Supplementary materials

1. The setting of the hypothetical actual parameter

In the experimental area, six parameter zones with six observation wells (OW) were designed according to the Voronoi diagram, and one pumping well (PW) was installed in each zone using Well Package (WEL). The Recharge Package (RCH) was introduced to model surface and boundary recharge parameters. Accordingly, the set specific yield across from Zone 1 to Zone 6 is 0.16, 0.20, 0.26, 0.18, 0.23, and 0.29, respectively; and the set specific storage across Zone 1 and Zone 6 is 1×10^{-3}, 1.5×10^{-3}, 2.5×10^{-3}, 2.0×10^{-3}, 3.0×10^{-3}, and 3.5×10^{-3} 1/m, respectively. There are four stress periods in 30 days of simulated time steps. The pumping rate of the well from PW1 to PW6 is assigned inversely proportional to the alluvial order, in which the corresponding values are set as -60, -50, -30, -40, -20, and -10 m^3/day, respectively. The aquifer bottom elevation is set as -10 m, and the initial head is set as 2 m. Considering the arid and semi-arid hydrogeological environment, the parameters across six zones are assigned according to the operation conditions from simulator MODFLOW-2005 embedded in ModelMuse v. 3.10 and from the UCODE solver in ModelMate v. 1.0.3 [1].

This study designed two hypothetical experiments to verify the capability and accuracy for identifying different kinds of inverse problems through the proposing SR3 VLS quasi-Newton algorithm. Experiment 1 tests six zonal hydraulic conductivities with single factor loading score constraints to approximate the Hessian and calculate the corresponding direction. The parameters to be identified in Experiment 2 are six zonal hydraulic conductivities, six surface recharges, and six boundary recharges that use overlain high–low factor loading scores to approximate and correct the Hessian. To enhance the identified accuracy, this study devises *LSE* of groundwater storage as the objective function. For verification and discussion of the causality associated with the ill-posed problem, the identified processes and results using the Jacobian quasi-Newton, and LMA from the USGS developed package UCODE embedded in software ModelMate v. 1.0.3, which uses *LSE* of groundwater head as the objective function, is also performed and compared.

2. Detailed optimization process and discussion of Experiment 1

The initial solution of hydraulic conductivity in Experiment 1 is set as a relatively larger value: 25 m/day. During the five iterations, the modified VLS quasi-Newton algorithm used the single factor loading score (i.e. symmetrical rank one structure) of higher rank components with an average of 3.33 and deeper depth components with an average of 3.20 for the Hessian approximation and for enlarging/scale along the direction which is corrected by the vectorized limited step sizes across multiple parameter zones, as shown in **Figure 1**(a). This indicates that hydraulic conductivity is the parameter that affects the fluctuation of groundwater storage to a lesser degree with longer travel time. The footprint of iterations vs. hydraulic conductivity in Experiment 1 optimized by the Jacobian quasi-Newton, LMA, and the SR1 VLS quasi-Newton algorithm is illustrated in **Figure 2**(a-1), **Figure 2**(b-1), and **Figure 2**(c-1), respectively. According to the footprint pattern, this study discovers that the use of single factor loading score is hard to detect the exact area of the global minimum, although the vectorized limited switchable step sizes were striving to accelerate convergence and correct the direction to approach a global optimum iteratively. Hence, the capability of converging to the true solution and achieving a well-posed problem by using SR1 VLS quasi-Newton is ordinary compared to those of the Jacobian quasi-Newton and LMA. A hybrid approach using multi-rank combined factor loading scores specialized for each zone would be promising to generate the lowest error in parameters and the groundwater head.

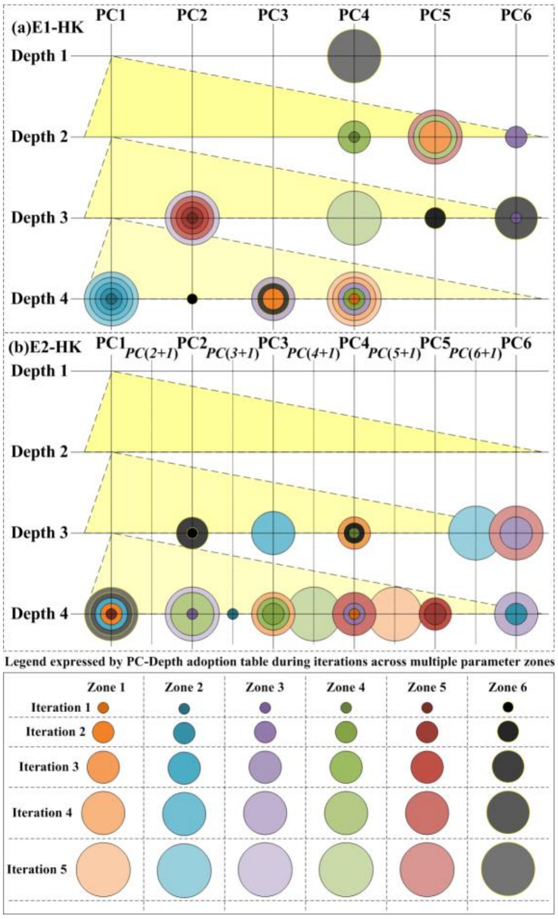

Figure 1. PC Rank Depth adoption diagram for identification of hydraulic conductivity during iterations across multiple parameter zones: (a) Experiment 1; (b) Experiment 2.

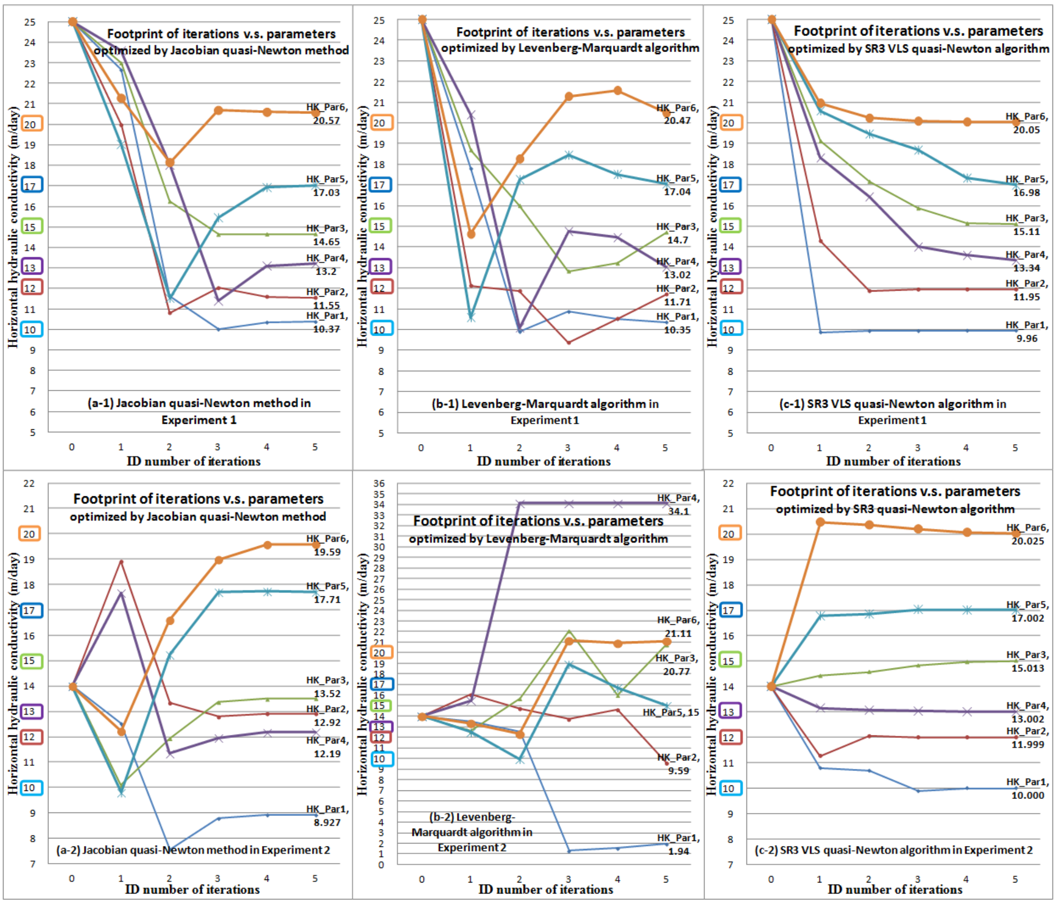

Figure 2. Footprint of iterations vs. hydraulic conductivity in Experiment 1 and Experiment 2 optimized by (a) Jacobian quasi-Newton method; (b) LMA; (c) SR3 VLS quasi-Newton algorithm.

3. Detailed optimization process and discussion of Experiment 2

The initial estimates of hydraulic conductivity in Experiment 2 use an assumed mean value of 14 m/day, and those of surface and boundary recharge rates use assumed averages of 8.667×10^{-4} m/day and 1.417×10^{-4} m/day, respectively. During the five iterations, for identification of hydraulic conductivity, the switchable SR3–SR1 VLS quasi-Newton algorithm used a low-rank (j=1) and high-rank factor loading score with an average of 3.35 in deeper depth components with an average of 3.71 from the simulated storage fluctuation between adjacent iterations to calculate the correction matrix for the Hessian and to enlarge/scale the direction corrected by the vectorized limited step sizes across multiple parameter zones, as shown in **Figure 1**(b). For surface recharge, all are distributed at shallow depth components with an average of 1.33 and mostly are distributed at low-rank components with an average of 3.57, as shown in **Figure 3**(a); for those of boundary recharge, the loading scores are distributed at middle-depth components with an average of 2.63 and are generally uniformly distributed across low-rank and high-rank components with an average of 4.13, as shown in **Figure 3**(b). This demonstrates that surface recharge is the largest and most direct factor affecting fluctuation in groundwater storage with shorter travel times, and boundary recharge greatly influences the groundwater storage fluctuations, albeit with longer response lag time.

The iterations vs. hydraulic conductivity footprints in Experiment 2 optimized by the Jacobian quasi-Newton, LMA, and switchable SR3–SR1 VLS quasi-Newton algorithms are illustrated in **Figure 2**(a-2), (b-2), and (c-2), and those of iterations vs. surface recharge and boundary recharge are illustrated in **Figure 4**. According to the footprint pattern, this study discovers that the combined high–low factor loading scores and partial application of single loading score can detect the global minimum area. Meanwhile, the super parameters with high sensitivity and simulation error in groundwater storage have priority for correction in front iteration, in which the vectorized limited switchable step sizes attempted to accelerate convergence along the corrected direction to move from the local to global optimum iteratively. Hence, the parameters identified by using switchable SR3–SR1 VLS quasi-Newton can converge to the true solution while solving nonlinear ill-posed problems. Besides, the VLS quasi-Newton only made 74 number of transient simulation times among five iterations for calculation of the Hessian matrix and step sizes, but that of the Jacobian quasi-Newton and LMA requires 192 number of simulation times. Hence, the VLS quasi-Newton only needs 38.47% of simulation times relative to the Jacobian quasi-Newton and LMA in the eighteen-zonal parameter system. Overall, according to the analysis results of Experiments 1 and 2, increasing three times of parameter's number in the Jacobian quasi-Newton and LMA would increase 0.63 times of model runs; while that in the VLS quasi-Newton, slightly reduces 1.3% of model runs.

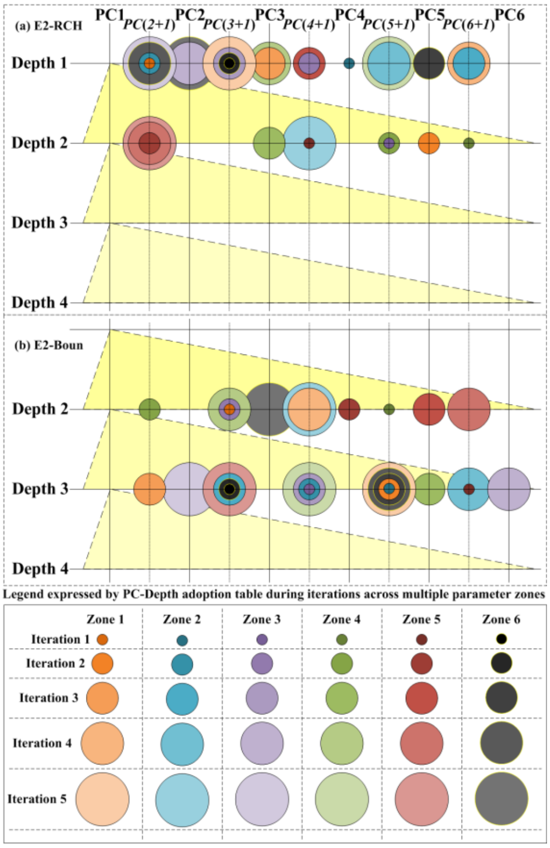

Figure 3. PC Rank Depth adoption diagram for identification of recharge during iterations across multiple zones in Experiment 2: (a) surface recharge; (b) boundary recharge.

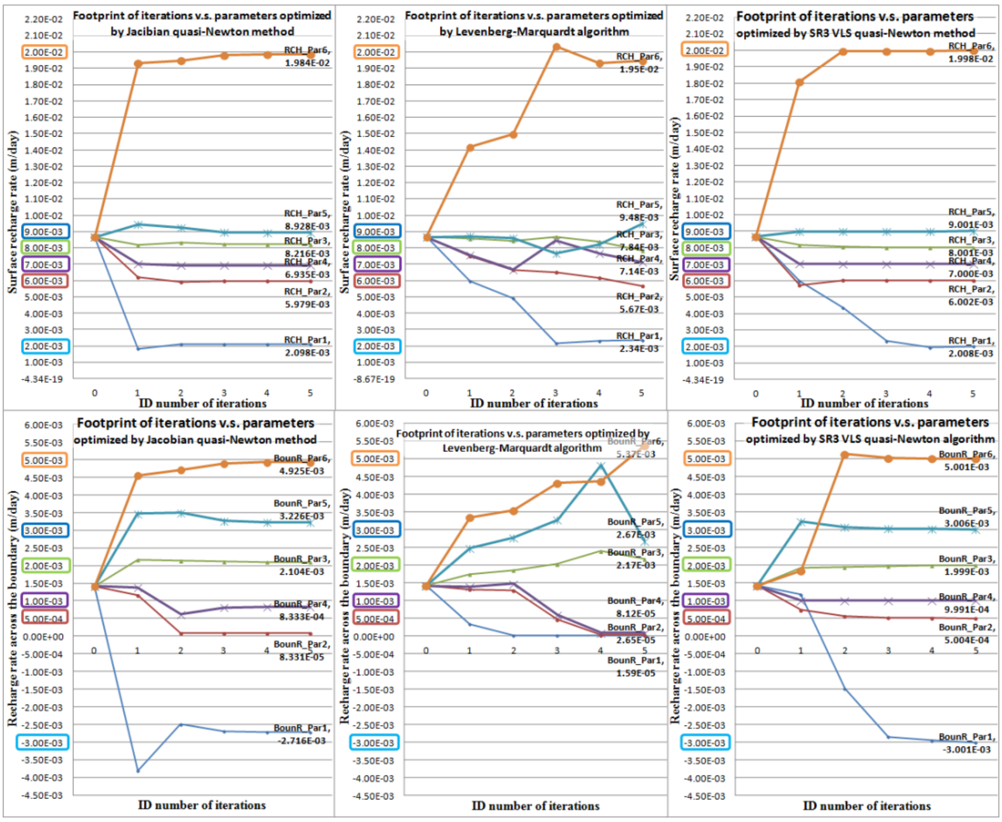

Figure 4. Footprint of iterations vs. surface recharge (-1) and boundary recharge (-2) in Experiment 2 optimized by (a) Jacobian quasi-Newton; (b) L–M algorithm; (c) SR3 VLS quasi-Newton algorithm.

References

1. Banta, E.R. Modelmate—a graphical user interface for model analysis. *U.S. Geological Survey Techniques and Methods*; USGS: Reston, Virginia, USA, **2011**.