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Non-Optimization Direct Method of the Inverse Problem (NODMIP) for Groundwater Modeling in a Large Scale Basin

大流域を対象とした地下水モデルのための逆解析非最適化直接法

LUO Qiang*

羅 強

Nobuyuki TAMAI**

玉井 信行

Guangwei HUANG***

黄 光偉

The University of Tokyo The University of Tokyo

(東京大学)

The University of Tokyo The University of Tokyo

(東京大学)

The University of Tokyo

(東京大学)

The indirect method and stochastic method are efficient and accurate in the inverse groundwater modeling in a small research area but inefficient in a large scale basin. Because the Kanto Plain is a large scale basin, to develop an inverse groundwater model in this basin, we are forced to turn to the direct method. The direct method is a conceptually simple method, but also faced by the ill-posedness problem that makes this method yield no solution in a large scale basin if the traditional optimization solution scheme is adopted. Therefore, the authors developed a non-optimization solution scheme, the NODMIP, to eliminate the ill-posedness problem, while overcoming the difficulties in groundwater modeling in a large scale basin at the same time. To do so, the following five steps are taken: 1) solving the governing equations one time step by one time step, 2) imposing constraints of the prior information while the equations are being solved, 3) eliminating the pumping term and the residual term in the discretized equation, 4) interpolating water table data by Kriging technique, 5) estimating the unique aquifer parameters by simple arithmetic averaging method. This model is validated by an application in the Kanto Plain.

Key Words : Groundwater, Inverse problem, Aquifer, Hydraulic conductivity, Specific yield

地下水問題の逆解析においては、間接法や確率法は効率が良く正確な方法として知られている。しかしながら、この評価は大流域のモデルに対しては当てはまらない。一方、直接法は概念的には簡単であるが、大流域では不良問題により解が得られないことがしばしば生ずる。

本論文は直接法において不良問題を取り除く解法を構築し、大流域における地下水理パラメータの逆解析を可能にした。解法の特徴は、1) 時間ステップごとに支配方程式を解く、2) 事前情報を制約条件として活用する、3) 揚水項と残差項を一定値と考え、差分表示式ではこれらを無視する、4) 地下水面資料をクリギング法で内挿する、5) 各時間の計算値の算術平均値を、その地点の固有の帯水層定数とした。本手法を関東平野に適用した結果は、観測値をほぼ良好に再現でき、本解法は合理的に構成されていることが確認できた。

キーワード : 地下水、逆解析、帯水層、透水係数、比貯留係数

I. INTRODUCTION

Groundwater models are developed sophisticatedly today, but they are mainly applied to small areas or basins with relative small numbers of

grids or nodes. For example, the research area of Clifton and Neuman (1982) is approximately 500km² with 122 grids; and another research performed by Neuman (1980) is on an area about 28 km² with 39 grids. Yeh, *et al.* (1983) made a re-

*Doctoral student of River and Environment Eng. Lab., Graduate school of Eng., the University of Tokyo (7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan)

**Prof. of the University of Tokyo (7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan)

***Associate Prof. of the University of Tokyo (7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan)

search on a very small area 5.8km² with 256 grids, while the study area by Sun and Yeh (1992) is even much smaller, 0.13km², in which they set 168 elements and 150 nodes. Limited research area guarantees the sufficiency and accuracy of observation data, and furthermore small number of grids ensures the efficiency of a model.

However, some times we have to simulate groundwater hydrologic processes in a large scale basin. According to Singh (1995), even though there is no strict definition, a basin of 1000km² or more in area is called large-scale. Being compared with a small scale basin, a two dimensional distributed groundwater model in a large-scale basin faces several difficulties. For example, 1) there is few detail distributed aquifer parameter data; 2) observation wells is severely deficient, and 3) seldom of them are for the purpose of hydrologic research. Therefore, the accuracy of observation data is not guaranteed. Additionally, large area means large grid size and/or huge grid numbers that may increase simulation error and/or computer time expense.

This paper proposes a methodology to overcome the above mentioned difficulties. A non-optimization direct method for inverse groundwater model is developed to estimate distributed aquifer parameters in a large scale basin, in which the influences of data deficiency, low data accuracy, large grid size, huge grid number and long computer time are diminished.

Today, inverse methods are well developed, which can be mainly classified into three categories: 1) the indirect method (Neuman, 1973), 2) the direct method, and 3) the stochastic method (Sun, 1994).

An indirect method or a stochastic method involves solving complex matrix equation. Of course, the solution itself is not difficult, and some standard programs can be obtained too. These two methods are accurate and convenient for a small research area. But for a large scale basin like the Kanto Plain, whose area is more than 20,000km² (about 3,600 grids in a grid size of 2.5km, 360,000 grids if the grid size is 250m), the expense of huge

computer time makes the indirect method and the stochastic method almost inapplicable. How about their alternative—the direct method?

The direct method is a conceptually simple method. Just as Anderson (1999) pointed out, a complex model is not necessary a better model, and we found that a simple model is not always a bad one.

The direct method identifies parameters directly and simply by solving a set of governing equations, which are always super-determinate. This method is also transferred into optimization problem through computer programming. However, in this method there is a fatal obstacle, that is, the so-called ill-posedness problem that the solution is highly sensitive to any noise associated with the observation data. According to our research, the solution is even more sensitive to measurement error with increasing grid size.

II. THE DIRECT METHOD AND ILL-POSEDNESS PROBLEM

1. Concepts of the direct method

The general form of groundwater models can be represented by the following operator equation:

$$L(S, P, \mathbf{x}, t) = 0 \quad (1)$$

where S is the state variable, P is the model parameter, $\mathbf{x}$ is the space variables and t is time. When the above equation is discretized, a set of algebraic equations are obtained and their compact form is:

$$L(S, P) = 0 \quad (2)$$

in which, if N_s and N_t are numbers of space and time steps respectively, and $N = N_s \times N_t$, then $S = (u_1, u_2, \dots, u_N)^T$. If N_p is the number of parameters and $M = N_s \times N_p$, then $P = (p_1, p_2, \dots, p_M)^T$. Number of state variable observation time series is always larger than the number of parameters, thus equation (2) is usually super-determinate. This kind of super-determinate equations can be solved by the optimization problem method, e.g. the L_1 -norm equation error criterion method, the L_2 -norm equation error criterion method and quasi-linearization method (Sun, 1994).

For the L_2 -norm equation error criterion

method, if w is the weight, the optimization equation is written as below:

$$\sum_{n=1}^N w_n L_n \frac{\partial L_n}{\partial p_m} = 0, (m=1, 2, \dots, M) \quad (3)$$

where L_n ($n=1, 2, \dots, N$) comprise linear equations of P_m ($m=1, 2, \dots, M$):

$$A p - b = 0 \quad (4)$$

Combining equation (3) and (4), a solution of p is yielded:

$$\hat{p} = (A^T W A)^{-1} A^T W b \quad (5)$$

If $w_n=1$ ($n=1, 2, \dots, N$), equation (5) will be reduced to the following:

$$\hat{p} = (A^T A)^{-1} A^T b \quad (6)$$

2. The ill-posedness problem and measures to eliminate it

Errors are always included in the observation data of the state variable, thus the state variable vector S become:

$$\tilde{S} = S + \delta S \quad (7)$$

which will also incur errors to A and b in turn and makes equation (4) change to:

$$\tilde{A} p - \tilde{b} = r \quad (8)$$

where r is the residual vector. Thus the final solution of p becomes:

$$\tilde{\hat{p}} = (\tilde{A}^T \tilde{A})^{-1} \tilde{A}^T (\tilde{b} + r) \quad (9)$$

According to Sun (1994), the square matrix $(\tilde{A}^T \tilde{A})$ in equation (9) is often nearly singular, and thus causes a large error to the identified parameters.

In the case of a large scale basin, data accuracy of state variable is even lower due to difficulties of observation and involving large quantity of interpolation. The square matrix $(\tilde{A}^T \tilde{A})$ in equation (9) always tends to be singular and makes equation (9) yield no solution (Luo, *et al.*, 1999). A program written in FORTRAN always tends to be stopped by the "overflow" error or "divided by zero" error while it is running.

Sun (1994) proposed two measures to overcome the difficulty of ill-posedness problem. One is imposing constrains of prior information and the other is parameterization. However, Sun's constrains must be imposed after the program already reached to a solution. Unfortunately, in a

large-scale basin model, the program tends to be stopped before it reaches any solution. Parameterization is meaningless for a large-scale basin, because the size of its grids is usually larger than the whole interested area of some researches for small areas.

Thus, then necessary first step is breaking out of the bindings of the stumbling huge square matrix in equation (9). And then impose constrains of the prior information while the equations are being solved. Based on these considerations, Luo, *et al.* (1999) developed a SILGROM (Simplified Inverse Large-scale Groundwater Model). The SILGROM identified parameters with high accuracy in an artificial basin of 20×20 grids. However, its application in Kanto Plain yielded less satisfactory results. Here, the authors provide another remedy to this problem: the NODMIP (non-optimization direct method of the inverse problem).

III. THE NON-OPTIMIZATION DIRECT METHOD

1. The governing equation - Boussinesq Equation and its discretization

When the groundwater is assumed to be unconfined and the aquifer is isotropic, the two dimensional groundwater equation, the Boussinesq Equation, is written as below (Anderson, 1992):

$$\frac{\partial}{\partial x} \left(K \frac{\partial h^2}{\partial x} \right) + \frac{\partial}{\partial y} \left(K \frac{\partial h^2}{\partial y} \right) = 2S_y \frac{\partial h}{\partial t} - 2(R - P) \quad (10)$$

where h is the elevation of water table, K is the hydraulic conductivity, S_y is the specific yield, and $(R - P)$ is the source term, in where R is the infiltration/re-charge and P is pumping of groundwater/extraction.

Executing partial differentiation inside brackets, equation (10) can be expanded like this:

$$\begin{aligned} & K \frac{\partial^2 h^2}{\partial x^2} + \frac{\partial K}{\partial x} \frac{\partial h^2}{\partial x} + K \frac{\partial^2 h^2}{\partial y^2} + \frac{\partial K}{\partial y} \frac{\partial h^2}{\partial y} \\ & = 2S_y \frac{\partial h}{\partial t} - 2R + 2P \end{aligned} \quad (11)$$

Using central difference for both spatial and temporal differentiation, equation (11) can be discretized as below:

$$\begin{aligned}
& K_{ij} \frac{h_{i+1j}^2 - 2h_{ijk}^2 + h_{i-1j}^2}{\Delta y^2} + (K_{i+1j} - K_{i-1j}) \\
& \times \frac{h_{i+1j}^2 - h_{i-1j}^2}{4\Delta y^2} + K_{ij} \frac{h_{ij+1k}^2 - 2h_{ijk}^2 + h_{ij-1k}^2}{\Delta x^2} \\
& + (K_{ij+1} - K_{ij-1}) \frac{h_{ij+1k}^2 - h_{ij-1k}^2}{4\Delta x^2} \\
& = S_{yij} \frac{h_{ijk+1} - h_{ijk-1}}{\Delta t} - 2R_{ijk} + 2P_{ijk} \quad (12)
\end{aligned}$$

where i is the spatial step for y and j is that for x , and k is the temporal step. It is noticed that the observed water table $\tilde{h}$ includes an error δh , and $\tilde{h} = h + \delta h$. If r_{ijk} represents the residuals of equation (12), equation (12) reduces to:

$$\begin{aligned}
& K_{ij} \frac{\tilde{h}_{i+1j}^2 - 2\tilde{h}_{ijk}^2 + \tilde{h}_{i-1j}^2}{\Delta y^2} + (K_{i+1j} - K_{i-1j}) \\
& \times \frac{\tilde{h}_{i+1j}^2 - \tilde{h}_{i-1j}^2}{4\Delta y^2} + K_{ij} \frac{\tilde{h}_{ij+1k}^2 - 2\tilde{h}_{ijk}^2 + \tilde{h}_{ij-1k}^2}{\Delta x^2} \\
& + (K_{ij+1} - K_{ij-1}) \frac{\tilde{h}_{ij+1k}^2 - \tilde{h}_{ij-1k}^2}{4\Delta x^2} \\
& = S_{yij} \frac{\tilde{h}_{ijk+1} - \tilde{h}_{ijk-1}}{\Delta t} - 2R_{ijk} + 2P_{ijk} + r_{ijk} \quad (13)
\end{aligned}$$

If S , R , P and r are known in equation (13) and there is a time series of observation data of water table, it is sure that equation (13) has a unique solution of K by solving the optimization problem if the square matrix is not singular. And vice versa for S , if K , R , P and r are known. However, as pointed out in II. 2, the square matrix always tends to be singular, there will be no solution for equation (13) by an optimization method. Thus, it must be abandoned.

We turn to the non-optimization method. In the non-optimization method, equation (13) is solved grid by grid (explicit) or one time step by one time step (implicit). Even though some grids or time steps may yield no solution, it is definite that there are solutions in many other time steps if the time series of water table is long enough. Finally, the unique parameters can be estimated from these solutions once an identification scheme is determined.

2. Deriving a practical form of the discretized equation

In equation (13), no detail data of P can be ob-

tained as mentioned before, therefore the residual term r is actually an unknown, too, and both vary with time. Moreover, the hydraulic conductivity K and specific yield S , must be identified simultaneously. Thus, this equation is practically indeterminate even if in the optimization method.

According to Japan Society of Water Supply (1993, 1994), the daily pumping of groundwater is conducted according to an annual plan, which means that the pumping will not vary violently from day to day. Thus it is assumed that pumping rates in the nearest two days are the same:

$$P_{ijk+1} - P_{ijk} \approx 0 \quad (14)$$

The residual term r_{ijk} is mainly related to measurement errors of water table, which is always taken as a stochastic variable. The usual treatment to this term in a deterministic model is simply to omit it. However, in our research, we consider that it is mainly affected by field measurement conditions, e.g. the weather of a measuring day. It is assumed that weather dose not change abruptly from day to day (this assumption may hold in most time in a year according to our daily experience). And thus, it may be reasonable to assume that the magnitudes of r_{ijk} in the nearest two days do not change obviously (if the time step is one day):

$$r_{ijk+1} - r_{ijk} \approx 0 \quad (15)$$

Under the above two assumptions, equation (13) of time step $k+1$ subtracting that of time step k , after rearrangement, yields:

$$\begin{aligned}
& a_{i-1j}K_{i-1j} + a_{ij-1k}K_{ij-1} + a_{ijk}K_{ij} \\
& + a_{ij+1k}K_{ij+1} + a_{i+1j}K_{i+1j} + b_{ijk}S_{yij} = c_k \quad (16)
\end{aligned}$$

where a , b and c are coefficients related to water table elevations of time steps $k-1$, k and $k+1$ and infiltration of $k+1$ and k . Doing the same with another two time steps, $k+2$ and $k+1$, yields another linear equation:

$$\begin{aligned}
& a_{i-1j}K_{i-1j} + a_{ij-1k}K_{ij-1} + a_{ijk}K_{ij} \\
& + a_{ij+1k}K_{ij+1} + a_{i+1j}K_{i+1j} + b_{ijk+1}S_{yij} = c_{k+1} \quad (17)
\end{aligned}$$

Equations (16) and (17) can be solved together by either an explicit method or an implicit method, and hydraulic conductivity and specific yield of aquifer are identified simultaneously.

3. Imposing constraints of prior information

After and only after the above processes are conducted, can constraints of prior information be imposed during the solution procedure.

For the explicit method, equations (16) and (17) are solved grid by grid, and for the implicit method, they are solved at all grids simultaneously, but one time step by one time step. When there is no solution in a grid for the explicit method or all grids at one time step, constraints of prior information are imposed, the upper bound will be assigned to the solution. Or, if the solutions of one grid or one time step are larger than the upper bound, they will be replaced by the upper bound, or by the lower bound if the solutions are smaller than the lower bound.

4. Interpolating water table observation data with Kriging technique

To solve equations (16) and (17), water table elevation in each grid is needed, which is obviously impossible. Moreover, in a large scale basin, observation data of water table are severely insufficient. In this study we have only 39 observation wells in the whole Kanto Plain. It is inevitable to involve some kinds of interpolation technique. Water tables in mountain slopes are roughly of an increment stationary field, and we suppose that water table elevation in the plain area of a basin is a variable of weakly isotropic stationary field. A weakly isotropic stationary field must be an increment stationary field (Sun, 1994), and thus, the Kriging estimation for increment stationary fields can be used:

$$\hat{h}_{ij} = \sum_{i=1}^n \lambda_i h_i \quad (18)$$

where $\hat{h}_{ij}$ is the interpolation of water table, n is the number of observation well, h_i is the observed water table at the site of well i , and λ_i is called Kriging estimator and given by the following equations:

$$\begin{cases} \sum_{i=1}^n \gamma_{lm} \lambda_i + \mu = \gamma_{m,0} & (m=1, 2, \dots, n) \\ \sum_{i=1}^n \lambda_i = 1 \\ \gamma(L) = \alpha L^\beta, \alpha > 0, 0 < \beta < 2 \end{cases} \quad (19)$$

where L is distances between observation wells or observation well and the computed grid, α and β are given coefficients, γ_{lm} and $\gamma_{i,0}$ are coefficients relating to distances between observation wells l and m or l and computed grid, respectively, and μ is an unknown Lagrangian multiplier.

The third equation in (19) is called polynomial variogram, which satisfies the necessary variogram conditions:

$$\begin{cases} \gamma(0) = 0, \gamma(L) > 0 \\ \lim_{L \rightarrow \infty} \frac{\gamma(L)}{L^2} = 0 \end{cases} \quad (20)$$

The cross validation technique can be used to check the Kriging estimators (Sun, 1994). However, the solution to equation (19) will automatically satisfy the cross validation conditions.

5. Estimating unique aquifer parameters

The solution of equations (16) and (17) by NODMIP will result in a series of identified parameters. How to estimate unique aquifer parameters from these series of outputs? We studied two kinds of algorithm, one is the statistic method and the other is simply arithmetic average. The accuracy of output by statistic method depends on the number of samples, here means the length of time series. Unfortunately, we do not have a very long time series of observation data in this research, the accuracy by stochastic method seems to be lower than that by the simple average method. Thus, the unique aquifer parameters are simply estimated by taking arithmetic averages over all outputs of the whole time series.

IV. AN APPLICATION TO THE KANTO PLAIN

1. Description of groundwater basin of the Kanto Plain

According to the River Bureau of the Ministry of Construction, Japan, the groundwater basin of Kanto Plain includes Tone River basin, Edo River basin and Ara River basin. The total area is approximately 21,000km².

In this research, a grid size of 2.5km is selected, in consistence with that of the water and heat bal-

Fig. 1 Research area and observation wells

ance model in the Kanto region we developed. The whole basin is covered by a rectangular area with 7780 grids, among which, about 3,600 grids are computed ones. Due to no digitized data of water table elevation, only data at 39 observation wells are utilized. The research area of the Kanto Plain and the observation wells are shown in Fig. 1. The coordinate unit is number of grids in the West–East and North–South direction.

2. Model development

Observation water table data of the year 1993 are used to develop the model. Spatial step is 2.5 km and temporal step is one day. According to Agriculture Ground-water Research Group of Japan (1986), the upper bound of hydraulic conductivity is 1.710^{-3} m/s, and that of specific yield is

Fig. 2 Polynomial variogram $\gamma(L) = aL^\beta$

0.6. Both values of lower bound are set to be 0. In this research, we assume that the unconfined aquifer is uniformly distributed, or the bottom of aquifer is flat. The Kriging interpretation coefficients α and β are set to be 5.0 and 1.5 respectively (Fig. 2).

3. Boundary conditions and initial condition

All land or mountainous boundaries are assumed to be impermeable boundaries, boundaries adjacent to the sea to be unchanging elevation boundaries (elevation: 0m). The initial condition is the observed water table data of the last 3 days of the previous year of computation.

4. Estimation of hydraulic conductivity and specific yield

The final estimated values of hydraulic conductivity and specific yield are shown in Fig. 3 and Fig. 4. According to Agriculture Ground-water Research Group of Japan (1986), generally, the hydraulic conductivity in Tochigi and Gunma Prefectures (northern part) are larger than that in Saitama Prefecture and Tokyo, as shown in Fig. 3.

5. Model validation and discussions

The observation data of water table in the year 1994 are used to validate the model. A comparison of computed water table with the observed one is

Fig. 3 Estimated Hydraulic conductivity

Fig. 4 Estimated Specific yield

Fig. 5 Comparison of water table

shown in Fig. 5. A computed contour line of water table and an observed one are shown in Figs. 6 and 7.

One can see from Fig. 5 that the computed line only simulates the averaged trend of water table. It is because, in the validation, a constant daily pumping rate of groundwater is used, which is from the water supply data. This may account for the disability of the model to simulate the decreasing peak. Moreover, due to the nature of fundamental research, we do not include an infiltration model here and the natural recharge to groundwater is simply assumed to be a unique percentage of rainfall only in the whole basin. This is the reason why the model cannot simulate the rising peak of the water table. However, we are confident that, once we obtain detailed pumping and recharge data and include an infiltration model

Fig. 6 Observed water table distribution on Dec. 31, 1994

Fig. 7 Computed water table distribution on Dec. 31, 1994

when an elaborate model is required, the simulation of time varying water table would result in better output.

However, from Figs. 6 and 7, one can see that the computed contour lines of water table and the observed ones fit quite well generally in the whole basin. The objective of this research is to estimate distributed aquifer parameters. NODMIP resorts to correct water table distributions at all time steps, but not some peak periods. Therefore, successful reproduction of water table contour lines ensures the correct estimation of distributed aquifer

fer parameters.

V. CONCLUSIONS

From this research, it can be concluded that:
(1) The direct method is not only a conceptually simple inverse method, but also an effective one that can be adopted to solve real problems for the groundwater modeling in a large scale basin. (2) For a large scale basin, an effective directive method needs not only to eliminate the ill-posedness problem, but also to overcome the difficulties faced by a large scale model. (3) The NODMIP is an effective inverse groundwater model applicable to large scale basins, in which detailed distributed aquifer parameter data are not always available.

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