The Use of Interval Analysis in Hydrologic Systems

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Abstract. Hydrological data are often highly inaccurate. Interval methods help to estimate inaccuracy caused by data uncertainty, both for *forward* problems (in which we predict how water will flow in the known medium), and for the *inverse* problems (in which we observe how water flows and determine the properties of the medium).

1. Introduction: Interval Computations are Needed

Geohydrology and its problems. Geohydrology describes how water flows in the subsurface. We know equations that describe this flow, but parameters of these equations are usually known only approximately. Two types of problems are of interest:

- forward problems, in which we know the parameters of the medium, and want to predict how water flows in the subsurface;
- *inverse* problems, in which we measure how the water flows, and attempt to estimate the corresponding parameters of the medium.

We must take uncertainty into consideration. In both problems, we must take uncertainty into consideration. The measurement result \tilde{X} may differ from the actual value X of the measured quantity:

- In some cases, we know the probabilities of different measurement errors.
- However, in most real-life cases, we only know the upper bound Δ on the measurement error $\Delta X = \tilde{X} X$ ($|\Delta X| \leq \Delta$). Therefore, the only information about X that we get from the measurement result is that X belongs to the *interval* $\mathbf{X} = [\tilde{X} \Delta, \tilde{X} + \Delta]$.

Interval computations are needed for solving the inverse problem. Due to the uncertainty in measurements, the parameters of the medium that we estimate or reconstruct from the measurements also contains uncertainty: different possible values $X \in \mathbf{X}$, generally speaking, can lead to different values of the estimated parameters. It is therefore desirable to estimate the range of parameter values:

ideally, to compute the *interval* of possible values of the parameters, or, at least, an *enclosure* for this interval. Thus, interval computations [1], [17], [21] are needed for solving the *inverse* problem.

Interval computations are needed for solving the forward problem. Similarly, interval computations are needed for the forward problem as well: To solve the forward problem, we must know the parameters of the media. Since these parameters are only known approximately (to be more precise, with interval uncertainty), we should only expect interval predictions for the forward problem.

Historical comment. The need for interval estimates in hydrological problems was suggested in [5] (see also [3]).

Interval computations are needed even if we know probabilities. In the inverse problem, if we know probabilities, we can use statistical methods to estimate the values of the desired parameters. Many known statistical methods (e.g., maximum likelihood method) are based on some *optimization*. This optimization can be rarely done analytically, so numerical methods are needed. Many known schemes for numerical optimization do not *guarantee* that the result is indeed optimal, i.e., the solution can be a local optimum. If we want to find the global optimum, we need to use methods of global optimization that lead to *guaranteed* results. Therefore methods of interval computations which provide guaranteed bounds are very suitable for such problems.

There is one more reason: In some cases, we do not know the *exact* probabilities, we only know the *intervals* of possible values of these probabilities (or of statistical characteristics of the corresponding probability distribution). Different values of these probabilities lead to a different optimal estimate; it is therefore desirable to find the *interval* of possible estimate values.

Interval computations can be used. In this paper, we show with several simple examples, that interval computations *can* be used to solve hydrologic problems, characterized by uncertainties.

2. Case Study: Linear 1D Hydrologic System—General Description

A brief description of the case system. Our examples will describe the simplest possible geohydrologic system: a 1D system represented by a linear differential equation, which describes (steady-state) flow through a confined porous medium (Figure 1).

How to describe the case system in mathematical terms: informal derivation of the corresponding differential equation. Let x be a coordinate in the direction of the flow. At any point x, the current state of the flow can be characterized by two variables:

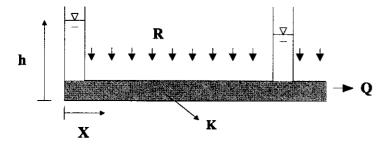


Figure 1. Flow through porous medium of hydraulic conductivity, k.

- The first variable is the hydraulic potential (head), h(x). This potential is defined as the height to which the water would rise if an open tube was attached to the system at point x.
- The second variable is the flux q(x) through the medium, which is defined as the quantity of water flowing per unit time at point x.

The resistance of the medium decreases the flow energy. The larger the flux and longer the travel distance, the more energy is expended, resulting in a larger drop in the hydraulic potential. Thus, the decrease Δh in the potential is proportional to the flux q and the travel length Δx : $\Delta h = -\rho(x) \cdot q \cdot \Delta x$, where the coefficient $\rho(x)$ describes the resistance of the medium.

This formula is precise if the flux is constant in x. In reality, at certain locations, water may enter or exit (discharge) the system, thus changing the flux. Therefore, to ensure validity of the governing equation, we will consider instead of finite intervals Δx , infinitesimal intervals dx. Then, the change in height dh is also infinitesimal, resulting in the differential equation $dh = -\rho \cdot q \cdot dx$, i.e.,

$$\frac{dh}{dx} = -\rho(x) \cdot q(x). \tag{2.1}$$

As in electric circuit analysis, it is often convenient to use instead of the resistance $\rho(x)$, the inverse quantity *conductivity* $k(x) = 1 / \rho(x)$. In terms of conductivity, equation (2.1) takes the form

$$q(x) = -k(x) \cdot \frac{dh}{dx}. (2.2)$$

Homogeneous case. The value of conductivity is usually not known precisely. In many practical cases, we can assume that the medium is:

- either homogeneous, in which case the value of conductivity k(x) does not depend on x at all,
- or at least consists of several homogeneous sub-domains (zones), in each of which the conductivity is constant.

The simplest case: no change in flux. If no water enters or exits the system, then the flux simply remains constant: q(x) = q.

If the flux remains constant in a homogeneous area, then, substituting q(x) =const and k(x) =const into equation (2.2), we can conclude that the derivative dh/dx is also constant (equal to -q/k), and therefore, the head h(x) changes linearly with x. In this case, the derivative dh/dx coincides with the ratio $\Delta h/\Delta x$, and therefore equation (2.2) takes the form

$$q = -k \cdot \frac{\Delta h}{\Delta r}.\tag{2.3}$$

In other words, the original approximate difference equation, which we used to derive the exact differential equation, is, in this particular case, exactly true.

Case of spatially varying flux. If the flux is not constant, but varies spatially, then the following differential equation describes the change in flux:

$$\frac{dq}{dx} = -R(x). (2.4)$$

where R(x) is the rate (per unit length) with which the flux changes. If we substitute expression (2.2) for the flux into (2.4), we get a more widely used form of this equation:

$$\frac{d}{dx}\left(k \cdot \frac{dh}{dx}\right) = R(x). \tag{2.5}$$

In particular, when the medium is homogeneous (k(x) = k), we get the simplified version of this equation:

$$k \cdot \frac{d^2h}{dx^2} = R(x). \tag{2.6}$$

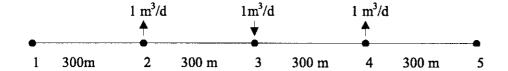
Comment. The equations (2.5) and (2.6) are usually solved by using finite difference methods, see, e.g., [2], [11], [12].

Case of concentrated flux. Another possibility for a change in water is when water enters or exits the system at a distinct point. If we denote by x_0 the point of this addition or retrieval, and by $Q(x_0)$, the amount of added or retrieved flux, then we can conclude that the flux $q(x_0+)$ right after this point is related to the flux $q(x_0-)$ right before this point by the relation

$$q(x_0+) = q(x_0-) + Q(x_0). (2.7)$$

In particular, if the areas immediately prior to x_0 (from x^- to x_0) and immediately following x_0 (from x_0 to x^+) are homogeneous, we can substitute expressions (2.3) instead of the values $q(x_0-)$ and $q(x_0+)$ and obtain the equation:

$$-k^{-} \cdot \frac{h(x_0) - h(x^{-})}{x_0 - x^{-}} = -k^{+} \cdot \frac{h(x^{+}) - h(x_0)}{x^{+} - x_0} + Q(x_0). \tag{2.8}$$



Hydraulic Conductivity: k=[40,50] m/d

Boundary Conditions: h₁=h₅=100m

Figure 2. Problem description for case study 1.

An even more simplified version of this equation can be obtained if we assume that the sub-domains $[x^-, x_0]$ and $[x_0, x^+]$ are of equal length Δx , and that the medium is homogeneous throughout the domain $[x^-, x^+]$. In this case, equation (2.8) takes the form:

$$k \frac{h(x_0 - \Delta x) + h(x_0 + \Delta x) - 2h(x_0)}{\Delta x} = Q(x_0).$$
 (2.9)

Comment. The left-hand side of this equation is proportional to the standard finite-difference approximation of the second derivative. Therefore, this equation can be viewed as a finite-difference approximation of the second-order differential equation (2.6). (It is worth mentioning that in the above case, equation (2.9) is exact, and not just approximately true.)

3. Case Study 1: Forward Problem

Formulation of the problem: what is known. Let us consider flow through a homogeneous porous domain of length 1200 m (Figure 2). The conductivity k is known to be within the interval [40, 50] m/day. The head at the endpoints is constant at 100 m ($h_1 = h_5 = 100$). The following additions and retrievals occur:

- at x_2 (300 m from x_1), 1 m³/day exits the system;
- at x_3 (600 m from x_1), 1 m³/day enters the system;
- finally, at x_4 (900 m from x_1), 1 m³/day exits the system.

Formulation of the problem: what we are interested in. We are interested in determining how the head h(x) varies with x.

What exactly do we need to compute. Since the medium is homogeneous, the head h(x) varies linearly in each of the intervals $[x_i, x_{i+1}]$. A linear function h(x) in the interval $[x_i, x_{i+1}]$ is uniquely determined by the values $h_i = h(x_i)$ and $h_{i+1} = h(x_{i+1})$

at the endpoints. Thus, to determine h(x) for all x, it is sufficient to determine $h_1, h_2, ..., h_5$.

Since $h_1 = 100$ and $h_5 = 100$, we are interested in three unknowns: h_2 , h_3 , and h_4 .

Equations: For the homogeneous case under consideration, we can use equation (2.9) for $x_0 = x_2$, $x_0 = x_3$, and $x_0 = x_4$, thereby obtaining the following three equations:

$$k \cdot \frac{100 + h_3 - 2h_2}{300} = 1;$$

$$k \cdot \frac{h_2 + h_4 - 2h_3}{300} = -1;$$

$$k \cdot \frac{h_3 + 100 - 2h_4}{300} = 1.$$
(3.1)

To simplify these equations, we can multiply both sides of each equation by C = 300 / k, resulting in:

$$100 + h_3 - 2h_2 = C; (3.2a)$$

$$h_2 + h_4 - 2h_3 = -C; (3.2b)$$

$$h_3 + 100 - 2h_4 = C. (3.2c)$$

These equations can be explicitly solved, resulting in:

$$h_2 = 100 - 0.5 \cdot C; \tag{3.3a}$$

$$h_3 = 100;$$
 (3.3b)

$$h_4 = 100 - 0.5 \cdot C. \tag{3.3c}$$

Since $k \in [40, 50]$, we conclude that $C = 300 / k \in [6, 7.5]$, and therefore, we have the following interval bounds for h_i :

$$\mathbf{h}_1 = [100, 100], \quad \mathbf{h}_2 = [96.25, 97], \quad \mathbf{h}_3 = [100, 100], \\ \mathbf{h}_4 = [96.25, 97], \quad \mathbf{h}_5 = [100, 100].$$
 (3.4)

Possible values of h(x) for $x \neq x_i$ can be obtained by linear extrapolation.

Comment 1: General piece-wise homogeneous case. In the general piece-wise homogeneous case, we have to consider the more general equation (2.8). Since we only know interval values for k and probably, for Q, we get *interval* linear equations. For solving such equations, we can use methods described in [7], [9], [10], [14], [16], [18], [19], [22], [23]. However, for our problems, these methods lead to huge overestimation, because:

 most of these methods assume that different coefficients can independently vary within the corresponding intervals, while • in our case, due to the homogeneity assumption, several different coefficients express the same value: conductivity k in a given zone.

To the author's knowledge, only one paper [13] describes interval methods that explicitly account for such dependencies between the coefficients.

Comment 2: Non-homogeneous case. What if we do not assume that the medium is homogeneous? In other words, what if we allow different values of k(x) for different x (but all within the interval [40, 50])?

In this case, on each interval $[x_i, x_{i+1}]$, the flux is constant, and therefore, from equation (2.1), we can conclude that $dh = -\rho(x) \cdot q \cdot dx$, implying

$$h_i - h_{i+1} = q \cdot \int_{x_i}^{x_{i+1}} \rho(x) \, \mathrm{d}x,$$
 (3.5)

where $\rho(x) = 1 / k(x) \in [1 / 50, 1 / 40]$. Due to the bounds on $\rho(x)$, and the fact that $x_{i+1} - x_i = 300$, the integral is within the interval

$$C = [300 \cdot 1 / 40, 300 \cdot 1 / 50] = [6, 7.5].$$

Thus, we can get the two-sided bounds on the difference $h_{i+1} - h_i$ that depend on the (unknown) value q.

Due to flow conservation (equation (2.7)), if flow in the subdomain $[x_1, x_2]$ is equal to q, then:

- the flow in the next subdomain $[x_2, x_3]$ is equal to q 1,
- the flow in the subdomain $[x_3, x_4]$ is again equal to q;
- the flow in the subdomain $[x_4, x_5]$ is equal to q 1.

Let us assume that the flow is positive on the subdomains $[x_1, x_2]$ and $[x_3, x_4]$, and negative (i.e., going in the opposite direction) in the domains $[x_2, x_3]$ and $[x_4, x_5]$. Thus, q > 0, q - 1 < 0, and we get the following bounds on the differences $h_i - h_{i+1}$:

$$6q \le 100 - h_2 \le 7.5q; \tag{3.6a}$$

$$7.5 - 7.5q < h_2 - h_3 \le 6 - 6q; (3.6b)$$

$$6q \le h_3 - h_4 \le 7.5q; \tag{3.6c}$$

$$7.5 - 7.5q < h_4 - 100 \le 6 - 6q. \tag{3.6d}$$

We thus get a system of 4 linear inequalities with 4 unknowns h_2 , h_3 , h_4 , and q. Using linear programming, we can find the intervals of possible values for each of these quantities.

Since in our formulation, we are only interested in the values h_2 , h_3 , and h_4 , and not in q, we can, instead of using the general linear programming techniques, first eliminate q from this system of inequalities. There is a standard method for eliminating q. Namely:

- we represent each inequality as a two-sided inequality in terms of q;
- then, the existence of the value q that satisfies all these inequalities is equivalent to the requirement that each lower bound does not exceed each upper bound.

For our system (3.6), this method leads to the following inequalities:

$$\frac{100 - h_2}{7.5} \le q \le \frac{100 - h_2}{6};\tag{3.7a}$$

$$1 - \frac{h_3 - h_2}{6} \le q \le 1 - \frac{h_3 - h_2}{7.5}; \tag{3.7b}$$

$$\frac{h_3 - h_4}{7.5} \le q \le \frac{h_3 - h_4}{6}; \tag{3.7c}$$

$$1 - \frac{100 - h_4}{6} \le q \le 1 - \frac{100 - h_4}{75}. (3.7d)$$

By comparing (3.7a) and (3.7b), we conclude that:

$$\frac{100 \quad h_2}{7.5} \le 1 - \frac{h_3 \quad h_2}{7.5}$$

and

$$1 - \frac{h_3 - h_2}{6} \le \frac{100 - h_2}{6},$$

i.e., we conclude that

$$100 + h_3 - 2h_2 \in [6, 7.5].$$

Similarly, we conclude that other second differences must belong to the interval C = [6, 7.5]. Then, we can solve the resulting system of linear inequalities with three unknowns.

If we additionally assume that the flow is *symmetric* with respect to the point x_3 , then we have $h_2 = h_4$, and from the equality of the flows in the subdomains $[x_1, x_2]$ and $[x_4, x_5]$, we conclude that q = |q - 1|, i.e., q = 0.5. In this case, from (3.6a) and (3.6d), we conclude that $h_2 = h_4 \in 100 - [6q, 7.5q]$, i.e., $h_2 = h_4$ can take arbitrary values from the interval $h_2 = h_4 = [96.25, 97.0]$. From the equation (3.6c), we can now conclude that $h_3 - h_2 \in [6q, 7.5q]$, and therefore, the possible values of h_3 is equal to $h_2 + [6q, 7.5q] = [96.25, 97.0] + [3.0, 3.75] = [99.25, 100.75]$. Thus:

$$\mathbf{h}_1 = [100.0, 100.0], \quad \mathbf{h}_2 = [96.25, 97.0], \quad \mathbf{h}_3 = [99.25, 100.75],$$

 $\mathbf{h}_4 = [96.25, 97.0], \quad \mathbf{h}_5 = [100.0, 100.0].$

Even with the additional symmetry assumption, some of the resulting intervals are wider than the intervals (3.4) for the homogeneous case: namely, we can get values $h_3 \neq 100$.

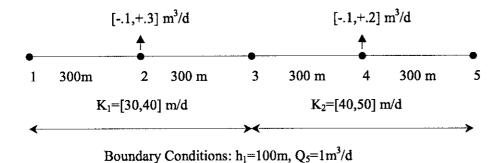


Figure 3. Problem description for case study 2.

4. Case Study 2: Forward Problem

Description of the example. In this example (Figure 3), we also discretized the domain by five equidistant points $x_1, ..., x_5$ ($\Delta x = 300 \text{ m}$). The head at x_1 is constant at 100 m. At points x_2 and x_4 fluxes Q_2 and Q_4 are applied. We do not know the exact values of these fluxes, however $\mathbf{Q}_2 = [-0.1, 0.3] \, \mathrm{m}^3/\mathrm{day}$ and $\mathbf{Q}_4 = [-0.1, 0.2] \, \mathrm{m}^3/\mathrm{day}$ contain these values. The flux at the right end is equal to 1 m³/day.

The system is piece-wise homogeneous:

- on the first sub-domain $[x_1, x_3]$, we have conductivity k_1 which is within the interval [30, 40] m/day;
- on the second sub-domain $[x_3, x_5]$, we have conductivity k_2 which is within the interval [40, 50] m/day.

Our goal is to find the possible values of the heads h_2 through h_5 .

How we solve the problem. When k_j and Q_j are known, the heads can be uniquely determined by equations (2.8) and (2.9). In general, we, thus, have an expression for h_i in terms of the unknown values of k_j and Q_j . It can be shown that for the case under consideration, i.e., a constant head at one end and a constant flux at the other end, the resulting dependency $h_i(k_1, ..., Q_1, ...)$ is monotonic in each of its variables, so, we can explicitly find the desired intervals by considering the corresponding endpoints of the intervals Q_j and k_j . The resulting values are:

$$\mathbf{h}_2 = [88.00, 96.25], \quad \mathbf{h}_3 = [77.00, 90.25],$$

 $\mathbf{h}_4 = [68.75, 85.45], \quad \mathbf{h}_5 = [61.25, 79.45].$

5. Case Study 3: Inverse Problem

General formula. The goal of the inverse problem is to find, based on observed values of heads h_i (and fluxes), the conductivities k_i of different subdomains.

Usually, we assume that measurement errors are normally distributed and independent. In this case, the least squares methods leads to the following formula for reconstructing the desired values k_i from the measurements \tilde{h}_i :

$$L = \sum_{i=1}^{n} \left(h_i(k_1, \dots) - \tilde{h}_i \right)^2 \to \min_{k_1, \dots},$$

where:

- n is the total number of measurements,
- \tilde{h}_i are the measured heads, and
- $h_i(k_1,...)$ are the values of heads computed by using the conductivities k_l .

In many cases, in addition to the current measurement results, we have some *prior* estimates $k_j^{(0)}$ for conductivities. These are estimated from previous measurements, or from knowledge of the system. In such cases, we know the covariance matrix for such estimates, and the least squares method takes the following modified form:

$$L = \sum_{i=1}^{n} (h_i(k_1, \dots) - \tilde{h}_i)^2 + [K - K^{(0)}]^T [V^{-1}][K - K^{(0)}] \to \min_{k_1, \dots},$$
 (5.1)

where:

- $K = (k_1, ...)$ is the vector of the (unknown) parameters k_j ;
- $K^{(0)} = (k_1^{(0)}, ...)$ is the vector of the prior estimates of the conductivities; and
- the matrix V^{-1} is the inverse of the covariance matrix (which is a measure of the correlation of the prior estimates).

How we can solve the inverse problem. One possibility to find the minimum is to find all extremal points, i.e., all points $K = (k_1, ...)$ in which

$$\frac{\partial L}{\partial k_i} = 0, \quad j = 1, ...,$$

and, if there are several such points, choose the point K for which $L \to \min$.

Example: description. We consider an example from [4], which is described in Figure 4. A flux of 1 unit flows through a system of unit length, with a constant head $h_1 = 5$ at the left end. The system is discretized into four equal intervals of length $\Delta x = 0.25$. The following observations for the heads exist:

- at point $x_2 = x_1 + \Delta x$, $\tilde{h}_2 = 4.5$;
- at point $x_3 = x_1 + 2\Delta x$, $\tilde{h}_3 = 4.0$; and
- at point $x_4 = x_1 + 3\Delta x$, $\tilde{h}_4 = 3.0$.

Water flows through two homogeneous domains:

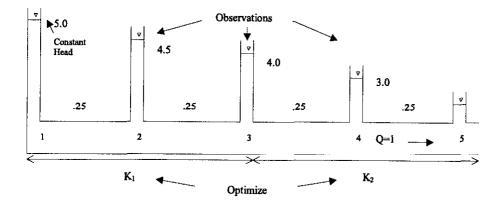


Figure 4. Problem definition for case study 3.

- $[x_1, x_3]$, with the (unknown) conductivity k_1 , and
- $[x_3, x_5]$, with the (unknown) conductivity k_2 .

No water is added or retrieved, therefore we can use equations (2.9) and (2.8) (with $Q(x_i) = 0$) to calculate the heads.

For each set of values $K = (k_1, k_2)$, these equations uniquely determine the actual values h_i of the heads. A prior estimate $k_1^{(0)} = 0.6$ and $k_2^{(0)} = 0.35$, along with an inverse inverse covariance matrix

$$V^{-1} = \begin{bmatrix} 50.5, 49.5 \\ 49.5, 50.5 \end{bmatrix},$$

was specified in [4].

Example: what was determined previously. By applying (heuristic) methods, the authors of [4] found *two* extremal points: $K^{(1)} = (0.465, 0.473)$ and $K^{(2)} = (0.723, 0.213)$, with values $L(K^{(1)}) = 0.2045$ and $L(K^{(2)}) = 0.1806 < L(K^{(1)})$.

Example: what we determined. We applied the Interval Newton method [1], [8], [10], [17] to the system of equations that describes the extremal points, and found not only the above two points, but also a third extremal point: $K^{(3)} = (0.582, 0.349)$.

In can be shown, by considering the Hessian of (5.1), that $K^{(3)}$ is a local maximum $(L(K^{(3)}) = 0.2232 > L(K^{(1)}))$. Therefore, in this particular case, the heuristic method computed the global minimum correctly. However, the very fact that this heuristic method missed one of the extremal points suggests that the global minimum too could have been missed.

This example illustrates the need to consider global methods, such as the Interval Newton method, to ensure guaranteed solutions of the optimization problem.

Future plans. The main objective of our study was to show the viability of interval techniques. Now that the viability is established, it is desirable to look for more

efficient ways of finding the global minimum. For example, we can use modifications of interval Newton method that enhance efficiency of the method [6], [15], or use alternative interval techniques (see, e.g., [20]).

6. Conclusion

The primary objective of our study was to demonstrate that interval techniques provide viable tools for solving the forward and inverse hydrological problems.

A major drawback of the existing interval techniques is the fact that they do not take into consideration the dependency between the medium coefficients, and, as a result, overestimate. It is, therefore, desirable to design methods that take this dependency into consideration.

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