model as the *a-priori* model.

This chapter focused on the estimation of 3-D moisture content distribution from electrical conductivity and neutron-derived moisture content using a cokriging technique. In Section 3.2, I described a water infiltration experiment in Socorro, New Mexico. Next, a difference inversion algorithm based on my stochastic inversion method was presented. Qualitative monitoring of water movement using the percent changes of electrical conductivity was demonstrated in Section 3.4. In Section 3.5, I gave a brief introduction to the cokriging method and presented the results of cokriging estimates. The effect of the number of neutron wells used for the cokriging was investigated to determine the optimum results for the least input. Section 3.6 compared and contrasted some different approaches to obtain the moisture content. Section 3.7 summarized the accomplishments in this chapter.

3.2 Experiment Description

The Socorro-Tech vadose zone (STVZ) facility was built on a southeast trending ridge bounded by drainages to the north and the south. The deposits of the site exhibit contrasting textures and sedimentary structures typical of similar deposits found in

various DOE sites in the west. The test site was installed in relatively unconsolidated heterogeneous fluvial deposits consisting of gravel, sand, and clays of fairly high hydraulic permeability. The near-surface layer, above 2 meters, consists of dry sands and pebbles. There is a clay layer at a depth of 5 to 6 meters. The rest of the site consists of fine sands with variable contents of clay and iron oxides.

A plan-view schematic of the site showing the locations of various instruments is given in Figure 3.1. Dense arrays of hydrologic probes such as time-domain reflectometer (TDR) probes and tensiometers, along with arrays of surface and subsurface ERT electrodes were installed at the STVZ site. Operation of TDR interferes with ERT data collection, so no TDR data were collected after infiltration began. XBGPR surveys and neutron probe measurements were achieved through the PVC access tubes. This provides the capability to construct 3-D images of the subsurface electrical conductivity, from which estimates of the subsurface geology, temporal moisture content distributions, and wetted bulb development can be derived.

The objective of the infiltration was to provide data to validate the HHGIT as a method for recovering in-situ estimates of subsurface hydraulic parameters. The innermost square shown in Figure 3.1 is the infiltrometer made of a matrix of 900 18-gauge medical needles. Infiltration began on March 11, 1999 at 12:05PM with a constant flux to a 3m by 3m infiltration surface at a rate of 2.7 cm/day. Above the infiltrometer a no-flow surface boundary condition was guaranteed by overlaying the whole site with an

impermeable tarp to eliminate both evaporation and precipitation. ERT, neutron probe, and tensiometer data have been collected frequently during early infiltration times to obtain as high of temporal resolution of the wetted bulb as possible, while GPR data have been collected slightly less frequently due to the acquisition time and labor that is necessary.

The neutron probe was the major moisture content measuring device installed at the site since TDR data were not collected due to the method's interference with ERT. The neutron probe is a geophysical logging tool based on neutron thermalization, an interaction between high-energy neutrons and hydrogen atoms. The direct measurement of a neutron probe is the count of thermal neutrons, which is converted into moisture content by a calibration curve. The sample size, the radius of influence sphere of neutrons, ranges from 8 centimeters to 35 centimeters depending on the moisture content of the medium (Stephens, 1996). The sources of error inherent with neutron probe measurements include the probabilistic nature of the neutron thermalization process, the nonlinearity of the calibration, soil heterogeneity and mineralogy, borehole diameter and casing materials, and so on.

Neutron probe data may be collected in the 13 boreholes throughout the site at a depth from 0.50m to 11.75m with a sampling interval of 0.25m. The borehole separation varies irregularly from 2.2m to 5.3m. At the initial stage of infiltration, neutron probe data were collected only in the five inner boreholes. As water spread out, more and

more boreholes were included. The moisture content measured by neutron probes will be cokriged with electrical conductivities for 3-D moisture content distribution at the site.

High-resolution XBGPR data were taken only along a single southwest–northeast transect due to the method's labor-intensive nature. Estimation of moisture content from GPR data is becoming a standard practice (Greaves et al., 1996; Hubbard et al., 1997; Eppstein and Dougherty, 1998; Paprocki and Alumbaugh, 1999). This conversion is a two-step approach. First, the electromagnetic wave velocity image is converted into a dielectric constant distribution image after GPR data reduction. Second, the moisture content can be estimated from the dielectric constant using an empirical Topp's equation (Topp, 1980).

Figure 2.3 shows the plan view of the ERT survey setup. There are a total of 8 vertical electrode arrays (VEAs) and 36 surface electrodes that were bundled into four cables (C, F, I and L). Four inner wells, or VEAs (A, D, H and K), were installed for monitoring the initial infiltration. This should save a lot of time in data collection and processing. Once the water spreads out of the bounds of the inner wells, four outer wells (B, E, G, and J) together with the four inner wells were designed for monitoring the water movement through the whole site. Both inner wells and outer wells were installed at the corners of a square. The well separation is 10.5 meters between wells B and G and 6 meters between wells A and D. There were seventeen electrodes in each well with

an electrode spacing of 0.762 meter (2.5 feet). Although the ERT VEAs can be emplaced via cone penetrometer (CPT), the method of emplacement was with a drill rig at the STVT site.

The inner dipole-dipole ERT data were collected everyday for 75 days, except for the period of ERT system breakdown from March 24 to April 7, 1999. As of April 8, inner dipole-dipole data were taken every other day. Another longer period of system breakdown happened from June 25 to July 21, 1999. The complete dipole-dipole data set, using all wells and electrodes, was collected once a week. It takes approximately 9 hours to collect one complete dipole-dipole ERT data set with about 40,000 measurements, one half of which are reciprocal measurements for the observation error check. Some sets of pole-pole data were taken as backups without further processing, since the introduction of infinity electrodes complicates the inverse problem and increases the CPU time for inversion greatly.

3.3 Difference Inversion Algorithm

The dramatic temporal change of electrical resistivities and potential differences in in-situ monitoring is usually uncommon. The background electrical conductivity obtained by standard inversion can be inputted as the *a-priori* model in the stochastic inversion. To achieve the same level of data fit, the background ERT data may be inputted as a reference. This leads to an innovative difference inversion strategy. There are several advantages to this new approach. First, convergence is much faster than a full inversion

without any *a-priori* knowledge, since the inverse process needs to find small perturbations about a good *a-priori* model. It is expected that this method will cut down the CPU time for difference inversion by a factor two to four compared with standard stochastic inversion. Second, systematic errors, such as those due to errors in the field configuration and the discretization error in the forward modeling algorithm, tend to cancel. The result is that I can fit the difference data far more closely than the individual potentials. Better data fits often equate to better resolution with fewer inversion artifacts.

For a nonlinear inverse problem, the data $\mathbf{d}$ is a nonlinear function of model parameters $\mathbf{m}$, $\mathbf{d} = \mathbf{g}(\mathbf{m})$. The data error to be minimized is given by

$$\Delta \mathbf{D} = (\mathbf{d}_{\text{obs}} - \mathbf{d}_{\text{obs}}^0) - [\mathbf{g}(\mathbf{m}) - \mathbf{g}(\mathbf{m}^0)] = [\mathbf{d}_{\text{obs}} - \mathbf{g}(\mathbf{m})] - [\mathbf{d}_{\text{obs}}^0 - \mathbf{g}(\mathbf{m}^0)]. \quad (3.1)$$

$\mathbf{d}_{\text{obs}}$ is the observed data vector. $\mathbf{d}_{\text{obs}}^0$ is the known background data vector. $\mathbf{m}^0$ is the known background model which is inputted as the *a-priori* model. Now data misfit has two parts. The first part is the same as the data misfit in standard Occam's and stochastic inversions described in last two chapters. The second part is the background data misfit, introduced as a correction term. The difference inversion is expected to achieve the same level of data fit as the background inversion with a model structure characterized by the model covariance matrix. The objective of difference inversion in the stochastic framework becomes

$$S(\mathbf{m}) = \Delta \mathbf{D}^T \mathbf{C}_D^{-1} \Delta \mathbf{D} + \alpha \cdot (\mathbf{m} - \mathbf{m}^0)^T \mathbf{C}_M^{-1} (\mathbf{m} - \mathbf{m}^0). \quad (3.2)$$

$\mathbf{C}_D$ is the data covariance matrix. $\mathbf{C}_M$ is the model parameter covariance matrix. α is a trade-off factor adapted from Occam's inversion. One may notice that the constraint on the model parameter in the objective function remains the same as in the standard stochastic inversion described in last two chapters. After minimization by Newton's method, one ends up with the following linearized iterative algorithm.

$$(\mathbf{C}_M \mathbf{G}_s^T \mathbf{C}_D^{-1} \mathbf{G}_s + \alpha \cdot \mathbf{I}) \Delta \mathbf{m}_s = \mathbf{C}_M \mathbf{G}_s^T \mathbf{C}_D^{-1} \Delta \mathbf{D} + \alpha \cdot (\mathbf{m}^0 - \mathbf{m}_s). \quad (3.3)$$

$\Delta \mathbf{m}_n = \mathbf{m}_{n+1} - \mathbf{m}_n$. Equation (3.3) is almost the same as equations (1.6) or (2.4) except for a different expression for $\Delta \mathbf{D}$. The asymmetric system (3.3) can be solved using QMRCGSTAB (Chan et al., 1994). QMRCGSTAB is the quasi-minimal residual extension to Bi-CGSTAB (van der Vorst, 1992) with smooth convergence behavior. QMRCGSTAB combines the local minimization in Bi-CGSTAB with a global quasi-minimization.

3.4 Percent Difference of Electrical Conductivity

The fast and cost-effective ERT method was the only high-resolution three-dimensional monitoring tool installed at the STVZ site. The 10.5m $\times$ 10.5m site was discretized into $28 \times 28 \times 34 = 26,656$ cells with a cell size of 0.375m $\times$ 0.375m $\times$ 0.381m. The mesh of

the inverse model, including boundary elements, consists of $40 \times 40 \times 39 = 62,400$ elements. The total number of electrical potential measurements is around 20,000 in a complete dipole-dipole data set.

A number of ERT data sets were taken before the infiltration began on March 11, 1999. A complete dipole-dipole data set collected on February 16, 1999, 23 days before infiltration, was chosen to reconstruct the background electrical conductivity model using standard stochastic inversion described in Chapter 1. The post-infiltration data were inverted using the fast, newly-developed, difference inverse algorithm.

For the standard stochastic inversion of background data, a 5% data noise was assumed. An exponential covariance model with a horizontal correlation length of 3 elements and no vertical correlation was used in the inversion. The trade-off factor, $\alpha = 10$, gave a satisfactory convergence and data fit. The factor n in equation (1.13) was set to 0.1. It took 87 hours 21 minutes and 17 iterations for the weighted data misfit to converge to the number of data. Occam's inversion took 45 hours 36 minutes to achieve the same level of data fit. One may notice that the run-time of stochastic inversion almost doubled that of Occam's inversion.

The inverted background resistivity model shows a strongly layered subsurface structure (Figure 3.2). A very resistive near-surface layer of 2 meters depth with a resistivity higher than $1000 \Omega\cdot\text{m}$ corresponds to the near-surface dry sands and gravels. A series of

thin conductive layers above 6 meters indicates the existence of thin clay layers or sand layers with a high content of iron oxides. There is also a conductive layer at the bottom of the image, with a resistivity lower than $100\ \Omega\cdot\text{m}$, corresponding to sand layers with a high content of iron oxides according to the core logs. The rest of site, consisting of fine sands, has a resistivity of a few hundred ohm-m. The resistivity of the site ranges from a few ohm-m to a few thousand ohm-m with three orders of contrast of the electrical property. Compared with an infiltration site at the Maricopa Agricultural Center located in Maricopa, Arizona (Stubben and LaBrecque, 1998), where the background resistivity ranged from $10\ \Omega\cdot\text{m}$ to $100\ \Omega\cdot\text{m}$ with only one order of contrast, the resistivity contrast at the STVZ site is very large. This poses great difficulties in the ERT data inversion and later cokriging processing due to severe non-linearity and non-stationarity.

The post-infiltration data sets were collected daily at the early stage, and weekly afterwards. The wetting fronts usually move fairly fast at the early stage in an infiltration experiment. Water downward movement becomes slower and slower later. I chose five data sets to demonstrate the development of the wetted bulb based on both the availability of data and an approximate temporal logarithmic scale. More data sets taken at the early stage were chosen. These data sets were collected during the 1st week (March 12), the 2nd week (March 20), the 6th week (April 15), the 11th week (May 18), and the 20th week (July 22).

Compared with the percent change of electrical resistivity, the percent change of electrical conductivity produces a larger anomaly in a case where the electrical conductivity tends to go up, for example, a water infiltration experiment in the vadose zone. In an opposite case like air-sparging in a water-saturated zone, where resistivity is most likely to increase, the percent change of resistivity gives a better visual effect. For example, a resistivity decrease from 200 $\Omega\cdot\text{m}$ to 100 $\Omega\cdot\text{m}$ will produce a 50% anomaly of resistivity change, but will give a 100% anomaly of conductivity change for the same case. I use the percent change of electrical conductivity for demonstration of water movement in the vadose zone.

Post-infiltration data were inverted using difference inversion described in the last section. The inversion control factors were kept the same as those in the background inversion except for the assumed level of data noise, since a data error correction term from the background data was introduced in the difference inverse algorithm (Equation 3.1). Instead of setting a 5% data error in the background data inversion using standard stochastic inversion, I employed a 4% data error estimate in the difference inversion. This will definitely increase the CPU time of difference inversion compared with a 5% error approximation.

It took only 24 hours for the inversion of data collected on March 12, one day after infiltration. This is a decrease in CPU time by a factor of 3.6 compared with more than 87 hours for standard stochastic inversion of background data. As the later data sets

differ more and more from the background data set, the difference inversion took longer to fit the data. For the July 22 data set, difference inversion took 46 hours to converge.

The percent difference images of electrical conductivity in a 3-D view are shown in Figure 3.3. A 30% cutoff for volume rendering was employed for image construction. The development of the wetted bulb can be seen clearly from the difference images. Though plot bounds of percent change are limited from -80% to 80%, the real maximum percent change was as high as 2426%.

The depth of wetting fronts can be estimated from the percent change images of electrical conductivity. The moisture content changes estimated from neutron probe measurements in the central neutron well, neutron well #1 in Figure 3.1, were shown in Figure 3.4. If I set the depth of wetting fronts at 1% moisture content change, the wetting front in the central neutron well was at a depth of about 0.9m on March 12, 3.2m on March 20, 6.2m on April 15, 6.8m on May 18, and 8.3m on July 22. These depths of the wetting front in the central neutron well can be identified from the percent difference of electrical conductivity. It is also clear that water movement was downwards and skewed toward the west (Figure 3.3).

The percent difference images of electrical conductivity provide a clear picture about water movement in the vadose zone. But, they are not convenient for hydrologists to incorporate them into their modeling. The final goal of this ongoing project is to

develop a joint hydrological-geophysical inverse technique by taking advantage of over-sampled ERT data. One feasible way to convert electrical conductivity into moisture content is to cokrige the neutron probe measurements and electrical conductivities.

3.5 Moisture Content Estimation Using Cokriging

Moisture content at the STVZ site, measured with neutron probes, was sampled in a sparse grid with a horizontal spacing of more than 3 meters through PVC-access boreholes. Cross-borehole ground penetrating radar (XBGPR) gives better resolution in moisture content estimation than ERT data, but was sampled only along a single southwest-northeast transect at the site. Neither neutron probe nor XBGPR data can provide a detailed three-dimensional picture of subsurface moisture distribution. ERT data were inverted over a dense grid with a cell size of $0.375\text{m} \times 0.375\text{m} \times 0.381\text{m}$. There has been no well-established relationship to convert electrical conductivity into moisture content. ERT data alone can only provide a qualitative interpretation about subsurface water movement. This makes an ideal case for the application of the cokriging technique to estimate under-sampled moisture content, from the over-sampled secondary variable – electrical conductivity.

3.5.1 Variogram Modeling

Spatial variability information about moisture content and electrical conductivity is required for cokriging estimation. The auto-correlation of an individual variable and cross-correlation between two variables can be obtained through variogram analysis.

Unlike the covariance and correlation functions, which are measures of the similarity of data, the variogram $\gamma(h)$ measures the average dissimilarity between data separated by a vector h . The variogram is defined as half the average squared difference between the components of every data pair:

$$\gamma(h) = \frac{1}{2N} \sum_{i=1}^N [z(x_i) - z(x_i + h)]^2, \quad (3.4)$$

where the random variable (RV) Z has N pairs of data which are a distance h apart. $z(x)$ is the realization of Z . The variogram function is also called a semi-variogram because of the factor $1/2$ in (3.4). Definition (3.4) is referred to as variogram hereafter. Note that an intrinsic hypothesis was assumed for (3.4). A random function $Z(x)$ is said to be intrinsic when: (1) its mean exists and does not vary with location; and (2) for all vectors h the difference $[Z(x+h) - Z(x)]$ has a finite variance which does not depend on the location x . The intrinsic hypothesis can be seen as the limitation of the second-order stationarity to the difference random function $[Z(x) - Z(x+h)]$ (Journel and Huijbregts, 1978, p.33). The major difference between the intrinsic hypothesis and second-order stationarity is that the intrinsic hypothesis requires that the variogram exists but second-order stationarity requires that the covariance exists with a finite *a-priori* variance. Equation (3.4) can be used to estimate the cross-variogram when one changes $z(x+h)$ into the realization or sample value of another variable. For more details about

variogram analysis, refer to Journel and Huijbregts (1978), and Isaaks and Srivastava (1989).

A 3-D variogram program, named gamv in Deutsch and Journel (1998), was used to compute the 3-D auto-variogram for neutron-derived moisture content and electrical conductivity inverted from ERT data, and the cross-variogram between neutron probe moisture content and electrical conductivity. Since the relationship between the moisture content and electrical conductivity follows an empirical power law (LaBrecque et al., 1999), I used the logarithm of the percentage of moisture content and the logarithm of electrical conductivity in milli-Siemens/meter in the variogram analysis in order to linearize the relation between them.

The moisture content from April 15 and electrical conductivity from April 13 were chosen for variogram modeling. Moisture content changes in a two-day period were small 32 days after the infiltration began. It is hoped that the partially-wet ground on April 13, 1999 was not too dry and not too wet. Thus the variogram models on April 13 should be representative throughout the infiltration period. The control parameter file for the variogram analysis is documented below.

Parameters for GAMV

START OF PARAMETERS:

apr15.in

\data file

1 2 3	\column for x,y, z coordinates
2 4 5	\nvar; column numbers...
-1.0e21 1.0e21	\tmin, tmax (trimming limits)
apr15v.out	\output file for variograms
10	\nlag - the number of lags
2.0	\xlag - unit separation distance
1.0	\xltol- lag tolerance
3	\ndir - number of directions
0.0 45.0 5.0 0.0 30.0 3.0	\azm,atol,bandwh,dip,dtol,bandwd
90.0 45.0 5.0 0.0 30.0 3.0	\azm,atol,bandwh,dip,dtol,bandwd
0.0 45.0 5.0 90.0 30.0 3.0	\azm,atol,bandwh,dip,dtol,bandwd
0	\standardize sill? (0=no, 1=yes)
3	\number of variograms
1 1 1	\tail, head, variogram type
1 2 2	\tail, head, cross-variogram
2 2 1	\tail, head, variogram type

Note that the number of lags is 10 with a lag distance of 2m and a lag tolerance of 1m. One may notice that 3-D variograms in the x, y and z directions are estimated. The half-window azimuth tolerance is 45° and the half-window of dip tolerance is 30°. The azimuth bandwidth is 5m and the dip bandwidth is 3m. The auto-variogram of moisture content, auto-variogram of conductivity, and cross-variogram between moisture content

and conductivity in the x , y and z directions are calculated respectively. Refer to Deutsch and Journel (1998, p.53) for more details about the meaning of these control parameters.

All sample variograms were fit fairly well by a Gaussian model with a horizontal (X and Y) range of 4m and a vertical (Z) range of 2m (Figure 3.5). This agrees with the layering subsurface structure of the site. It is necessary to point out that the variogram model fitting is not unique. The conductivity sample variogram may fit an exponential model better. I employed a Gaussian model for approximation in order to take advantage of the linear model of coregionalization implemented in the cokriging algorithm (Deutsch and Journel, 1998).

3.5.2 Cokriging

Kriging is a generalized linear regression technique that provides a minimum-variance unbiased linear estimator of the unknown characteristic studied. The kriging method is usually used to estimate the attribute value at unsampled locations using weighted linear combinations of the observed values. Kriging retains the observed data at the sample locations. Fundamentals of various kriging methods can be found in Journel and Huijbregts (1978), Isaaks and Srivastava (1989), Goovaerts (1997), and Deutsch and Journel (1998).

Cokriging takes advantage of the spatial cross-correlation of two or more variables, in addition to the auto-correlation of the individual variable itself, to estimate the primary variable at unsampled locations. Cokriging is particularly useful when the primary variable, for example moisture content from neutron probes at the Socorro site, is undersampled. More discussions on cokriging can be found in Journel and Huijbregts (1978), Isaaks and Srivastava (1989), Goovaerts (1997), and Deutsch and Journel (1998).

Consider a simplest cokriging case with only two variables: moisture content as the primary variable and electrical conductivity as the secondary variable. Given m samples of moisture content, θ , with a stationary mean of m_θ and n samples of electrical conductivity, σ , with a stationary mean of m_σ , the cokriging estimate of moisture content at an unsampled location can be expressed as

$$\hat{\theta}_0 - m_\theta = \sum_{i=1}^m \alpha_i [\theta_i - m_\theta] + \sum_{j=1}^n \beta_j [\sigma_j - m_\sigma]. \quad (3.5)$$

The $n + m$ cokriging weights α and β are determined so as to ensure unbiasedness and minimum error variance. For simple cokriging, local means m_θ and m_σ are assumed constant and known *a-priori*, but there is no constraint on the weights. Ordinary cokriging accounts for local variations of the means by limiting the domain of stationarity of both the primary and secondary means, which are unknown, to the local

neighborhood. The unknown means are filtered from the linear estimator by setting constraints on the weights. For traditional ordinary cokriging, the weights applied to the primary variable sum to unity (1), and the weights applied to any other variable sum to zero (0). For more details about cokriging, refer to Journel and Huijbregts (1978), Isaaks and Srivastava (1989), and Goovaerts (1997).

A 3-D cokriging program named cokb3d in Deutsch and Journel (1998) was used to estimate the 3-D moisture distribution in a dense grid by cokriging a limited number of neutron probe moisture contents and over-sampled electrical conductivities inverted from ERT data. The variogram modeling results from the last section served as the cokriging control parameters. Listed below is the cokriging input parameter file.

Parameters for COKB3D

START OF PARAMETERS:

mar12.in	\input data file
2	\number of variables primary+other
1 2 3 4 5	\columns for X,Y,Z and variables
-1.0e21 1.0e21	\trimming limits
0	\co-located cokriging? (0=no, 1=yes)
somedata.dat	\file with gridded covariate
4	\column for covariate
1	\debugging level: 0,1,2,3

cokb3d.dbg	\file for debugging output
mar12s.out	\file for output
28 -5.063 0.375	\nx,xmn,xsiz
28 -5.063 0.375	\ny,ymn,ysiz
34 0.1905 0.381	\nz,zmn,zsiz
1 1 1	\x, y, and z block discret
1 8 16	\min, max primary, max secondary
2.0 2.0 1.0	\maximum search radii: primary
2.0 2.0 1.0	\maximum search radii: all secondary
0.0 0.0 0.0	\angles for search ellipsoid
0	\kriging type (0=SK, 1=OK, 2=OK-trad)
0.6278 0.6434	\mean(i),i=1,nvar
1 1	\semivariogram for "i" and "j"
1 0.001	\nst, nugget effect
3 0.055 0.0 0.0 0.0	\it,cc,ang1,ang2,ang3
4.0 4.0 2.0	\a_hmax, a_hmin, a_vert
1 2	\semivariogram for "i" and "j"
1 0.0	\nst, nugget effect
3 0.043 0.0 0.0 0.0	\it,cc,ang1,ang2,ang3
4.0 4.0 2.0	\a_hmax, a_hmin, a_vert
2 2	\semivariogram for "i" and "j"
1 0.08	\nst, nugget effect

```

3  0.15  0.0  0.0  0.0          \it,cc,ang1,ang2,ang3
4.0 4.0  2.0          \a_hmax, a_hmin, a_vert

```

The cokriging mesh is the same as that of conductivity: $28 \times 28 \times 34$ with the cell size of $0.375\text{m} \times 0.375\text{m} \times 0.381\text{m}$. I used the simple cokriging method for 3-D moisture content estimation. The disadvantage of simple cokriging is that it requires that both variables have a stationary mean throughout the mesh. Ordinary cokriging was expected to work better in this case with a high contrast in conductivity. Unfortunately, my tests did not give satisfactory results. The variogram structure derived in the last section (Figure 3.5) is the critical input here. For a thorough understanding of the parameters listed above, consult the GSLIB user's guide (Deutsch and Journel, 1998, p.100)

The search radius for both variables is 2m in the horizontal direction and 1m in the vertical direction. I found that the search radius used in the cokriging to be critical in the moisture content estimates. For points in the mesh closer than one search radius to a neutron well, the neutron data dominated the estimate of moisture content, and electrical conductivity data were largely ignored.

3.5.3 Results and discussions

A large amount of neutron probe data is usually not available in practical applications, while densely-sampled ERT data can be obtained relatively readily. I tested a few cases with a different number of neutron probe wells to see the importance of neutron probe

data on the cokriging estimates. There are a total of 13 neutron probe wells installed at the site. One central well is numbered as #1. Four inner wells are numbered from #2 to #5, and four outer wells are numbered from #6 to #9. The additional 4 wells outside the cokriging mesh are #10 through #13. Refer to Figure 3.1 for the neutron well numbering scheme.

3.5.3.1 2-D Images of moisture content

Figure 3.6 shows the cokriging estimates of moisture content with neutron probe data superimposed on it. The comparison was made along a southwest-northeast transect extracted from the 3-D cokriging output using three data sets: the pre-infiltration background data set, data taken 9 days after infiltration, and data taken 33 days after infiltration. The temporal moisture content changes and the effect of the number of neutron wells can be seen from these images. I attempted to find out how many neutron wells were needed for cokriging to obtain a realistic moisture content distribution.

The moisture content data from the central neutron well played an indispensable role in cokriging estimates of moisture content. Cokriging using over-sampled conductivity and moisture content from a single central neutron well provided an acceptable 3-D estimate of moisture content throughout the site. The cokriging estimates using a single central neutron well agreed fairly well with the estimates using all 13 neutron wells. ERT data produced a satisfactory estimate of moisture content at the locations where neutron data were not available. There is no doubt that the more neutron data I used for cokriging,

the better estimate of moisture content I would expect. Cokriging with the data from all 13 neutron wells gave the best moisture content estimates.

ERT has the worst resolution along the transect shown in Figure 3.6, especially in the center of the transect, since no ERT wells are even close to the transect. Cokriging estimates without the central neutron well data but with the data from the four outer wells did a poor job below the infiltrometer where the greatest moisture content changes took place. This does not imply that ERT is not sensitive to moisture content change, since I already demonstrated above that the percent change of electrical conductivity successfully monitored the development of the wetted bulb.

The fundamental assumption in the simple cokriging is the intrinsic hypothesis that requires both neutron and electrical conductivity data to have a stationary mean throughout the site. The sharp contrast in conductivity in the site indicates a non-stationary conductivity field. The severe non-linearity between neutron data and electrical conductivity ruined some cokriging results, especially in the top resistive layer.

I attempted cokriging using percent change of conductivity and relative change of neutron moisture content. Unfortunately I ended up with erratic auto- and cross-variograms. I also made an effort to divide the conductivity field into a top resistive

zone above 2m and a bottom relatively conductive zone. But, I did not have enough neutron data to come up with appropriate variogram models.

Though some unfavorable results were presented above, I showed that cokriging is still a feasible approach to estimate moisture content from conductivity and neutron data. Cokriging is particularly useful in the case where the background electrical conductivity contrast is not too strong.

3.5.3.2 3-D Moisture content changes

ERT is a 3-D characterization tool. The 3-D electrical conductivity field was transformed into 3-D moisture content distribution by cokriging. Figure 3.7 shows the 3-D background moisture content distribution cokriged using a single central neutron well and all 13 neutron wells. It can be seen that there were few differences between the two images of background moisture content. This implies that a single neutron well in the center of the ERT configuration may be adequate for ERT to provide a 3-D moisture content distribution via cokriging.

Before going further, I must make clear the definitions of some nomenclatures that will be used below. The volumetric moisture content is dimensionless. It is expressed either as a fraction or as a percentage. When I talk about percent change of moisture content, it is really confusing. So, I use the term absolute change to express the mathematical difference between the post-infiltration moisture content and the pre-infiltration one.

The term relative change is the same as percent change of conductivity, given by the absolute change divided by the preinfiltration moisture content.

Absolute changes in moisture content after infiltration were pretty small. According to neutron-derived moisture content estimates, the average absolute change of moisture content was around 2 ~ 3%. Figure 3.8 shows 3-D volume rendering images with a 1% threshold. It is obvious that neutron data dominated the difference images. With a 2% threshold the volume images would leave only a few small drops of “water”. The horizontal water spreading in the top layer clearly showing on the percent difference images of conductivity (Figure 3.3) did not exist in the absolute change images. Because the top layer was too dry and resistive, a large increase in conductivity did not result in a large increase in moisture content due to the severe nonlinear behavior between the two.

When I plotted the relative changes of moisture content, the images appear to be more realistic (Figure 3.9). The effect of dramatic changes of electrical conductivity can be seen from the relative changes of cokriged moisture content. Images produced using a single central neutron-well restored the resolution of ERT and were bounded with the neutron data. The images generated with all 13 neutron-wells seem overly sensitive to the neutron data. An artifact at a depth of about 12m was more evidence of noisy neutron data.

The neutron probes are usually less accurate at very low or very high moisture content. The STVZ site is very dry with an average moisture content of 5% ~ 7%. Stephen (1996) also stated that the PVC casing I used tends to absorb the slow neutrons, thus lowering the accuracy of the neutron probes.

3.6 Comparison of Estimation Methods of Moisture Content

In this section, I are going to compare five approaches for moisture content estimation. The first approach is a quasi-direct moisture logging tool – neutron measurements, which is the most accurate technique I installed at the STVZ site. The second tool is XBGPR, which is an indirect moisture measurement technique. XBGPR data may be converted into moisture content by a two-step process (LaBrecque et al., 1999; Paprocki and Alumbaugh, 1999). LaBrecque et al. (1999) proposed an empirical power relationship between the moisture content and electrical conductivity. In the third and fourth approaches I will use their power law relation to derive moisture content from electrical conductivity obtained from Occam's and stochastic inversions respectively. The fifth approach is the cokriging method derived above.

The power law relationship described in LaBrecque et al. (1999) had some errors. The correct power law relationship is of the form

$$\theta = a \cdot \rho_t^{-b} \quad (3.6)$$

where ρ_t is the resistivity of partially-saturated sediments; θ is moisture content; and a and b are empirical constants determined by comparing resistivity values to neutron derived moisture contents. I have found good comparisons between ERT and Neutron data using $a = 0.3$ and $b = 0.31$. The changes in resistivity caused by increased moisture content during infiltration also follow a power law relationship (Equation 3.6). Using laboratory studies of resistivity versus saturation for core samples from the site, I chose a value of $b = 0.66$. Using this value of b and the background values of moisture content and resistivity (determined using the background constants in Equation 3.6), I can solve Equation (3.6) for a different value of the constant, a , for each element of the inverse mesh.

The comparison was made along the XBGPR' transect due to availability of GPR data. All ERT-derived moisture contents along the XBGPR' transect were extracted either from the 3-D cokriging output or from 3-D power law conversion.

It is beyond doubt that cokriging using neutron data in all 13 wells provided the best estimate among the five approaches (Figure 3.10). Neutron data alone can only characterize moisture content changes around boreholes. Cokriging of neutron and ERT data produced moisture content estimates over a much denser grid while retaining neutron-derived moisture contents at measurement locations.

XBGPR-derived moisture contents agreed very well with neutron measurements. In the sense of moisture content measurements, GPR and neutron probes shared an identical physical basis, i.e., water content versus dielectric constant. It is also noted that GPR and neutron probes had co-located measurements by sharing the same boreholes and the same depth reference. These all guaranteed a good match between moisture contents derived from the two data sets.

Moisture contents converted using the empirical power law relationship show overall a good agreement with the neutron-derived moisture contents. LaBrecque et al. (1999) listed a few reasons explaining why ERT-derived moisture contents had a relatively poor fit to the neutron-derived ones. A large electrode separation and poor resolution along the imaging transect, due to no ERT well being present, most likely caused less accurate estimates of moisture content. As stated above, the severe non-linearity between the moisture content and electrical conductivity probably smeared the results of a simple conversion using the power law relationship.

Stochastic inversion did not resolve the region directly below the infiltrometer very well. The inappropriate *a-priori* model tended to force the inverse process toward the wrong direction due to the nonuniqueness of underdetermined inverse problems.

3.7 Conclusions

Stochastic inversion was successfully applied to monitoring a water infiltration experiment at the Socorro-Tech Vadose Zone (STVZ) facility, New Mexico. A new difference inverse algorithm was two to three times faster than standard stochastic inversion. The percent changes of electrical conductivity provided a qualitative view for monitoring the development of wetted bulb during the infiltration.

Under the assumption of a power law relationship between conductivity and moisture content, the logarithm of conductivity and logarithm of moisture content can be approximated by a linear model. The auto-variogram and cross-variogram of these two transformed variables were all fit to a Gaussian variogram model with a 4m horizontal range and a 2m vertical range. Therefore, a linear model of coregionalization was employed in cokriging for interpolation.

Cokriging results indicated that 3-D electrical conductivity data together with neutron-derived moisture contents provided an excellent estimate of the 3-D moisture content distribution. The effect of the number of neutron wells used for the cokriging was investigated to determine the optimum results for the least input. We found that a neutron well in the center of ERT mesh where no VEA exists played an indispensable role in cokriging estimates. The center neutron well along with the ERT data provided a fairly good result for limited amount of data used. The results suggests that cokriging of

ERT and neutron data is a fast and effective technique for obtaining the 3-D in-situ moisture content distribution and for 3-D monitoring of an advancing wetting front.

The relative changes of moisture content estimated from simple cokriging demonstrated better resolution to show the development of the wetted bulb than the absolute changes.

Compared with GPR-derived moisture contents, ERT-derived moisture contents using an empirical power law had a relatively poor agreement with neutron-derived moisture contents. The high contrast of the electrical conductivity field at the STVZ site posed great difficulties for the 3-D inversion of ERT data and conversion of conductivity into moisture content and cokriging of neutron and conductivity data. These techniques will produce more favorable results at a less heterogeneous site.

- Two-Nested Tensiometer Locations. Each hole has two instrument clusters consisting of a tensiometer, a suction lysimeter, and a TDR probe from top to bottom. The clusters are about 3.5 and 6 meters below the ground surface.
- Four-Nested Tensiometer Locations. The tensiometer porous cups are about 2, 4, 6, and 8 meters below the ground surface. A TDR probe is installed at the bottom of each hole with a suction lysimeter immediately above. The TDR probe/suction lysimeter pair is located just below deepest tensiometer porous cup.
- Infiltrometer tensiometers nested at 0.5 and 1.0 meter below the surface.
- PVC Cased Wells used for collecting neutron and GPR data.
- ERT vertical electrode arrays (VEAs).

Figure 3.1. A plan-view schematic of the STVZ site showing the locations various instruments. The innermost square of 3 meters by 3 meters is the infiltrometer made of a matrix of medical needles. The dotted line along the southwest-northeast direction is the 2-D XBGPR imaging plane.

Figure 3.2. Background electrical conductivity image of the STVZ site. The distance unit in the figure is meters. Plotted is $\log_{10}(\text{conductivity})$ image with the conductivity unit of mS/m. 2.0 corresponds to $10 \Omega\cdot\text{m}$ and 0.0 to $1000 \Omega\cdot\text{m}$.

Figure 3.3. Percent change of electrical conductivity at the STVZ site. The cut-off for the volume rendering is 30%. Refer to Figure 2.3 for ERT well locations.

Figure 3.4. Absolute change of moisture content in the central neutron well at the STVZ site. The background neutron measurements were taken on February 5, 1999, about five weeks before infiltration.

Figure 3.5a. Variogram analysis and model fitting of neutron moisture content data. The dotted line is sample variogram, and the solid line is a best-fit Gaussian model.

Figure 3.5b. Variogram analysis and model fitting of electrical conductivity data. The dotted line is sample variogram, and the solid line is a best-fit Gaussian model.

Figure 3.5c. Cross-variogram analysis and model fitting of neutron moisture content and electrical conductivity data. The dotted line is sample variogram, and the solid line is a best-fit Gaussian model.

Figure 3.6a. Cokriging estimates of background moisture content along a southwest-northeast transect at the STVZ site. ERT data were collected on Feb. 16, 1999, while neutron data on Feb. 5, 1999. Captions show the data from which neutron wells are used in cokriging. Refer to Figure 3.1 for neutron well numbering scheme and well locations. Central well is well #1. Four outer wells are numbered from #6 to #9.

Figure 3.6b. Cokriging estimates of moisture content along a southwest-northeast transect at the STVZ site on March 20, 1999. Neutron data were taken on March 18. Captions show the data from which neutron wells are used in cokriging. Refer to Figure 3.1 for neutron well numbering scheme and well locations. Central well is well #1. Four outer wells are numbered from #6 to #9.

Figure 3.6c. Cokriging estimates of moisture content along a southwest-northeast transect at the STVZ site on April 13, 1999. Neutron data were taken on April 15. Captions show the data from which neutron wells are used in cokriging. Refer to Figure 3.1 for neutron well numbering scheme and well locations. Central well is well #1. Four outer wells are numbered from #6 to #9.

Figure 3.7. 3-D background moisture content estimated by cokriging electrical conductivity and neutron-derived moisture contents from a single central neutron well and all 13 neutron wells respectively.

Figure 3.8. Absolute changes of moisture content estimated by simple cokriging.

Figure 3.10. Relative changes of moisture content estimated by simple cokriging.

Figure 3.10a. Comparison of background moisture content obtained from five different approaches along a southwest-northeast transect at the STVZ site. Neutron moisture content data are superimposed in columns on the images. In ERT – cokriging approach all 13 neutron well data were used.

Figure 3.10b. Comparison of moisture content obtained from five different approaches along a southwest-northeast transect at the STVZ site using data taken on March 20, 1999. Neutron moisture content data are superimposed in columns on the images. In ERT – cokriging approach all 13 neutron well data were used.

Figure 3.10c. Comparison of moisture content obtained from five different approaches along a southwest-northeast transect at the STVZ site using data taken on April 13, 1999. Neutron moisture content data are superimposed in columns on the images. In ERT – cokriging approach all 13 neutron well data were used.

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