WATER RESOURCES RESEARCH, VOL. 34, NO. 8, PAGES 2077–2079, AUGUST 1998

Comment on "Minimum relative entropy inversion: Theory and application to recovering the release history of a groundwater contaminant" by Allan D. Woodbury and Tadeusz J. Ulrych

Z. J. Kabala
Department of Civil and Environmental Engineering, Duke University, Durham, North Carolina

Todd H. Skaggs
U.S. Salinity Laboratory, Riverside, California

1. Introduction

In our paper [*Skaggs and Kabala*, 1994] we posed the problem of recovering the release history of a groundwater contaminant plume that evolves for some time before it is discovered and its spatial distribution measured. This problem often arises in assigning liabilities for cleanup of an aquifer contaminated by a number of parties. We pointed out that this is an ill-posed problem and obtained an approximate solution via Tikhonov regularization (TR), using *Provencher*'s [1982] *F* distribution criterion to select the regularization strength. Later, we developed an algorithm based on the concept of quasi-reversibility and obtained another approximate solution to the same problem [*Skaggs and Kabala*, 1995]. Each methodology has its own limitations. Since we believe the more tools that are available to the hydrologist the better, we welcome the related paper by *Woodbury and Ulrych* [1996], who developed two variants of the minimum relative entropy (MRE) algorithm, one with presmoothing and one without, and applied them to the problem we posed. Both MRE methods appear to be powerful probabilistic approaches to linear inversion. However, in applying the methods to the problem of recovering a contaminant release history, *Woodbury and Ulrych* [1996] did not mention the fundamental characteristic of the problem at hand, its ill-posedness, and made a number of vague statements that could mislead the reader about the uniqueness, nature, and uncertainty of MRE and TR solutions. In addition, *Woodbury and Ulrych* [1996] made incorrect statements about the structure of measurement errors and its effect on regularized solutions. They did not recognize that in general it is not possible to assign conventional confidence intervals to a solution of an ill-posed problem and in particular to a recovered contaminant release history. Finally, *Woodbury and Ulrych* [1996] used flawed procedures in their comparison of the MRE and TR solutions and therefore reached conclusions that are unsupported by the evidence they presented. We take this opportunity to clarify these issues.

2. The Nature and Uniqueness of the Solutions

Woodbury and Ulrych [1996, p. 2676] state

> ... Skaggs and Kabala's solution is "regularized" or smoothed in some sense and is only one solution out of an infinite number possible for this problem. Our solution is different in that it represents a unique average obtained from the pdf which in the context of MRE is the most probable...

The authors clearly indicate a special status for their solution by claiming the MRE solution is "different" from the TR solution that "is only one ... out of an infinite number possible." However, this statement can be interpreted in more than one way. The reader may infer that *Woodbury and Ulrych* [1996] are claiming nonuniqueness is associated with the TR methodology and not with the MRE approach. This is wrong. The nonuniqueness of the solution is caused by the ill-posed nature of the physical problem and is not associated with any particular solution methodology, nor can nonuniqueness be eliminated with any particular procedure.

An alternative interpretation is that *Woodbury and Ulrych* [1996] are claiming the MRE procedure selects a solution in an objective and unambiguous way, whereas the TR procedure is ambiguous due to the need to select a value for the regularization parameter. Again, this is wrong, and wrong on two counts. First, our TR solution is obtained unambiguously by letting *Provencher*'s [1982] *F* distribution criterion determine the regularization strength. Second, it is the MRE procedure that requires as input a subjective prior estimate of the release history and, if presmoothing is used, a subjective level of smoothing of the measured data. The Tikhonov regularization approach, on the contrary, requires no subjective inputs.

In summary, *Woodbury and Ulrych*'s [1996] MRE solutions to the ill-posed problem of identifying the contaminant release history do not and cannot resolve the inherent nonuniqueness. In general, a unique solution to the problem does not exist.

3. Measurement Error Structure and Its Effect on the Solution

Woodbury and Ulrych [1996, p. 2675] state that they "have discovered some inconsistencies in the treatment of noise in Skaggs and Kabala's work," which they later (p. 2677) clarify

> Notice that (26) of *Skaggs and Kabala* [1994], namely,
>
> $$C^*(x_n, t) = C(x_n, t) + \varepsilon\delta_n C(x_n, t)$$
>
> produces noise that has a skewed distribution in that the noise level is now a percentage of the measurement value at that point. Skaggs and Kabala used Tikhonov regularization, which requires that random measurement error and the expected value of the errors to be zero. Therefore we are uncertain with what impact the skew as noted above affected Skaggs and Kabala's results.

Finally, they conclude (p. 2680) that

Paper number 98WR01337.
0043-1397/98/98WR-01337$09.00

For noisy data we find that our model for observation noise produces pseudo-random measurement error. The approach adopted by *Skaggs and Kabala* [1994] to produce noisy data does not.

As noted by *Macdonald* [1995], the two simplest error structures are additive (normally distributed, uncorrelated, zero mean, constant variance) and multiplicative (according to (26) cited above). *Woodbury and Ulrych* [1996] used the simpler additive errors, whereas we [*Skaggs and Kabala*, 1994] used multiplicative errors. We agree that the multiplicative form creates plume measurement errors that are not normally distributed, but we disagree with *Woodbury and Ulrych*'s [1996] dismissal of this error model. In fact, one could argue that the multiplicative model is closer to reality. Consider that analytical methods for measuring chemical concentrations frequently require diluting samples of high concentration. If the analytical technique introduces a normally distributed, additive measurement error, the plume measurement errors will exhibit the skewed distribution of the multiplicative model because the analytical errors will be multiplied by the concentration-dependent dilution index. However, if some samples require dilution and some do not, the measurement errors will then have a stochastic structure that is more complicated than either the additive or multiplicative models.

Of course, errors can arise in a number of places, and one might be tempted to invoke the central limit theorem to argue that the net effect of all errors can be represented as a normally distributed additive error. However, this argument is undermined by the fact that synthetic data sets created with additive errors are simply unrealistic, as generated measurements near the edges of the sampling grid do not tend toward zero and are frequently negative. Common sense dictates that if we are measuring a plume's spatial distribution for purposes of recovering a contaminant release history, we should continue taking measurements until we are confident our sampling grid encompasses the full extent of the plume, that is, until measurements at the edges of our grid are consistently near zero. When synthetic data sets are created with additive errors, measurements near the edges of the sampling grid are characterized by physically nonsensical negative concentrations and significantly large positive concentrations (neither of which are precluded by the multiplicative form, but both are much less likely). An example of such an unrealistic data set can be seen in Figure 13 of *Woodbury and Ulrych* [1996]. Given this data set, it is unlikely that anyone would conclude that the full extent of the plume had been sampled (or that anyone would continue to retain the services of a chemist who reports such large negative concentrations). In addition, negative concentrations are inconsistent with the convection-dispersion equation used by both *Woodbury and Ulrych* [1996] and *Skaggs and Kabala* [1994], and are inconsistent with nonnegativity constraints imposed in both works.

Although *Woodbury and Ulrych* [1996, p. 2677] are incorrect in claiming Tikhonov regularization "requires that random measurement error and the expected value of the errors to be zero"; what they probably meant was Tikhonov regularization requires errors that are normally distributed with a zero mean. If this is the case, they are partially correct. Tikhonov regularization makes no assumptions about the structure of measurement errors, and thus the multiplicative form of error is consistent with the method. However, the F distribution criterion we used to obtain a value for the regularization parameter, α, does implicitly assume errors are normally distributed with zero mean, but as *Provencher* [1982] notes "slight deviations from normality are not nearly as critical as unaccounted for systematic errors or presmoothed data." Our experience indicates the F distribution criterion is robust and that results are similar when obtained using comparably sized multiplicative or additive errors. If one knows beforehand that measurement errors are multiplicative, this information can be incorporated into the Tikhonov regularization method by appropriately weighting the data [see, e.g., *Provencher*, 1982]. However, it seems unlikely that a hydrologist would know with certainty that measurement errors are strictly multiplicative. We note that for real measurement errors, which are not normally distributed, the MRE methodology faces exactly the same dilemma that *Woodbury and Ulrych* [1996] found for Tikhonov regularization.

In summary, contrary to statements made by *Woodbury and Ulrych* [1996], both additive and multiplicative models can be used to generate measurement errors, although the additive form used by *Woodbury and Ulrych* [1996] tends to create unrealistic data sets that are inconsistent with physically based transport models and with the nonnegativity constraints of the Tikhonov regularization methodology used by *Skaggs and Kabala* [1994] and the MRE methodology used by *Woodbury and Ulrych* [1996]. It is unlikely that true plume measurement errors follow a simple form, and consequently any technique that relies heavily on the assumption of a simple error structure is of lesser value.

4. Confidence Intervals

Woodbury and Ulrych [1996, p. 2671] write

In this paper we show that given prior information in terms of a lower and upper bound, a prior bias, and constraints in terms of measured data, minimum relative entropy (MRE) yields exact expressions for the posterior probability density function (pdf) and the expected value of the linear inverse problem. In addition, we are able to produce any desired confidence intervals.

Later, they elaborate on how to interpret a particular 90% confidence interval in terms a recovered contaminant release history [*Woodbury and Ulrych* 1996, p. 2676]: "Therefore there is an 90% probability that the "true" source function will lie within this range by chance." *Woodbury and Ulrych*'s [1996] use of the term confidence interval is misleading in the context of solving this ill-posed problem. The reason is that on average, the true contaminant release history does not need to be contained in *Woodbury and Ulrych*'s [1996] "90%-confidence interval" in 90% of their MRE applications, contrary to their statement. In fact, their 90%-confidence intervals may on average contain the true release history in an arbitrarily small fraction of cases. The same is true about confidence intervals associated with Tikhonov regularization or any other solution methodology for an ill-posed problem. This becomes clear when one considers recovering the contaminant release history from measurements of a highly dispersed plume, one measured long enough after the release to have its details dispersed beyond detection level. A simple thought experiment demonstrates this point. Assume we have a source function consisting of two narrow pulses of equal strength released one shortly after another. Initially, the plume will evolve with two peaks, but after sufficient time the two peaks will coalesce and the plume will look, within measurement error, as though it was created by a single-peak release. Suppose for a given evolution time we generate a series of plume measurement data sets, each with a different realization of measurement error, and solve for the contaminant release history. Depending on the realization of the measurement error, some solutions (TR or MRE) will have two peaks (or more), many will have a single peak, and so will the related, say, 90%-confidence intervals. In these latter cases, the true solution will lie partially outside the confidence intervals. The frequency of single-peak solutions and confidence intervals, and consequently the frequency that the true solution lies partially outside the confidence intervals, will depend on the degree of plume dispersal at the time of measurement, with the frequency increasing as the plume becomes more dispersed. For a sufficiently long evolution time, the plume will be highly dispersed and the 90%-confidence intervals may on average contain the true release history in an arbitrarily small fraction of cases. This demonstrates that the term confidence interval is in general meaningless for this ill-posed problem, especially in the practically important case of no a priori knowledge about the nature of the release.

This does not mean that solutions with reasonable accuracy cannot be found. They can as long as information about the release history has not yet dissipated too much. Obviously, when a plume becomes fully dispersed in the aquifer, no release history can be recovered; information about it is then irretrievably lost. We cannot thus ask for a solution of every contaminant release history problem. We should ask instead "How far into the past can we recreate the history of the contaminant release with reasonable accuracy?" We close this issue by quoting *Provencher* [1982]:

> "Care must be exercised in making statements about error estimates and confidence regions, since the errors in solutions to ill-posed problems are generally unbounded."

5. Comparison of the MRE and Regularized Solutions

In several places, including the abstract and conclusions, *Woodbury and Ulrych* [1996] claim that the MRE method appears to be superior to the TR approach used by us [*Skaggs and Kabala*, 1994]. Upon reading this, one might be under the impression that the authors present strong supporting evidence. However, even a cursory look at their evidence reveals that this is not the case and that *Woodbury and Ulrych* [1996] used a flawed procedure in conducting their comparison.

A proper comparison of the MRE and Tikhonov regularization methods should be conducted using many contaminant release scenarios, measurement error realizations, and plume evolution times. The two methods should be tested using the same data sets and conclusions should be drawn only after a reasonable number of cases are considered. *Woodbury and Ulrych*'s [1996] comparison falls far short of this ideal. Although they assert that the problems they address are "similar" to those considered by us [*Skaggs and Kabala*, 1994], the problems actually differ significantly in three respects. First, in our simulations we used a data set consisting of only 25 synthetic plume measurements [*Skaggs and Kabala*, 1994, Figures 4 and 5], whereas *Woodbury and Ulrych* [1996, Figures 10 and 14] used a data set consisting of 61 points, that is, more than twice as many. Second, in generating their data, *Woodbury and Ulrych* [1996] used a different realization of measurement error than we [*Skaggs and Kabala*, 1994] did, and generated it from a different probability distribution, as discussed earlier. Third, *Woodbury and Ulrych* [1996] reached their conclusions based on just a single contaminant release function.

In summary, we take no stance regarding which method would prove superior in a proper comparison, but the comparison made by *Woodbury and Ulrych* [1996] is fundamentally flawed and even a measured conclusion such as their "qualitatively appears superior" is not justified.

We note in closing that neither of the authors of this note were permitted to see the paper of *Woodbury and Ulrych* [1996] while it was in review for publication, despite its criticism of and comparisons to our earlier work. Had we been allowed to see the paper in review, we could have readily and clearly pointed out its flaws along with its misleading and incorrect statements, to the benefit of all concerned.

Acknowledgment. This research was partially supported by the USDA CSRS under grant 93-37102-9393.

References

Hadamard, J., *Lectures on Cauchy's Problem in Linear Partial Differential Equations*, Yale University Press, New Haven, Conn., 1923.

Macdonald, J. R., Solution of an "impossible" diffusion-inversion problem, *Comput. Phys.*, *9*(5), 546–553, 1995.

Provencher, S. W., A constrained regularization method for inverting data represented by linear algebraic or integral equations, *Comput. Phys. Commun.*, *27*, 213–227, 1982.

Skaggs, T. H., and Z. J. Kabala, Recovering the release history of a groundwater contaminant, *Water Resour. Res.*, *30*(1), 71–79, 1994.

Skaggs, T. H., and Z. J. Kabala, Recovering the history of a groundwater contaminant plume: Method of quasi-reversibility, *Water Resour. Res.*, *31*(11), 2669–2673, 1995.

Woodbury, A. D., and T. J. Ulrych, Minimum relative entropy inversion: Theory and application to recovering the release history of a groundwater contaminant, *Water Resour. Res.*, *32*(9), 2671–2681, 1996.

Z. J. Kabala, Department of Civil and Environmental Engineering, Duke University, Durham, NC 27708. (kabala@copernicus.egr.duke.edu).

T. H. Skaggs, U.S. Salinity Laboratory, 450 West Big Springs Road, Riverside, CA 92507. (tskaggs@ussl.ars.usda.gov).

(Received February 28, 1997; revised March 3, 1998; accepted April 16, 1998.)