Soft Constraints in Identification of Distributed Parameters

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Abstract—In this article, we introduce an idea of using soft constraint to improve effectiveness of existing optimization methods for identifying unknown parameter zones for distributed parameter identification problems. The constraint is put on the projected size of each parameter zone. But the constraint is only softly imposed due to uncertainty consideration. Two identification procedures based on such a constrained optimization idea are described. Results on three examples are presented to illustrate the advantages of this new approach.

I. INTRIDUCTION

We have developed over the past several years procedures for identifying unknown parameters of distributed parameter systems (cf. [1], [2]). Applications of those methods to parameter identification for groundwater flow and solute transport can be found in a newly developed comprehensive package vPIMM, Visual Parameter Identification for MODFLOW and MT3DMS (cf. [3]). In this article, we introduce soft constraints in those optimization methods for identifying distributed parameters of groundwater systems. We first discretize the unknown parameter into a number of zones. But unlike existing zonation based identification schemes that require a priori information regarding the shape and/or even the complete configuration of all the parameter zones, we do not impose any one of such assumptions regarding parameter zones. Instead, we assume that all the different types of zones have been observed at least in one location for each zone type and that each parameter zone is connected to an observation site of the same zone type. We also assume that each parameter zone occupies roughly a certain percentage of the entire system domain or is roughly of certain kind of shape. It is not realistic to assume an exact percentage of the entire domain and an exact kind of shape for each zone. Thus we only impose soft constraints in parameter identification procedures. Our objective is to find a good parameter distribution that would generate basically the same observation data at the observation locations.

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Even if the distributed parameters are discretized into a fairly small number of zone types, identification of such parameters usually leads to a large scale ill-conditioned optimization problem because zone shapes and boundaries are still unknown. We have observed in our tests of unconstrained parameter identification methods that significant disproportionality may occur among the sizes of identified zones (as evidenced in Figs. 1c, 1f, and 3c below). They could prevent the algorithms from escaping local minimum solutions without restarting. This disproportionality phenomenon occurs more often when the domain of the state variable of the distributed system becomes larger. We have been investigating effectiveness of using soft constraints on size and shape for improving the overall quality of the final solution. Soft constraints are enforced only up to a certain (prescribed) degree of tolerance. Preliminary results on soft size constraints are reported in this article. The identification algorithms will be described and hypothetical examples will be used for illustrating effectiveness of the proposed methods.

II. PARAMETER ZONE IDENTIFICATION UNDER SOFT SIZE CONSTRAINT

A distributed parameter identification problem is defined in terms of a state simulation model, a choice of unknown parameters distributed over the spatial domain of the system, and specification of an objective function along with some state and parameter observation data. For the state simulation model, we consider a 2-dimensional steady state saturated groundwater flow equation

$$\frac{\partial}{\partial x}(K(x,y)\frac{\partial}{\partial x}h(x,y))+\frac{\partial}{\partial y}(K(x,y)\frac{\partial}{\partial y}h(x,y)) + Q = 0 \qquad (2.1)$$

plus boundary conditions

with the hydraulic conductivity K as the unknown spatially varying parameter that needs to be identified, and the hydraulic head h as the state of the system. A slightly different case would use the transmissivity T in the flow equation instead of the hydraulic conductivity K (cf. [4]). In (2.1), u = h(x, y) is the state variable, Θ = K(x, y) or T(x, y) the unknown spatially varying

parameter to be identified. Observed data at observation locations can be denoted by u_O for the states and Θ_O for the parameter values. Our parameter identification problem is to find a "best" estimate of $\Theta(x, y)$ given u_O and Θ_O. To be more specific, we introduce a weighted output least squares error function

$$f(\Theta_S) = 0.5\,(u_O - u_S)^T P\,(u_O - u_S) + 0.5(\Theta_O - \Theta_S)^T Q\,(\Theta_O - \Theta_S), \qquad (2.2)$$

which is used to measure performance of the current estimate Θ_S. $u_S(x, y)$ is the simulated state under the parameter Θ_S using the state equation (2.1). P and Q are appropriate weighting matrices. Our state equation (2.1) is currently stated as a second order partial differential equation. We could have included additional time variable or another spatial variable z in the state model. Even other types of distributed systems could be considered. The identification problem is restated as an optimization problem.

Minimize $f(\Theta_S)$ subject to (2.1)
and other possible constraints.

Equation (2.1) along with the unknown parameter is discretized by the usual finite difference method. Since we are mainly concerned with large domains (especially three-dimensional ones) over which the parameter will be distributed, we need to make a couple of assumptions.

(A1). Parameter zonation. The unknown parameters can take on a finite number of values. Each distinct value defines a zone type. We assume that all different types of parameter zones have been observed.

(A2). Zone connection to an observation site. Every type of zone is connected to at least one observation site of the same type. Thus the number of parameter observation sites limits the total number of zones of the parameter distribution.

However we impose no assumptions regarding zone boundary locations and shapes of zones. The current assumptions are reasonable from both theoretical and practical considerations as explained in [1].

At least five individual parameter identification methods were originally proposed in vPIMM [3]. They didn't take into account any soft constraints on zone sizes and shapes (that is, ZC = 0 in the examples below). The soft size constraint is considered below. A desirable size percentage (denoted by ZP in the figures) is specified along with a nominal tolerance for each zone type (10% is used in the examples). We now introduce two approaches to implement the soft size constraint.

In the first approach (ZC = 1 in the examples), we simply introduce an additional step in the existing methods to modify proposed nominal unknown parameter configuration by trying to impose the soft size constraint before the trial configuration is evaluated by the objective function. Thus in the extra procedure, we take a trial solution that is already zoned. Check the size constraint and order the zone types according to the degree of size violations. For each violated zone type (starting from the one with the most violation) move portions of its zone boundary outward or inward depending on whether the current size is too small or too big. This is done for several cycles or until the soft size constraint is satisfied.

In the second approach (ZC = 2 in the examples), we integrate one of the original zonation procedures (cf. [2]) with addition of a constraint on zone sizes. The zonation procedure has been one of the key components of our original parameter identification methods. Thus in this case, we take a trial solution that may not be zoned. As zones are being build up starting from the observation sites, size constraints are constantly checked. This is done for several cycles or until the entire domain is zoned.

In order to compromise accuracy with efficiency, only a small number of cycles of internal soft size constraint loop are gone through in both approaches. Presumably no precise zone size information will be available anyway. There is rarely a need for complete enforcement of hard size constraints. Instead, we treated size constraints as soft ones. Consequently, it is possible that our final zone configurations may still violate the desired size constraints.

In summary, there are at least three major features of our approaches: zone classification capability under fairly weak assumptions, no a priori assumptions regarding zone shape and zone configuration of unknown parameters, and control of degree of uncertainty of zone sizes. We use the soft size constraint as a mechanism for restricting the search domain and consequently improving effectiveness and liability of the overall parameter identification method.

III. TEST EXAMPLES

To test performance of the new approaches, two versions of the simulated annealing algorithm have been applied to three examples, coupled with both soft size constraint strategies. They are indirect optimization methods, called ZMSA1 and ZMSA2 in vPIMM. In all the test results, we run each optimization method for up to 30 seconds or until no improvement in the best error. Repeat the process until no improvement in the best error in two consecutive runs.

Example 1. We consider a rectangular site with no-flow boundary conditions on the left and the right sides and constant head conditions at the top (h = 20 m) and the bottom (h =10 m). It is a hypothetical site with the

true parameter distribution (use T for this example) illustrated in Fig. 1b. We have discretized the spatial domain into 11x11 cells. Although the true global solution is shown in Fig. 1b, such information is never used in the entire search process. We assume that the true T takes on four different values (say, 0.01, 0.40, 1.50, and 5.00, in square meters per day), representing four significantly different types of the geological zones. The type indicators are shown in the figure. Observation locations are marked by the circles. Test results are shown in different parts of Fig. 1. Without the soft size constraint, very small zones have resulted as shown in Figs. 1c and 1f. But they are undetectable from the objective function values alone. The results of the two constrained runs are clearly better with the second run slightly better than the first.

Example 2. This is also a hypothetical example of another rectangular site with no-flow boundary conditions on the top and along the right side, a constant head condition at the bottom (h =100 m), and a constant flow condition on the left side (Q = 0.25 m/d). This time we use K for the unknown parameter with the true configuration illustrated in Fig. 2b. We assume that the true K takes on four different values (say, 5, 50, 150, and 300, in meters per day), representing four types of zones again. We used 30x30 discretized cells. Test results for this example are shown in different parts of Fig. 2. The true zone sizes are more uniform for this example. Procedures without soft size constraint perform better than the same procedures applied to example 1. ZC = 1 still outperforms ZC = 0. ZC = 2 leads to a quite different zone #1. But the objective function values are compatible.

Example 3. This is essentially the example 2 with the exact solution changed to the one shown in Fig. 3b. This is a more difficult problem with the true zone sizes being far from uniform. Test results for this example are shown in different parts of Fig. 3. Fig. 3c shows the worst. Procedures with soft size constraint options seem to offer better results.

Based on the test results, a number of observations can be made.

(1). The advantage of the new algorithm is more significant when the spatial domain of the system becomes larger or zone sizes are more nonuniform.

(2). In terms of the number of function evaluations (although not shown explicitly), the soft size constraint options are more efficient to reach a competitive level of objective function values.

(3). One noticeable disadvantage of the new approaches is that it is more likely to stop improving the objective function value after reaching a fairly desirable level. However, this kind of behavior is more or less expected since restriction on the search domain will inevitably lose some searching power for capturing certain detailed features of the solution. But this effect is not completely negative. After a certain level, a smaller error does not necessarily imply a better solution because of imperfection in the quality and quantity of the observation data.

IV. ACKNOWLEDGMENT

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V. REFERENCES

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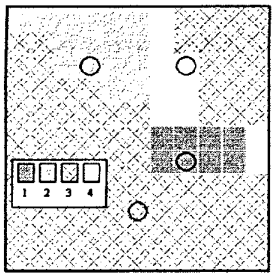

Fig. 1a Initial solution of example 1
with f=0.734, ZP = (6.6, 13.2, 71.9, 8.3)

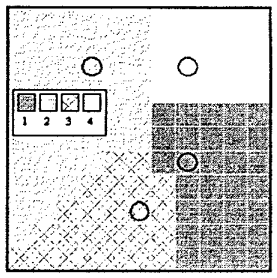

Fig. 1b True solution of example 1
with f=0, ZP = (38.1 25.6 19.8 16.5)

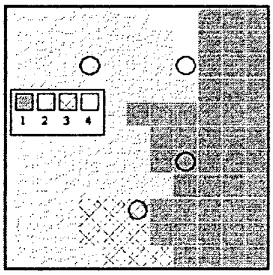

Fig. 1c Final solution of example 1 by ZSA1
f=.00243, ZP=(38.0, 51.2, 7.4, 3.3), ZC=0

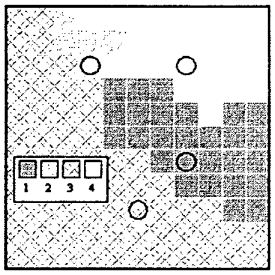

Fig. 1f Final solution of example 1 by ZSA2
f=.00416, ZP=(22.3, 4.1, 52.1, 21.5), ZC=0

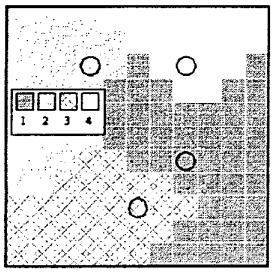

Fig. 1d Final solution of example 1 by ZSA1
f=0.107, ZP=(35.5, 25.62, 23.1, 15.7), ZC=1

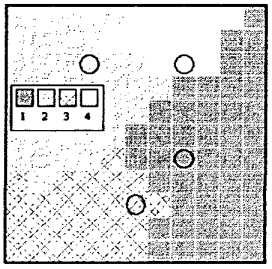

Fig. 1g Final solution of example 1 by ZSA2
f=.00245, ZP=(37.2, 31.4, 20.7, 10.7), ZC=1

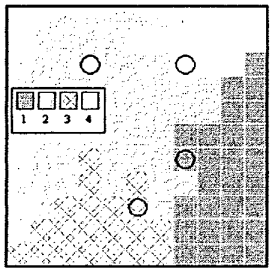

Fig. 1e Final solution of example 1 by ZSA1
f=.00818, ZP=(23.1, 49.6, 16.5, 10.7), ZC=2

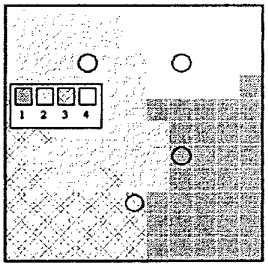

Fig. 1h Final solution of example 1 by ZSA2
f=.00122, ZP=(27. 3, 34.7, 20.7, 17.4), ZC=2

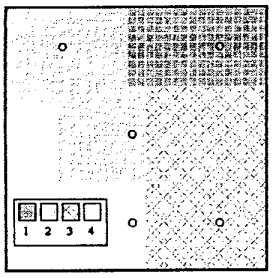

Fig. 2a Initial solution of example 2
f =53.01, ZP = (16.0, 27. 6, 32. 7, 23.8)

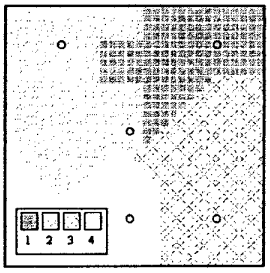

Fig. 2b True solution of example 2
with f = 0, ZP = (19.2, 30.7, 28.0, 22.1)

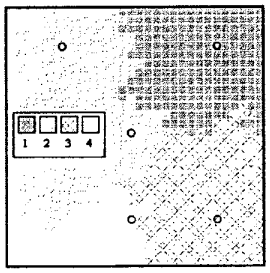

Fig. 2c Final solution of example 2 by ZSA1
f=0.678, ZP=(23.1, 41.9, 25.3, 9.7), ZC=0

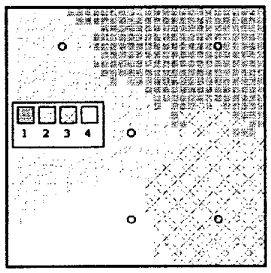

Fig. 2f Final solution of example 2 by ZSA2
f=0.223, ZP=(25.3, 35.8, 22.8, 16.1), ZC=0

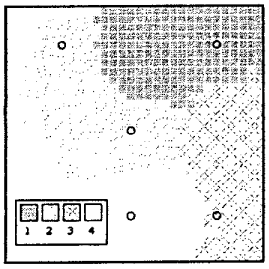

Fig. 2d Final solution of example 2 by ZSA1
f=0.593, ZP=(21.0, 31. 8, 19.1, 28.1), ZC=1

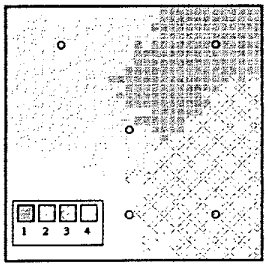

Fig. 2g Final solution of example 2 by ZSA2
f=0.127, ZP=(19.1, 31. 6, 27.1, 22.2), ZC=1

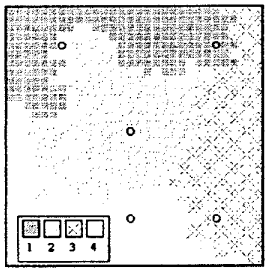

Fig. 2e Final solution of example 2 by ZSA1
f=0.302, ZP=(21.2, 34.3, 23.2, 21.2), ZC=2

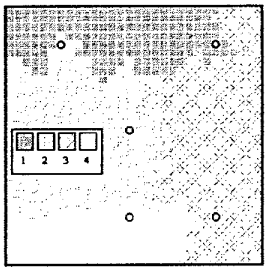

Fig. 2h Final solution of example 2 by ZSA2
f=.0414, ZP=(18. 8, 34. 7, 32.2, 14.3), ZC=2

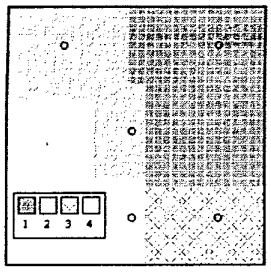

Fig. 3a Initial solution of example 3
f =184.56, ZP = (34.7,23.6,14.0,27.8)

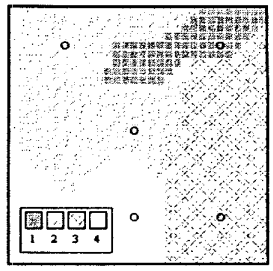

Fig. 3b True solution of example 3
with f = 0, ZP = (9.8 37.3 30.8 22.1)

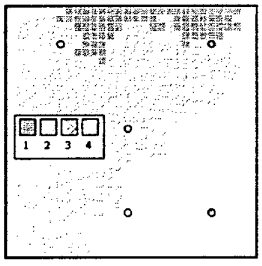

Fig. 3c Final solution of example 3 by ZSA1
f=0.157, ZP=(8.3, 56.4, 0.001, 35.1), ZC=0

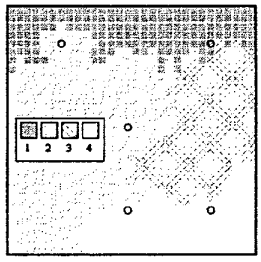

Fig. 3f Final solution of example 3 by ZSA2
f=0.228, ZP=(17.9, 43.7, 21.8, 16.7), ZC=0

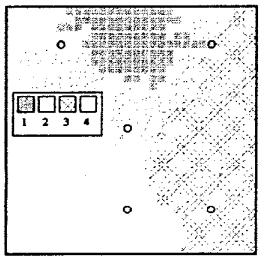

Fig. 3d Final solution of example 3 by ZSA1
f=0.156, ZP=(10. 9, 38.4, 29. 8, 20.9), ZC=1

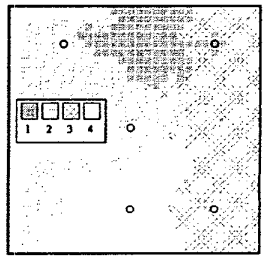

Fig. 3g Final solution of example 3 by ZSA2
f=0.3804, ZP=(10. 6, 40.0, 29. 8, 19.7), ZC=1

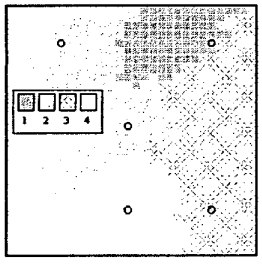

Fig. 3e Final solution of example 3 by ZSA1
f=0.261, ZP=(10.3, 40.0, 29.4, 20.2), ZC=2

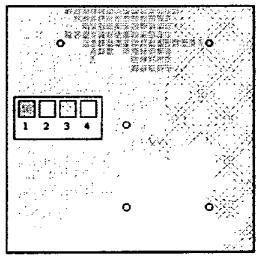

Fig. 3h Final solution of example 3 by ZSA2
f=0.0364, ZP=(9. 6, 41.1, 25.4, 23.9), ZC=2