Applicability of the most frequent value method in groundwater modeling

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Abstract The Most Frequent Value Method (MFV) is applied to groundwater modeling as a robust and effective geostatistical method. The Most Frequent Value method is theoretically derived from the minimization of the information loss called the I-divergence. The MFV algorithm is then coupled with global optimization (Very Fast Simulated Annealing) to provide a powerful method for solving the inverse problems in groundwater modeling. The advantages and applicability of this new approach are illustrated by means of theoretical investigations and case studies. It is demonstrated that the MFV method has certain advantages over the conventional statistical methods derived from the maximum likelihood principle.

Résumé On a appliqué la méthode de la valeur la plus fréquente (VPF) comme une méthode géostatistique robuste et efficace pour modéliser les eaux souterraines. Du point de vue théorique, la méthode de VPF part de la minimisation de l'information perdue, dénommée I-divergence. On couple après l'algorithme de la méthode de VPF avec la méthode d'optimisation globale affin de réaliser une méthode performante pour résoudre le problème inverse dans le domaine des eaux souterraine. Les avantages et les possibilités d'application de cette nouvelle approche sont illustrées par des investigations théoriques, ainsi que par des études de cas. On montre que la méthode de VPF présente certains avantages par rapport des méthodes statistiques conventionnelles basées sur le principe de la probabilité maximale.

Resumen El Método del Valor Mas Frecuente (VMF), es aplicado al modelamiento de agua subterránea, como un método geoestadístico simple y efectivo. Este método es derivado teóricamente de la acción de reducir al mínimo la pérdida de información, llamada así divergencia – I. El algoritmo del VMF es entonces acoplado con optimización global(Very Fast Simulated Annealing), para obtener así un método efectivo que resuelva los problemas inversos en el modelamiento de aguas subterráneas. Las ventajas y aplicabilidad de esta aproximación nueva son ilustradas a través de investigaciones teóricas y estudios de caso. Se demuestra que el método VMF tiene ciertas ventajas sobre los métodos estadísticos convencionales derivados del principio de la probabilidad máxima.

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Introduction

One of the main objectives of groundwater modeling is to determine the properly working earth models in order to adequately explain the hydrogeological observations. From the mathematical point of view, such solutions can be found by optimization (Lee 1999). Frequently, the inverse methods are used to determine the optimal parameter values of the groundwater models. Adjusting the estimates of the model parameters minimizes a special objective function, as a measure of the misfit or error, characterizing the deviation between the measured and calculated data. In Earth science applications, the objective functions may have multiple hills and valleys in the multi-dimensional parameter space. The conventional local search algorithms are usually trapped in one of the local minima instead of approaching the global minimum (Sen and Stoffa 1995). Such limitations of the conventional methods for hydrogeological problems can be circumvented by the application of the global optimization methods.

The calculated or theoretical data can be determined from the solution of mathematical models by assigning a set of prescribed values to the model parameters. This constitutes the forward problem. An accurate forward problem solution is vital for an effective inverse algorithm. Besides the forward and inversion problems, the

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applied statistical principle is also a key factor in successful modeling as the objective or error functions are based on different statistical norms and principles. Unfortunately, the old dogma still exists in that the estimation or the measuring errors are approximately normally (Gaussian) distributed (Huber 1981). Therefore, the application of the least-squares principles based on the maximum likelihood theory has been widespread even in geosciences. However, the efficiency of such classical algorithms is questionable when the actual error is not a Gaussian distribution.

The most frequent value (MFV) procedure (Steiner 1991, 1997) has been introduced as a robust and resistant method for geo-statistical data analysis and processing. This paper combines the MFV method with global optimization to provide more accuracy and reliability in parameter estimation in groundwater modeling and hydrogeology problems.

Theory of inverse procedures

A synthetic data set generated from a mathematical model using a set of assumed values for model parameters is compared with measured data. If the match is acceptable, the model parameter values are accepted as the best estimates. Otherwise, the parameters are modified to generate a new calculated data set and the quality of the match is investigated. This procedure is continued until a satisfactory match between the measured and calculated data is obtained. Therefore, the inverse procedures are usually regarded as optimization. The discrete data used in groundwater modeling is usually composed into a column vector as (Sen and Stoffa 1995):

$$d_{\text{measured}} = [d_1, d_2, d_3, \ldots, d_{\text{ND}}]T, \tag{1}$$

where ND is the number of measured data, and T denotes a matrix transpose. The parameters of a groundwater model are also given in a column vector:

$$m = [m_1, m_2, m_3, \ldots, m_{\text{NM}}]T, \tag{2}$$

where NM is the number of model parameters. The calculated or synthetic data (d_{cal}) can be generated by the solution of the forward problem, namely the g-operator, as:

$$d_{\text{cal}} = g(m). \tag{3}$$

Generally, the forward problem operator is not linear in hydrogeology. The objective is to determine the best estimate values of the model parameters, leading to the minimization of the difference between the measured (d_{measured}) and calculated (d_{cal}) data. For this purpose, properly-set objective or error functions are defined and referred to as statistical norms. The general L_p-norm of the error vector is given as (Menke 1984):

$$||e||_p = \left[\sum_{i=1}^{\text{ND}} |e_i|^p\right]^{1/p}. \tag{4}$$

The least-square norm, referred to as the L_2-norm, is the most common form derived from the L_p norms (Lines and Treitel 1984):

$$||e||_2 = \left[\sum_{i=1}^{\text{ND}} |e_i|^2\right]^{1/2}. \tag{5}$$

The L_2-norm divided by the number of data points (ND) yields the empirical square-root of variance or standard deviation, known as RMS (root-mean square) error (Isaaks and Srivastava 1989; Dobróka et al. 1991). Weighted L_2-norms can also be used when there is additional information about the measurements. When the observation errors are independent of each other and normally distributed, the optimal weighting coefficients can be the standard deviations of the observation errors. In practice, however, the standard deviations and the distribution types are usually unknown. The particular type of norm used in modeling determines the effectiveness and accuracy of parameter estimation. As the measured data can be originated from a very wide range of distributions and some errors or outliers can also be expected, the application of the L_2-norm has certain disadvantages in Earth science applications (Sun 1994). Hence, the use of the robust and resistant L_1-norm is more advantageous under these circumstances. However, the following P_k-norm, based on the MFV method (Steiner 1991, 1997), provides additional advantages over the L_1- and L_2-norms, as a robust and resistant measure of the model fitness:

$$P_k = \varepsilon \left[\prod_{i=1}^{\text{ND}} \left(1 + \frac{(d_i^{\text{measured}} - d_i^{\text{cal}})^2}{(k\varepsilon)^2}\right)\right]^{1/2\,\text{ND}}, \tag{6}$$

where ε denotes the scaling parameter or dihesion of the differences, as determined later.

When the relationship between the model parameters and the calculated data is not linear, a suitable linearization method, such as based on the truncated Taylor series expansion, can be resorted to simplify the solution. Thus, neglecting the second and higher order terms in the Taylor series leads to the following equations:

$$d_{\text{measured}} = g(m_0 + \Delta m) \quad \text{and} \quad \mathrm{d_{cal}} = \mathrm{g(m0)}, \tag{7}$$

$$d_{\text{measured}} = d_{\text{cal}} + \left.\frac{\partial g(m_0)}{\partial m}\right|_{m=m_0} \Delta m, \tag{8}$$

$$\Delta d = G_0 \Delta m, \tag{9}$$

where $\Delta d = d_{\text{measured}} - d_{\text{cal}}$. G_0 denotes a sensitivity matrix, including the partial derivatives of the calculated data with respect to various model parameters.

Frequently, the number of measured data (ND) is much larger than the number of model parameters (NM), leading to over-determined systems (Sen and Stoffa 1995). Hence, an important issue involving the inverse problems is to determine whether a unique solution exists (existence and uniqueness), and the solution can be regarded as

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being stable (stability). Inverse problems that do not possess uniqueness and stability are called ill-posed inverse problems. Otherwise the inverse problem is called well-posed. Nevertheless, techniques known as regularization can be applied to ill-posed problems to restore their being well-posed. Well-posed and over-determined inverse problems were investigated in this paper to demonstrate the usefulness of the proposed MFV algorithms. Resuming to Eq. (9), the L_2-norm yields a solution as:

$$\Delta m_{\mathrm{est}} = [GTG]^{-1} GT\Delta d. \tag{10}$$

To characterize the model parameters obtained by the inversion, consider the covariance given by:

$$[\mathrm{cov}\,\Delta \mathrm{m}_{\mathrm{est}}] = \sigma d^2 [GTG]^{-1}, \tag{11}$$

where σ_{d} is the root-mean-square difference between the computed and measured data. The discussion so far presupposes that all observations carry equal weights in the parameter estimation process. However, this will not always be the case as some measurements may be prone to different experimental errors than the others (Lebbe 1999). This means that the measured data can be weighted with a diagonal W-matrix if additional information is available for different observations. Consequently, Eqs. (10) and (11) can be modified, respectively, as:

$$\Delta m_{\mathrm{est}} = \left[G^T W G\right]^{-1} G^T W \Delta d, \tag{12}$$

$$[\mathrm{cov}\Delta m_{\mathrm{est}}] = \sigma_d^2 \left[G^T W G\right]^{-1}. \tag{13}$$

Applying the Marquardt–Levenberg algorithm, Eq. (12) can be modified as following to improve the search properties by an iterative procedure:

$$\Delta m_{\mathrm{est}} = \left[G^T W G + \alpha I\right]^{-1} G^T W \Delta d, \tag{14}$$

where α is called the Marquardt parameter, whose value gradually decreases to zero as the iteration progresses. Thus, initially the Marquardt–Levenberg method, frequently named as ridge-regression, operates based on the gradient principle. It then transforms into the Gauss–Newton method to seek an optimal solution. Although the Marquardt–Levenberg calculation can provide more stability, the effective operation still depends strongly on the initial guess assumed for the values of the model parameters for starting the iterative search. If the objective function has several local minima, the above-mentioned local search algorithms cannot provide the global minimum as a solution in case of a "bad" start of the parameter values search. This can be demonstrated by the following simple test problems. For example, consider the two-dimensional sinus cardinalis error function, given as (see Fig. 1):

$$z(x, y) = 1.1 - \sin\mathrm{c}(\mathrm{x}) \sin\mathrm{c}(\mathrm{y}). \tag{15}$$

This error-norm surface has several local minima and one global minimum location (x=0, y=0). Their locations are shown in Fig. 1. If the Levenberg–Marquardt algorithm is started from x=3.5 and y=0, the local minimum at

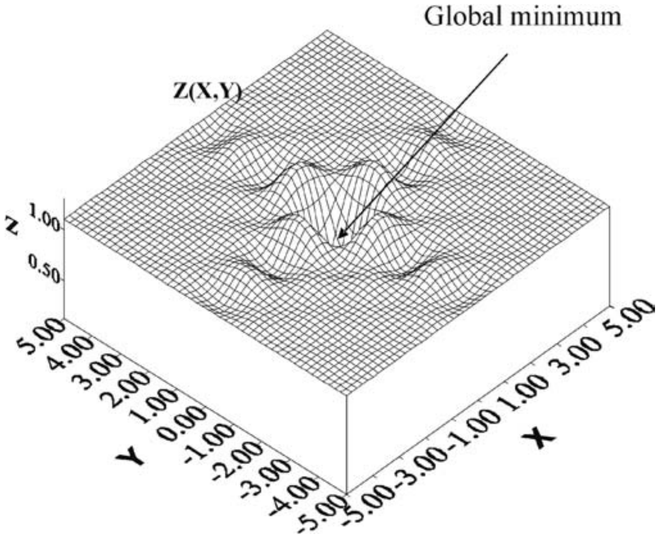

Fig. 1 Two dimensional error surface with several local minima and a global minimum at x=0 and y=0

x=3.53 and y=0 will be obtained as the solution. The experiment was repeated several times with different starting values to check the effectiveness of the global minimum search. The global minimum solution was obtained by the Levenberg–Marquardt method only when the starting point remained inside the "big pit." In contrast, the simulated annealing algorithm, described later, could easily solve this task without being trapped in the local minima locations. The solution x=0, y=0 was achieved in all cases regardless of the start of the model.

Complex groundwater models require numerical approaches for evaluation of the partial derivatives in the above-mentioned G sensitivity matrix. Consequently, additional numerical errors would be involved in the inversion process during the inverse matrix calculation of an inverse problem. These drawbacks of the local search algorithms underline the advantages of the global optimization methods for applications not only in hydrogeology but also in different branches of geosciences (Szucs and Civan 1996).

Global optimization and simulated annealing methods

Besides the genetic algorithms (GA), the simulated annealing (SA) methods have been applied widely to seek for global optimum in different engineering and natural science problems (Sen and Stoffa 1995). The works by Kirkpatrick et al. (1983) has shown that the model for simulating the annealing of solids, proposed by Metropolis et al. (1953), could be used for optimization problems, where the objective function to be minimized corresponds to the energy states of the solid and the control parameter corresponds to temperature, as defined later in the following. There are several modifications besides the classical Metropolis algorithms. The very fast simulated annealing (VFSA) method introduced by Ingber (1989)

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seems to be the fastest and most effective in multi-variable problems. The SA algorithms are easy to program and sufficiently fast even for cases involving a large number of unknown model parameters. Creating a classical Metropolis algorithm for a given groundwater modeling problem is relatively simple. The initial parameter vector is denoted as m_i. Consider the objective function (or error norm) denoted as $E(m_i)$. First, a new parameter vector (m_j) and the corresponding objective function $E(m_j)$ are generated. Then, the change in the value of the objective function, given as following, is examined:

$$\Delta E_{\mathrm{ij}} = E(mj) - E(mi). \tag{16}$$

If $\Delta E_{\mathrm{ij}} \leqslant 0$, then the new m_{j} parameter vector is always accepted. Contrary, if $\Delta E_{\mathrm{ij}} > 0$, then the probability of the acceptance of m_{j} parameter vector is determined using the Metropolis criterion, given by:

$$P = \exp\left(-\frac{\Delta \mathrm{E_{ij}}}{\mathrm{T}}\right), \tag{17}$$

where T corresponds to the temperature. This acceptance criterion provides an opportunity for avoiding entrapment in local minima. The temperature is decreased following a cooling schedule. An appropriate cooling schedule guarantees the convergent behavior of the method. Several studies have shown that decreasing temperature may result very rapidly in entrapment in a local minimum of the objective function (Sen and Stoffa 1995). Typically recommended choice considers a temperature variation proportionally to $1/\ln(n+1)$ at the n-th iteration (Szucs and Civan 1996).

Usually, the model parameters in practical problems may have different finite ranges of variations and may affect the error function differently. Therefore, it is reasonable to allow the various model parameters different amounts of perturbations from their current positions. Hence, Ingber (1989) modified the metropolis algorithm to elaborate VFSA method. Thus, consider that a model parameter m_i at iteration (annealing step or k) is bounded within a range of

$$m_i^{\min} \leqslant m_i^k \leqslant m_i^{\max}, \tag{18}$$

where $m_i^{\min}$ and $m_i^{\max}$ are the minimum and maximum values of the model parameter m_i. At iteration (k+1), the m_i model parameter value is perturbed using a random number generator ($u_i = (U[0,1])$ as:

$$m_i^{k+1} = m_i^k + y_i\left(m_i^{\max} - m_i^{\min}\right), \tag{19}$$

where

$$y_i = \mathrm{sgn}\left(\mathrm{u_i} - \frac{1}{2}\right)\mathrm{T_i}\left[\left(1 + \frac{1}{\mathrm{T_i}}\right)^{\left|2\mathrm{u_i}-1\right|} - 1\right]. \tag{20}$$

Ingber proved also that the following cooling schedule was effective in providing a global minimum:

$$T_i(k) = T_{0i}\exp\left(-\mathrm{c_i}\mathrm{k}^{1/\mathrm{NM}}\right). \tag{21}$$

The most frequent value (MFV) method

Besides a suitable optimization scheme, the formulation of an appropriate objective or error function also has a significant importance during any inverse calculation seeking for the best estimate values of the model parameters. The particular form of the statistical norm determines the performance of the optimization for a given error distribution. As proven previously by several geoscience applications and examples (Steiner 1972, 1988; Ferenczy et al. 1990; Steiner and Hajagos 1994; Szucs and Civan 1996), the application of the MFV procedure provides several advantages over the least-squares or other conventional statistical techniques in hydrogeology and groundwater modeling.

Having measured and calculated the data vectors in modeling as described earlier, the element of the residual vector (Δd) can be calculated by:

$$X_i = d_i^{\mathrm{mesasured}} - d_i^{\mathrm{cal}}. \tag{22}$$

The optimization objective of a groundwater modeling problem requires some kind of a norm of the residuals to be minimum. In most cases, the principle of the least-squares is applied. The classical statistics is based on this well-known principle, which can be easily formulated by the X_i residuals. Hence, the best model parameters set fulfils the minimum condition stated by:

$$\sum_{i=1}^{\mathrm{ND}} X_i^2 = \text{minimum}. \tag{23}$$

Although this minimum condition is commonly used, it has several disadvantages concerning the effectiveness and outlier sensitivity. Steiner (1965) alleviated this difficulty by introducing a principle of maximum reciprocals as:

$$\sum_{i=1}^{\mathrm{ND}} \frac{1}{X_i^2 + S^2} = \text{maximum}, \tag{24}$$

where S is a scaling parameter, characterizing the measurement error. A comparison of the above-defined principles reveals that the outliers heavily influence Eq. (23). Large measuring errors associated with one or more X_i–S may lead to unreal or misleading results in some cases. In such cases, the value of the expression given by Eq. (24) changes only by a negligible amount compared to Eq. (23). This property of the statistical procedure is referred to as resistance. Therefore, in this sense, the least-squares principle is not a resistant statistical procedure.

Applying the principle of the maximum reciprocals in a geostatistical analysis leads to the MFV technique (Steiner 1988, 1990, 1991, 1997; Hajagos and Steiner 1991). A statistical method is called an “MFV” technique if the X_i residuals are most frequently small (or even near zero) values. The condition stated by Eq. (24) forces the X_i residuals to be as small as possible in the overwhelming majority and it does not matter if therefore

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some X_i values become eventually very large. Consequently, statistical procedures derived from Eq. (24) are MFV procedures. However, this is not at all a unique property of the condition Eq. (24). For example, also the following condition results in an MFV technique:

$$\prod_{i=1}^{ND}\left(X_i^2+S^2\right)=\text{minimum}. \quad (25)$$

In case of a single unknown, that is if the location parameter (T) is to be determined, both Eqs. (24) and (25) can provide "the most frequent value" (MFV) in the sense that the $d_i^{\text{measured}}-S$ occur most frequently near the value of T, fulfilling the conditions stated by Eqs. (24) or (25). Now there is only one calculated data, i.e. the T, the residuals can be written as: $X_i=d_i^{\text{measured}}-T$. The value of T (or d_i^{cal}) obtained from the m parameter vector in a general case) resulting from the application of Eq. (23) requires that only a few X_i–S can be allowed to be large. However, even the largest values are required to be less than (one or) some X_i which can occur as a result of the same d_i^{measured} (i=1, 2,..., ND) sample while using Eq. (24) or Eq. (25). To achieve this, however, Eq. (23) sacrifices eventually the best d_i^{measured} values, because they cannot influence significantly the result T, or the resulting m parameter vector in a general case. Broadly speaking, Eq. (23) can provide such a T local parameter value, which is far away from the densest occurrence of the measured data.

The MFV procedures are sometimes called "modern statistical methods" (Steiner 1997), based on the idea first introduced by Steiner (1965). The hegemony of classical statistics even today can be perhaps excusable with the acceptance of the old dogma that "error distributions are always Gaussian" (Steiner and Hajagos 1995). Szucs (1994) showed that the frequently used statistical hypothesis tests, like the chi-square test (the χ^2-test), might lead to greatly misleading results. Monte Carlo simulations proved that the χ^2-test could not be recommended for the normality tests of different distributions occurring in practice. Even when the data samples significantly deviate from the Gaussian distribution, the χ^2-test accepts them as normally distributed with high probabilities at the most frequently used significance levels. As a result, when applying the χ^2-test the seemingly predominant presence of a Gaussian parent distribution may contribute to the survival of the traditional (non-robust and non-resistant) statistical algorithms. Assuming the observations to be normally distributed, the classical estimations are based on the maximum likelihood principle (MLE–maximum likelihood estimators). The MFV algorithm follows a completely different theoretical approach. The MFV method tends to achieve minimization of the I-divergence (information divergence) (Steiner 1997). I-divergence can be called as relative entropy and Kullback–Leibler distance, or a measure of information loss (Huber 1981). In the I-divergence theory, a substitute distribution is introduced and characterized to express the information loss.

Based on the minimization of the I-divergence, the theoretical background is elaborated to calculate the scale parameter (S) for the MFV criterion given by Eq. (25). Steiner (1991, 1997) presents a solution scheme for determining the scaling parameter in a way to minimize the information loss during statistical calculations. Therefore, the scaling parameter is also called dihesion, denoted by ε. Generalizing for the residuals, the expression for dihesion is given by:

$$\varepsilon^2=\frac{3\sum_{i=1}^{ND}\frac{X_i^2}{\left[X_i^2+\varepsilon^2\right]^2}}{\sum_{i=1}^{ND}\frac{1}{\left[X_i^2+\varepsilon^2\right]^2}}. \quad (26)$$

In turn, this implicit equation is also used for determination of the dihesion ε iteratively. It is very important to emphasize that ε is resistant against the outliers. In contrast, the standard deviation belonging to the least-squares approach is extremely sensitive to the outliers. It is more suitable to define S in Eqs. (24) and (25) as a multiple of or k-times the dihesion, that is $S=k\varepsilon$ The best value of k to be used depends upon the actual probability distribution type of the residuals. The dihesion plays a key role in the MFV procedures.

It is also important to describe the distribution types for the residuals (or the errors). For the sake of simplicity, all types of density functions will be given for the standard case, i.e. the case when the symmetry point lies in the origin and the value of the scale parameter is equal to unity. In classical statistics, the error distribution is assumed always nearly Gaussian. The corresponding density function is well known and given by:

$$fG(X)=\frac{1}{\sqrt{2\pi}}\exp\left(-\frac{X^2}{2}\right) \quad (27)$$

Because the error distribution cannot be known exactly apriority, it is more convenient to define a so-called supermodel distribution function, which can represent various distributions by changing a supermodel parameter. Although the actual distributions are probably not Gaussian, a symmetric distribution is expected for the residuals. This condition is satisfied in most cases. However, the distribution of the residuals may not be unimodal and symmetric. Then, a simple transformation can be sought in order to express a distribution as a symmetrical one (Kitandis 1997). For this purpose, various Earth science data and error distributions may be described effectively by using a $f_a(X)$ supermodel, given as (Steiner 1991, 1997):

$$f_a(x)=\frac{\Gamma(a/2)}{\sqrt{\pi}\Gamma((a-1)/2)}\frac{1}{(1+X^2)^{a/2}}, \quad (28)$$

where "a" is the supermodel parameter (a>1), and Γ denotes the usual gamma function, given by:

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$$\Gamma(z) = \int_0^\infty e^{-t} t^{z-1}\, dt, \quad z > 0 \tag{29}$$

For example, f_a=2(X) corresponds to the Cauchy distribution, given by:

$$f_{a=2}(X) = f_{\mathrm{Cauchy}}(X) = \frac{1}{\pi}\frac{1}{1+X^2} \tag{30}$$

The special Gaussian-bell shaped curve is obtained in the limit case as $a \rightarrow \infty$. The so-called geostatistical probability function is obtained when a=5 (Dutter 1987; Hajagos and Steiner 1995):

$$f_{a=5}(X) = \frac{3}{4}\frac{1}{(1+X^2)^{5/2}}. \tag{31}$$

Dutter (1987) showed that this probability density would be the most representative type in the geosciences. Instead of the classical L_p-norms (Eq. (4)), the so-called P_k-norms can be defined based on the MFV method (see also Eq. (6)):

$$P_k = \varepsilon \left[\prod_{i=1}^{\mathrm{ND}} \left(1 + \frac{\left(d_i^{\mathrm{measured}} - d_i^{\mathrm{cal}}\right)^2}{(k\varepsilon)^2} \right) \right]^{1/2\,\mathrm{ND}} \tag{32}$$

This norm corresponds to the principle of minimum products (Eq. (25)). For more accurate numerical calculations, the following form of the P_k-norms based on the principle of maximum reciprocals (Eq. (24)) would be preferred using the residuals (X_i):

$$P_k = 2\varepsilon\left(k^2+1\right)\frac{1}{\mathrm{ND}}\sum_{i=1}^{\mathrm{ND}} \frac{X_i^2}{3(k\varepsilon)^2 + X_i^2}. \tag{33}$$

It was also proved that the MFV method could be formulated as a so-called "iteratively re-weighted least-squares (IRLS) algorithm". Although the most-frequent value can be defined this way, its theoretical foundation and derivation are not related to the least-squares principle as discussed earlier. In case of a single unknown, i.e. if the location parameter (T) is to be determined, a double-iteration formula should be used for the calculation of T and ε, given as:

$$T = \frac{\sum_{i=1}^{\mathrm{ND}} X_i W_i(X_i)}{\sum_{i=1}^{\mathrm{ND}} W_i(X_i)}, \tag{34}$$

where the weights $W_i(X_i)$ and the dihesion are computed, respectively, by:

$$W_i(X_i) = \frac{(k\varepsilon)^2}{(k\varepsilon)^2 + (X_i - T)^2}, \tag{35}$$

$$\varepsilon^2 = \frac{3\sum_{i=1}^{\mathrm{ND}} (X_i - T)^2 (W_i(X_i))^2}{\sum_{i=1}^{\mathrm{ND}} (W_i(X_i))^2}. \tag{36}$$

Ths selection of k value is related to the efficiency calculations. The best value of k can be determined for a given error distribution. On the other hand, the MFV method is a very robust statistical procedure. This means that the choice of the k value affects the statistical efficiency very slightly. Therefore, only three different k values are proposed here. The value of k=2 is recommended if no previous information exists about the type of the actual distributions. If short flanks are expected, then k=3 should be used. If the actual distribution is of the Cauchy type, then k=1 provides the best statistical efficiency (Steiner 1991, 1997). It was further proven by Steiner (1991, 1997) that the MFV procedures are not only resistant but also robust. The attribute denoted as being "robust" generally indicates the efficiency of the statistical procedure is not very sensitive to the type of change. The estimates of T have a finite asymptotic variance, i.e. the law of large numbers is always fulfilled for the MFV calculations. The least-squares method does not satisfy this law if for example the error distribution is of the Cauchy type (Steiner 1991, 1997). Steiner (1991, 1997) proved that L_1-methods (based on the median principle) have a general robustness (efficiency) of 50.1% for the expected geosciences error distributions. This is much higher than the general robustness of the classical statistics (based on the L_2-norm). The latter does not have a higher efficiency than 7.8%. The general robustness of the MFV-methods are, however, always significantly greater than that of the L_1-procedures. The general robustness is higher than 90% for the Pk-norms. The theoretically most adequate definition of the efficiency of an arbitrary statistical procedure is given by:

$$\text{Statistical efficiency}\,(\%) = \frac{\text{extracted information}}{\text{total information}} \times 100 \tag{37}$$

Undoubtedly this definition provides a real measure of the statistical efficiency. However, a practically usable definition for numerical calculation of the statistical efficiency, denoted by e, is given by:

$$e\,(\%) = \frac{\text{minimum possible asymptotic variance}}{\text{asymptotic variance}} \times 100 \tag{38}$$

The denominator can be calculated for the actual applied statistical procedure. The nominator is the so-called Cramer–Rao bound, which can be found in almost every handbook of mathematical statistics, such as in Huber's (1981) famous book about robust statistics. The Cramer–Rao bound ($A^2_{\min}$) can be computed for the supermodel f_a for a given parameter as (Steiner 1997):

$$A_{\min}^2 = \frac{a+2}{a(a-1)}. \tag{39}$$

Steiner (1997) also derived the asymptotic variances for the least-squares method and MFV procedures if the actual error distribution is from the f_a supermodel:

$$A_{L_2}^2 = \frac{1}{(a-3)}, \tag{40}$$

and

$$A_{\mathrm{MFV}}^2 = \frac{\int_{-\infty}^{\infty} \frac{x^2}{\left((k\varepsilon)^2+x^2\right)^2} f_a(x)\,\mathrm{dx}}{\left[\int_{-\infty}^{\infty} \frac{(k\varepsilon)^2-x^2}{\left((k\varepsilon)^2-x^2\right)^2} f_a(x)\,\mathrm{dx}\right]^2}. \tag{41}$$

Applying these expressions, the efficiency relationships can be also derived for the least squares and MFV procedures if the actual error distribution is coming from the f_a supermodel. As mentioned earlier, the f_a supermodel can represent a very wide variety of actual geoscience data or error distributions as the supermodel parameter "*a*" is assigned appropriate values (from a Gaussian to the Cauchy type).

$$e(L_2) = \frac{(a+2)(a-3)}{a(a-1)}, \tag{42}$$

$$e(\mathrm{MFV}) = \frac{(a+2)}{a(a-1)A_{\mathrm{MFV}}^2}. \tag{43}$$

Figure 2 describes these efficiency relationships as a function of t=1/(a–1). This simple parameter transformation has a particular advantage in mapping the semi-infinite range of the supermodel parameter "*a*" value, varying from 2 to ∞, to the finite range of 0–1 for variation of the "*t*" value. Using the transformed t value for the horizontal axis, Fig. 2 provides a clear depiction of the robustness of this mapping function. The least-squares procedure works with 100% efficiency if the error distribution is Gaussian. This is not surprising because the least-squares estimate is the best when the distribution is Gaussian. Unfortunately, its efficiency diminishes sharply to zero for error distributions having longer tails. Therefore, the least-squares principle should not be applied for any type of distribution other than the Gaussian type. In contrast, the MFV procedure is very highly efficient (>90%) regardless of the distribution type. The MFV procedure performs the best statistics for the geo-statistical distribution (a=5), where the efficiency value is 100%. Therefore, the general high robustness of the MFV procedure is unarguable.

Besides their robustness, the MFV methods are also resistant. It can be seldom guaranteed that data are outlier-free. The appearance of the outliers may be very different (even rhapsodic). Statistical algorithms should be tested about their sensitivity or insensitivity (resistance) against the outliers. The outliers are due to measurement as well as model errors (Valstar et al. 2004). It does not matter to the MFV algorithms whether the greatness of the residuals is influenced by the measurement errors or the model errors. The above-mentioned double iteration process of the MFV methods guarantees a convergent solution to find the MFV and the dihesion or the inverse problem solution independently from the initial model parameter estimates. A large initial misfit does not influence the MFV method in finding the solution. When the solution is automatically provided the outliers of the residuals can be detected based on the MFV weights. A residual having a very small weight (W_i close to 0) can be identified as an outlier. Alternatively, if a certain measurement value is actually correct and reliable, then a large value or a small MFV weight of the outlier residual may be attributed to a model parameter error. Obviously, this may be important information for the hydrogeologist. This way of judgment was also applied in the discussion in the following field problem.

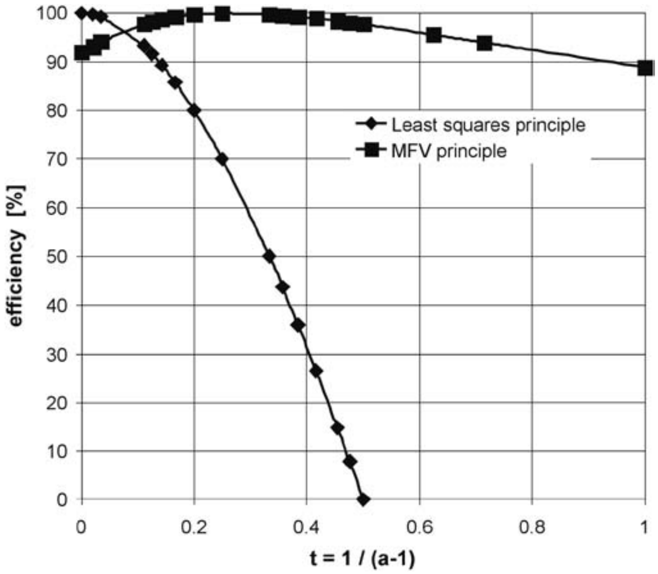

Fig. 2 Efficiency curves for the least squares and MFV procedures for the $f_a(X)$ supermodel

Applications for model and field problems

Although a natural science approach, that a groundwater reservoir is a general geologic medium, is very important in hydrogeology (Tóth 1999), sophisticated mathematical and statistical methods are also inevitable to increase the accuracy and efficiency of the relevant interpretation processes. Marsily et al. (2000) present an outstanding review about the inverse problems in hydrogeology. This study also reveals that this research area is very diverse and challenging. Although Carrera and Neuman (1986a, b, c) offer a very effective summary of the standard inverse techniques available in groundwater modeling, further work is necessary in order to make the inverse algorithms as a routine approach for practitioners (Poeter

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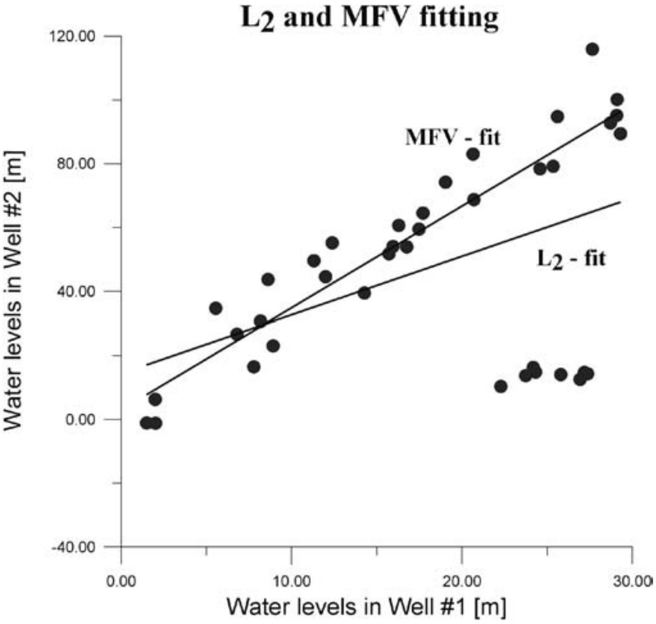

Fig. 3 Linear regression for water level data using the least-squares and MFV principles

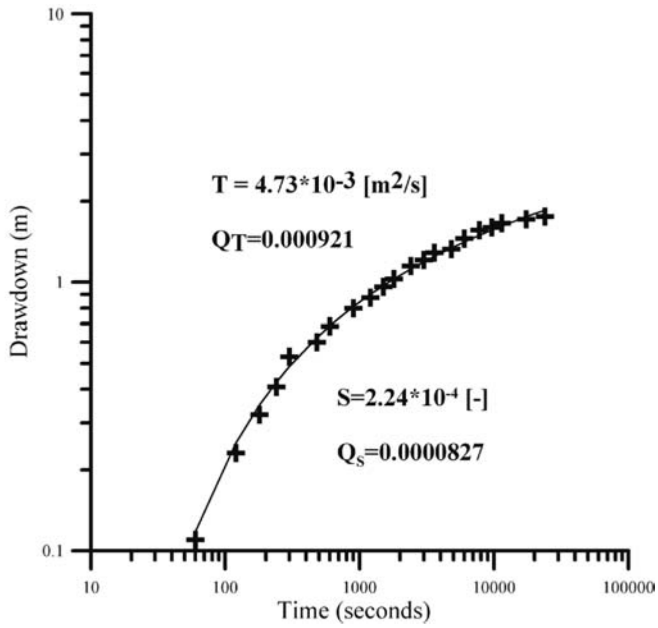

Fig. 4 Results of a pumping test interpretation using the MFV method. The uncertainties of the hydraulic parameters (Q_T and Q_S) are also determined

and Hill 1997). New techniques, like the representer-based inverse method (Valstar 2001; Valstar et al. 2004), have been elaborated for groundwater flow and transport applications. These are especially advantageous in such problems that the number of independent unknowns is proportional to the number of measurements. The representer-based procedure replaces the original inverse problem by an equivalent problem.

The MFV procedures may be facilitated for many problems in hydrogeology. Figure 3 shows an example of a simple linear fitting of the water level data derived from a thick Pleistocene aquifer. Water levels were measured in two different wells, where there was a strong correlation between the levels because of hydraulic communication between the screened layers. This strong relationship was also given by the generalized and robust correlation factor (Steiner 1997). Although it was derived from the traditional Pearson correlation coefficient, the generalized correlation factor has also a robust and resistant behavior. The traditional (Pearson-type) linear correlation factor showed only a weak relationship due to presence of the outliers. Figure 3 indicates that the linear relationship based on the least-squares principle can be heavily influenced by the presence of outliers (produced artificially by human error in this case). Whereas, the MFV procedure clearly avoids the misleading bunch of data and provides a realistic linear physical relationship instead of a statistically distorted one. For the MFV fitting, the following expression was minimized by the SA method to derive the values of the fitting parameters (a and b) for the linear regression equation.

$$P_2 = \varepsilon \left[\prod_{i=1}^{\mathrm{ND}} \left(1 + \frac{\left(h_{2,i} - \left(ah_{1,i} + b\right)\right)^2}{(2\varepsilon)^2} \right) \right]^{1/2\,\mathrm{ND}}, \qquad (44)$$

where $h_{1,i}$ and $h_{2,i}$ values are the measured water levels in wells #1 and #2, respectively.

Szucs (2002), and Szucs and Ritter (2002) applied the MFV procedures successfully for interpretations of several pumping tests. A well-defined geo-statistical method based on the MFV concept has been elaborated to determine the hydraulic parameters and their uncertainties. These are the necessary input data for a reliable groundwater modeling. The suggested algorithm is well posed from the point of existence, uniqueness, stability, and robustness. This new evaluation method is proven and validated for different pumping test interpretation methods (Kruseman and Ridder 1990). The main advantage of the suggested inverse procedure is that the uncertainty or the reliability of the hydraulic model parameters can also be determined by the MFV procedure and Monte Carlo simulations using one set of measured field data (Fig. 4). Artificial measuring errors are superimposed to the original measurements, and the inversion process is repeated several times. The applicability and usefulness of the introduced procedure have been demonstrated by means of several case studies on the ground water modeling problems concerning the northern Hungarian region (Szucs 2002; Szucs and Ritter 2002).

The following case studies give simple examples of the MFV inverse applications to improve groundwater modeling calibration results. The hydraulic head prediction that comes from a flow model is commonly used as the

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basis for model calibration. Calibration is a process of adjusting the model parameters to achieve a satisfactory match between the predicted (or calculated) and measured hydraulic heads (Hill 1998). Practically, calibration is an inverse process. Most commonly, calibration is accomplished by a trial-and-error adjustment of the model parameters based on the expert experience to achieve the best match between the measured and calculated data. The calibration based on the above-mentioned mathematical approaches is referred to as the automated inverse procedures in groundwater modeling (Hill 1992). Frequently, the objective function used as a calibration criterion is based on the mean error, the mean-absolute error (L_1 norm), or the root-mean-square error (RMS error, L_2 norm) (Anderson and Woessner 1992). Concerning the hydraulic heads (h), the RMS error can be defined as:

$$\mathrm{RMSE} = \left[\frac{1}{\mathrm{ND}}\sum_{\mathrm{i}=1}^{\mathrm{ND}}\left(\mathrm{h}_{\mathrm{i}}^{\mathrm{measured}} - \mathrm{h}_{\mathrm{i}}^{\mathrm{calculated}}\right)^2\right]^{0.5}. \tag{45}$$

Szucs and Ritter (2002) introduced the above-mentioned P_k-norm for groundwater model calibration purposes. Because the real data, and the error or residual distribution can never be known in advance, the usage of $P_{k=2}$-norm is most favorable for groundwater modeling. The definition of the $P_{k=2}$-norm is given based on above-mentioned theory as:

$$P_{k=2} = \varepsilon\left[\prod_{i=1}^{\mathrm{ND}}\left(1 + \frac{\left(\mathrm{h}_{\mathrm{i}}^{\mathrm{measured}} - \mathrm{h}_{\mathrm{i}}^{\mathrm{cal}}\right)^2}{(2\varepsilon)^2}\right)\right]^{1/2\,\mathrm{ND}}. \tag{46}$$

To demonstrate the advantage of the MFV procedure and global optimization in groundwater modeling, two main examples are provided here. First, the above-described methodology is tested and verified by means of the synthetic data of a predefined groundwater model. Then, a practical wellhead protection zone delineation example is carried out in order to illustrate the application of the suggested method.

Test problem

A simple one-layer unconfined steady-state groundwater model has been facilitated to describe and investigate the behavior of the proposed global optimization (SA) method and the MFV procedure. The x–y dimension of the test model is 1 km by 1 km. The top of the model layer is on 25 m. The bottom of the model layer is 0.0 m. The basic grid size is 20 m. A constant recharge rate at 0.0003 $m^3/(m^2$ day) was applied on the top of the grid system. Four polygons were delineated to represent the layer heterogeneity in the aquifer. The horizontal hydraulic conductivity is assumed to be constant in each polygon. Specified head boundary conditions were introduced on the west and east borders to simulate the natural groundwater flow from west to east. One production well was seated in each of polygon I (–400 m^3/s), II (–500 m^3/s) and III (–300 m^3/s). There is no well in polygon IV. As over-determined systems are preferred for any statistical interpretation, 12 observation points were stationed in the model for the groundwater calibration. As a general working frame, the Groundwater Modeling System 4.0 package (EMRL 2002) was applied for the test problem investigation. The flow model has been created with the help of the MODFLOW-2000 package (Harbough et al. 2000) using the prescribed model parameters.

Creating a flow model based on the actual model parameters is called a forward solution. The water levels could be derived exactly for the 12 observation points. To simulate real measured water level data at the observation points, 2% random geostatistical error was superimposed on the exact water levels. Having a pre-defined hydrogeological model and the "measured data set," the inverse investigations could be started. The GMS 4.0 system provides three built-in possibilities for automated inverse parameter estimation. These are the PEST (Doherty 2000), the UCODE (Poeter and Hill 1998), and the MODFLOW-2000 PES (Hill et al. 2000) procedures. They are similar in effectiveness and all of them are based on the classical statistical approaches. The MODFLOW-2000 PES method has been selected for comparison of the investigations with the present MFV based inverse algorithm using a global (metropolis simulated annealing) optimization (noted as MFV–SA). The MFV–SA inverse method has been also linked to the popular MODFLOW-2000 package, which provides the forward solution. In addition to the well-described error functions (RMSE and P-norm), the relative model distance (RM) given by Eq. (47) has also been used to characterize the accuracy of the compared inversion procedures.

$$\mathrm{RM} = \left(\frac{1}{\mathrm{NM}}\sum_{i=1}^{\mathrm{NM}}\left(\frac{m_i^0 - m_i}{m_i^0}\right)^2\right)^{1/2}, \tag{47}$$

where NM is the number of model parameters (NM=4 in the present case), m_i^0 is the value of the i-th true model parameter (hydraulic conductivities in the present test case), m_{i} is the i-th model parameter estimated based on the actual inverse procedure. In synthetic investigations, the relative model distance can also be used because the predefined model is known. Whereas in actual inversions involving the field problems, this useful parameter cannot be calculated, because the true model parameter values are never known exactly.

The present application of the MFV procedure utilized the classical simulated annealing global optimization search, because there were only four model parameters. However, for large-scale groundwater models, the application of the VFSA is recommended to reduce the computer running time. For illustration, the metropolis (SA) algorithm was applied with the parameter values given as follows. The initial temperature is T_0=1.0. The final temperature is T_{f}=0.0001. The temperature reduction constant is α=0.975. The number of iterations at each temperature is $R(t)$=300. Table 1 gives a summary of the most important results obtained by the MODFLOW-2000 PES and MFV+SA algorithms. The results clearly indi-

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Table 1 The main results of the inverse procedures carried out by MODFLOW-2000 PES and MFV–SA methods in case of 2% geostatistical distribution error added to the theoretical heads at the observation points

Test problem investigated by different inversion methods			
Model polygon	Prescribed model parameters	Model parameters from inversion	
		MODFLOW-2000 PES	MFV–SA
I	25 m/day	11.52 m/day	18.72 m/day
II	35 m/day	27.65 m/day	32.14 m/day
III	15 m/day	6.46 m/day	10.92 m/day
IV	10 m/day	1.90 m/day	7.38 m/day
Error function		RMSE=0.203 m	*P*-norm = 0.172 m
Relative model distance		RM=0.58	RM=0.27

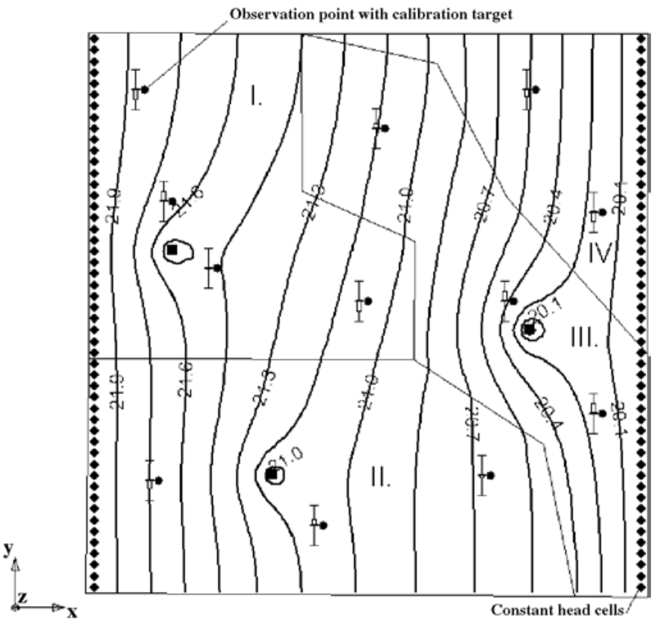

Fig. 5 Water levels in the flow model obtained using the most frequent value inverse procedure

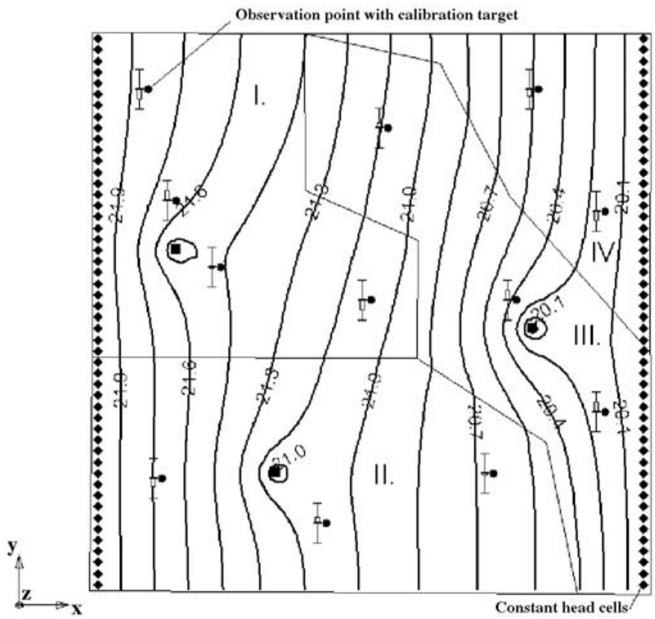

Fig. 6 Water levels in the flow model obtained using the MODFLOW-2000 PES inverse procedure

cate a great difference in the relative model distance (RM) values although the objective function values (RMSE and *P*-norm) are not far from each other. The relative model distance (RM=0.58, MODFLOW-2000 PES) reduces by half when the MFV based inverse procedure is applied (RM=0.27). Figures 5 and 6 also indicate the advantage of the MFV approach. Figure 5 shows nearly the same flow pattern as that of the original model. Figure 6 reflects the general trends of the original model, but it involves many more disturbances. The four polygons, where the hydraulic conductivity values are different, can also be seen on Figs. 5 and 6. Note that even the MFV–SA method was not able to give back the original model parameters. This is truly understandable because a complication in groundwater problems arises when the information about the head distributions is incomplete (Anderson and Woessner 1992). In this example, only 12 "observed data" are present. Therefore, it is important to appreciate and consider every piece of information concerning the heads. Hence, the statistical methods with high efficiency should be used during the interpretation.

Field problem

In general, the field experts prefer to use the commercially available professional groundwater modeling packages for hydrogeological evaluation and interpretation, such as the above-mentioned Groundwater Modeling System (GMS 4.0) or the Processing Modflow (Chiang and Kinzelbach 2001). Although these packages have built-in inverse modules like PEST, UCODE or MODFLOW-2000 PES, the trial-and-error calibration is still preferred in many cases because the modeler's expertise and experience can be involved in the process easily. In the following, the advantage of the MFV-based inverse groundwater modeling is demonstrated by a field example. Creating an inverse modeling program is not an easy task because it is difficult to incorporate the present improved subroutine to the existing standard groundwater modeling packages. Nevertheless, the following example demonstrates how easily and advantageously the MFV procedure can be applied to improve the interpretation results even in the case of traditional trial-and-error calibration.

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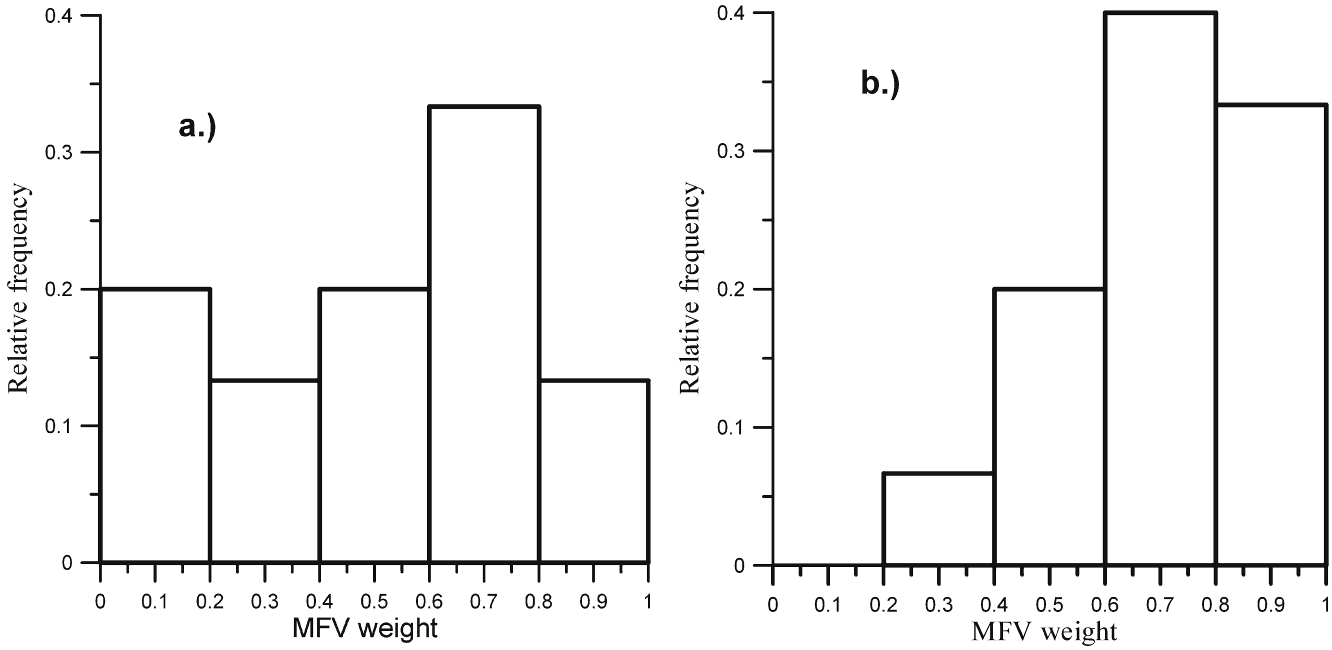

Fig. 7 Histograms of the MVF weights during the calibration process. The *left histogram* (**a**) shows an early stage and the *right histogram* (**b**) reflects the end of the trial-end error calibration

There is an ongoing national project supported by the Hungarian government to delineate the wellhead protection zones for vulnerable groundwater resources. The particle tracking MODPATH module (Pollock 1994) enables the delineation of the wellhead protection zones around the investigated production wells. Using the measured and calculated water level data at the observation points during the calibration process, the elements of the residuals can be determined as:

$$X_i = d_i^{\text{measured}} - d_i^{\text{cal}}. \quad (48)$$

Based on Eqs. (34), (35), (36), the most frequent value (T) and the dihesion parameter of the head residuals can be derived readily by means of a double-iteration process. Then, the MFV weights can be computed for each observation point as:

$$W_i(X_i) = \frac{(k\varepsilon)^2}{(k\varepsilon)^2 + (X_i - T)^2}. \quad (49)$$

Because the type of the residual distribution is not known, the value of k=2 is preferred as discussed previously. During each step of the trial-end-error calibration, the MFV weights can provide very visible and useful information for every observation point about the actual groundwater model condition concerning the strength of matching. The closer the MFV weight is to 1.0, the better the match between the measured and calculated head data for the actual observation points. Besides the individual weight interpretation, the histogram of the MFV weights can also give useful insight about the state of calibration. Figure 7 shows that the histogram has high relative frequency values at small MFV weights during the beginning of the calibration when the model parameter values are far from their real values. The right histogram is significantly different from the left one. This was obtained at the end of the trial-end-error calibration. If the calibration is carried out successfully and the measured data are reliable, the histogram should reflect highly on the relative frequency at the greater intervals of MFV weights. In this way, the MFV weights derived from the residuals can easily accelerate the trial-and-error process.

Conclusions

It has been demonstrated that the MFV method can be applied successfully for effective solution of various problems involving groundwater modeling under certain conditions, such as when the measurement errors are not Gaussian and the model concept errors are insignificant. This robust and resistant geostatistical procedure provides a high general efficiency. Well-posed and over-determined inverse problems investigated in this paper have demonstrated the usefulness of the MFV algorithms.

The application of the P-norms based on the MFV principle has been shown to be advantageous over the other types for inverse parameter estimation calculations. The automated parameter estimation method facilitating the MFV method and linked to the MODFLOW-2000-reference flow code has been shown to be effective for deriving the groundwater model parameters. The use of the MFV weights of the head residuals readily improves the groundwater interpretation results during traditional trail-and-error calibration processes. The VFSA optimization method has been shown to be reliable without

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requiring the initial guess of the model parameter values to be sufficiently close to the actual values.

The present study has proven that the MFV method provides certain advantages over the conventional statistical methods derived from the maximum likelihood principle. Consequently, the application of the MFV method coupled with global optimization is expected to become a more widespread practice in groundwater modeling. However, the proposed method is not a remedy for ill-posed groundwater modeling problems. Also, the slightly high computational effort requirement of the MFV method may be a drawback. Further improvements and refinements are recommended for future studies in order to make the MFV method much more versatile for groundwater modeling applications.

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