Development of subsampling ANOVA methods for sensitivity analysis with low calculation requirement

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Abstract

Quantifying parameter sensitivities is a key issue in hydrological simulation and the choice of sensitivity analysis method play an important role during this process. The Analysis of Variance (ANOVA) approach is based on a biased variance estimator and the estimated variance contributions would be biased, depending on the sample sizes of the different variance sources. To diminish the effect of the biased variance estimator on the sensitivity analysis, three developed subsampling ANOVA approaches (single-, multiple- and full-subsampling ANOVA) are established in this research. Two case studies including one simplified regression model and one hydrological model are used to illustrate the performance of the approaches. The traditional sobol's method is used as benchmark method. Results find that: (1) The subsampling effectively diminishes the bias introduced by the biased variance estimator. (2) The difference of sampling densities among parameters has great influence on quantification of parametric sensitivities in hydrologic modeling. (3) Compared with sobol's method, the subsampling ANOVA methods can significantly reduce the calculation requirements while achieve similar calculation accuracy. The approaches proposed in this study can serve as a first basis for the application of subsampling ANOVA in conceptual hydrological model sensitivity analysis under multiple uncertainties.

Keywords:

Sensitivity Analysis, Model parameters, Subsampling, ANOVA, calculation

requirement

1、Introduction

Hydrologic simulation is widely used for many water resource management such as water allocation, reservoir operation, and flood risk assessment (Ma et al., 2016, Fan et al., 2016, Fan et al., 2017). Temporally dynamic and spatially distributed processes in watershed systems are described through simple mathematical equations in conceptual hydrological model (Jin et al., 2010). However, significant uncertainties are associated with such descriptions resulting from uncertainties in model parameters, structures and inputs (Refsgaard and Storm, 1990, Vrugt, 2016, Liu et al., 2017, Bárdossy, 2007, Bárdossy and Singh, 2008). Good modeling practice requires an evaluation of the confidence in the model outputs, which includes quantification of the uncertainty in model results (i.e., uncertainty analysis) and an evaluation of how much each input/parameter contributes to the output uncertainty (i.e., sensitivity analysis) (Loosvelt et al., 2013, Song et al., 2015, Götzinger and Bárdossy, 2008). Without a realistic assessment of various uncertainties, decision makers may encounter troubles in accurately describing hydrologic processes and assessing regional water resources situation (Kelly et al., 2013, Zhang et al., 2016). Therefore a key issue in hydrological simulation is to quantify and reduce the various uncertainties in order to provide reliable hydrologic predictions (Jin et al., 2010, Song et al., 2015, Pianosi et al., 2016, Gamerith et al., 2013).

To analyze the sources of uncertainty, evaluate the contribution of each uncertainty factor and identify the key factors that affect model performance, various sensitivity analysis methods such as local or global methods, and qualitative or quantitative methods have been proposed in recent decades (Song et al., 2015, Tian, 2013, Pianosi et al., 2016). Local sensitivity analysis addresses sensitivity relative to point estimates of parameter values while a global sensitivity analysis examines the effects of input variations on the outputs in the entire allowable ranges of the input space (Hamby, 1995, Zhan et al., 2013). With the ability to reflect the effects of interactions between different parameters, particularly the nonlinear relationship, global sensitivity analysis is more popular in hydrological applications (Van Griensven et al., 2006, Cibin et al., 2010, Hu et al., 2015, Khorashadi Zadeh et al., 2017, Bennett et al., 2018). A series of global sensitivity analysis methods including qualitative screening methods (Morris, 1991, Campolongo et al., 2007) and quantitative techniques based on variance decomposition (Saltelli et al., 2010, Sobol', 2010, Saltelli et al., 2008, Vega et al., 1998, Bosshard et al., 2013) are available. The choice of sensitivity analysis method has an important impact on model parameters sensitivities results (Saltelli et al., 2019, Pianosi et al., 2016).

Among quantitative global sensitivity analysis methods, Analysis of Variance (ANOVA) has been widely used for identifying important uncertainty sources, quantifying individual and interactive impacts of contributors and guiding efforts (Qi et al., 2016b). This method has been used to investigate the influence of pollutants and seasonality on the river water quality (Vega et al., 1998), the contribution of hydrological model parameters to the discharge projection uncertainty (Addor et al., 2015), and the impact of climate changes on flow frequency (Giuntoli et al., 2015). Compared with other approaches, ANOVA is handy for handling small samples and more computationally efficient in uncertainty quantification (Tang et al., 2006, Qi et al., 2016c). However, it has been argued that the estimated variance contributions using the ANOVA method would be biased, depending on the sample size differences (Bosshard et al., 2013). To diminish the effect of the sample size on contribution quantification (Bosshard et al., 2013) proposed a subsampling scheme based on the theory of the ANOVA (here, we refer this method as single-subsampling ANOVA) and applied it to assess the importance of different uncertainty sources in an ensemble of hydrological climate-impact projections. By calculating the multiplicative bias of the variance ratio in the synthetic experiment without subsampling and with subsampling, the results indicated that the bias introduced by the variance estimator of ANOVA can be diminished effectively by the subsampling (Bosshard et al., 2013). To improve hydrological model calibration, (Qi et al., 2016c) used single-subsampling ANOVA to quantify the individual and interactive influence of algorithm parameters dynamically. (Qi et al., 2016a) also evaluated global fine-resolution precipitation products and their uncertainty quantification in ensemble discharge simulations by using single-subsampling ANOVA. In these investigations, single-subsampling-ANOVA has shown good performance in quantifying respective contributions of various uncertainty sources to the overall output variance. However, only single factor is subsampled in the above studies. There is a lack of comparison and analysis of the influence on uncertainty quantification when different factors are subsampled in ANOVA. The influence may also be uncertain if multiple factors are subsampled at the same time. How will the results change if all the factors are subsampled whereas the levels of subsampling are different? Moreover, it is necessary to compare subsampling ANOVA methods with some widely used sensitivity analysis methods to demonstrate the applicability of the subsampling ANOVA approaches.

The objectives of this paper is to (i) investigate impacts of subsampling different factors separately on the resulting sensitivity results; (ii) propose multiple-subsampling and full-subsampling ANOVA approaches to enhance the applicability of ANOVA in sensitivity analysis; (iii) reveal the influence of subsampling schemes in multiple-subsampling and full-subsampling ANOVA approaches on sensitivity analysis. The applicability of different subsampling ANOVA methods is illustrated through two case studies based on a three-parameter simplified model (Chen et al., 2019) and a four-parameter daily lumped rainfall-runoff model (GR4J model) (Perrin et al., 2003). The traditional sobol's method is used as benchmark method to evaluate the performance of different subsampling ANOVA approaches.

2、 Methodology

2.1 ANOVA sensitivity analysis techniques

In order to use the same terminology to present each sensitivity technique, a generalized model is defined as:

$$Y = F(X_1, X_2, \ldots X_k) \tag{1}$$

Where $X_1, X_2, \ldots X_k$ represent the independent variable (such as model parameters, or model structure) and Y represents the response (such as the model performance). Variance-based methods use a variance ratio to estimate the importance of parameters. According to the ANOVA theory, the total sum of the squares (SST) can be divided into the sum of squares due to individual model parameters and their interactions as follows (Saltelli et al., 2008., Saltelli et al., 2010).

$$SST = \sum_{i=1}^{k} SS_i + \sum_{i=1}^{k} \sum_{j>i}^{k} SS_{ij} + \ldots + SS_{1,2,\ldots,k} \tag{2}$$

where SS_i represents the squares due to the individual effect of X_i and SS_{ij} to $SS_{1,2,\ldots,k}$ represent the squares due to interactions among k factors. In this model, we summarize all interaction terms into the term SSI.

$$SSI = \sum_{i=1}^{k} \sum_{j>i}^{k} SS_{ij} + \ldots + SS_{1,2,\ldots,k} = SST - \sum_{i=1}^{k} SS_i \tag{3}$$

Then, for each effect, the variance fractions η^2 are derived as follows:

$$\eta_i^2 = \frac{SS_i}{SST} \tag{4}$$

$$\eta_I^2 = \frac{SSI}{SST} \tag{5}$$

where:

$$SST = \sum_{t_1=1}^{T_1}\sum_{t_2=1}^{T_2}\cdots\sum_{t_k=1}^{T_k}(Y^{t_1,t_2\cdots t_k} - Y^{o,o\cdots o})^2 \tag{6}$$

$$SS_i = \sum_{t_1=1}^{T_1}\sum_{t_2=1}^{T_2}\cdots\sum_{t_k=1}^{T_k}(Y^{o,o,\cdots t_i\cdots o} - Y^{o,o\cdots o})^2 \tag{7}$$

The symbol "o" indicates averaging over the particular index. Values of 0 and 1 for the variance fraction η^2 correspond to a contribution of an effect to the total ensemble variance (uncertainty) of 0% and 100%, respectively. Obviously:

$$\sum_{i=1}^{k}\eta_i^2 + \eta_I^2 = \sum_{i=1}^{k}\frac{SS_i}{SST} + \frac{SSI}{SST} = \frac{\sum_{i=1}^{k}SS_i + SSI}{SST} = 1 \tag{8}$$

2.2 Subsampling

To diminish the effect of the sample size on contribution quantification in ANOVA, (Bosshard et al., 2013) proposed a subsampling scheme. Assume that there are $\mathrm{T_i}$ elements for each parameter X_{i}, the vector X_{i} can be represented as $x_{\mathrm{i,1}}, x_{\mathrm{i,2}}, x_{\mathrm{i,3}} \cdots x_{\mathrm{i,T_i}}$. In each subsampling iteration, two elements are selected out of the total $\mathrm{T_i}$ elements which results in a total of $\mathrm{C}_{\mathrm{T_i}}^{2}$ (specify that C is the combination symbol) possible element pairs for X_{i}. Therefore, for element $x_{\mathrm{i,t_i}}$, the $\mathrm{t_i}$ is replaced by $g(\mathrm{h,j})$, which is a $2 \times C_{T_i}^{2}$ matrix as Formula (9). Here h means the row number and j means the column number. The total number of columns is defined as J. Therefore, h=1 or 2 and j=1, 2, 3,……,J. For more details of subsampling scheme, please refer to the literature (Bosshard et al., 2013).

$$g(h,j) = \begin{pmatrix} 1 & 1 & \cdots & 1 & 2 & 2 & \cdots & \mathrm{T}_{i-2} & \mathrm{T}_{i-2} & \mathrm{T}_{i-1} \\ 2 & 3 & \cdots & \mathrm{T}_{i} & 3 & 4 & \cdots & \mathrm{T}_{i-1} & \mathrm{T}_{i} & \mathrm{T}_{i} \end{pmatrix} \tag{9}$$

2.3 Single-subsampling ANOVA

Single-subsampling ANOVA means that only one parameter from the parameter vector ($X_1, X_2, \ldots X_k$) is subsampled before the ANOVA. Assuming that the X_n is subsampled, which mean the two elements selected from vector $x_{n,1}, x_{n,2}, x_{n,3} \cdots x_{n,T_n}$ are used for X_n. As for all other parameter X_i, there are still T_i elements for each X_i. We estimate the terms in equations (2) and (3) using the subsampling procedure introduced in section 2.2 as follows.

$$SST^{j} = \sum_{t_1=1}^{T_1}\sum_{t_2=1}^{T_2}\cdots\sum_{h=1}^{2}\cdots\sum_{t_k=1}^{T_k}(Y^{t_1,t_2\cdots g(h,j)\cdots t_k} - Y^{o,o\cdots g(o,j)\cdots o})^2 \tag{10}$$

For $i = n$:

$$SS_i^{j} = T_1 T_2 \cdots T_{n-1} T_{n+1} \cdots T_k \sum_{h=1}^{2}(Y^{t_1,t_2\cdots g(h,j)\cdots t_k} - Y^{o,o\cdots g(o,j)\cdots o})^2 \tag{11}$$

For $i \neq n$:

$$SS_i^{j} = 2 \times T_1 T_2 \cdots T_{i-1} T_{i+1} \cdots T_{n-1} T_{n+1} \cdots T_k \sum_{t_i=1}^{T_i}(Y^{o,o\cdots t_i\cdots g(o,j)\cdots o} - Y^{o,o\cdots g(o,j)\cdots o})^2 \tag{12}$$

The symbol o indicates averaging over the particular index. Then, for each effect, the variance fraction η^2 is derived as follows:

$$\eta_i^{\,2} = \frac{1}{J}\sum_{j=1}^{J}\frac{SS_i^j}{SST^j} \tag{13}$$

$$\eta_I^{\,2} = 1 - \sum_{i=1}^{k}\eta_i^{\,2} \tag{14}$$

2.4 Multiple-Subsampling ANOVA

The single-subsampling ANOVA may lead to biased results if different parameters are chosen for subsampling. As an extension of the single-subsampling ANOVA, a multiple-subsampling scheme is introduced to ANOVA, leading to a multiple-subsampling ANOVA approach. Multiple-subsampling ANOVA means that more than one parameter from the parameter vector ($X_1, X_2, ...X_\mathrm{k}$) are going to be subsampled at the same time before the ANOVA is calculated. Assume that $X_\mathrm{p}, \cdots X_\mathrm{q}$ are subsampled then $\mathrm{t_p}, \cdots \mathrm{t_q}$ are replaced by $g(h_\mathrm{p}, j_\mathrm{p}), \cdots g(h_\mathrm{q}, j_\mathrm{q})$ respectively. We estimate the terms in equations (2) and (3) using the subsampling procedure as follows:

$$SST^j = \sum_{t_1=1}^{\mathrm{T}_1}\sum_{t_2=1}^{\mathrm{T}_2}\cdots\sum_{h_\mathrm{p}=1}^{2}\cdots\sum_{h_\mathrm{q}=1}^{2}\cdots\sum_{t_\mathrm{k}=1}^{\mathrm{T_k}}\left(Y^{t_1,t_2\cdots g(h_\mathrm{p},j_\mathrm{p})\cdots g(h_\mathrm{q},j_\mathrm{q})\cdots t_\mathrm{k}} - Y^{o,o\cdots g(o,j_\mathrm{p})\cdots g(o,j_\mathrm{q})\cdots o}\right)^2 \tag{15}$$

For $i = \mathrm{p}\cdots\mathrm{q}$:

$$SS_i^j = \mathrm{T}_1\times\mathrm{T}_2\times\cdots\times\mathrm{T_k}\sum_{h_\mathrm{p}=1}^{2}\cdots\sum_{h_\mathrm{q}=1}^{2}\left(Y^{t_1,t_2\cdots g(h_\mathrm{p},j_\mathrm{p})\cdots g(h_\mathrm{q},j_\mathrm{q})\cdots t_\mathrm{k}} - Y^{o,o\cdots g(o,j_\mathrm{p})\cdots g(o,j_\mathrm{p})\cdots o}\right)^2 \tag{16}$$

For $i \neq \mathrm{p}\cdots\mathrm{q}$:

$$SS_i^j = 2\times\cdots\times 2\times \mathrm{T}_1\times \mathrm{T}_2\cdots \mathrm{T}_{\mathrm{i-1}}\times \mathrm{T}_{\mathrm{i+1}}\cdots \mathrm{T}_{\mathrm{k}}\sum_{t_i=1}^{\mathrm{T}_i}(Y^{o,o\cdots t_i\cdots g(o,j_{\mathrm{p}})\cdots g(o,j_{\mathrm{q}})\cdots o} - Y^{o,o\cdots g(o,j_{\mathrm{p}})\cdots g(o,j_{\mathrm{q}})\cdots o})^2$$

(17)

Then, for each effect, the variance fraction η^2 is derived as follows:

$$\eta_i^2 = \frac{1}{J}\sum_{j=1}^{J}\frac{SS_i^j}{SST^j} \tag{18}$$

$$\eta_I^2 = 1-\sum_{i=1}^{k}\eta_i^2 \tag{19}$$

2.5 Full-Subsampling ANOVA

Moreover, a full-subsampling approach can be formulated when all parameters are going to be subsampled. In detail, the full-subsampling ANOVA means that all parameters $X_1, X_2, ...X_k$ are subsampled before ANOVA is calculated. Consequently, $t_1, t_2, \cdots t_{\mathrm{k}}$ are replaced by $g(h_1, j_1), g(h_2, j_2), \cdots g(h_{\mathrm{k}}, j_{\mathrm{k}})$ respectively. We estimate the terms in equations (2) and (3) using the subsampling procedure as follows:

$$SST^j = \sum_{t_1=1}^{2}\sum_{t_2=1}^{2}\cdots\sum_{t_{\mathrm{k}}=1}^{2}(Y^{g(h_1,j_1),g(h_2,j_2)\cdots g(h_{\mathrm{k}},j_{\mathrm{k}})} - Y^{g(o,j_1)g(o,j_2)\cdots g(o,j_{\mathrm{k}})})^2 \tag{20}$$

$$SS_i^j = \sum_{h_1=1}^{2}\sum_{h_2=1}^{2}\cdots\sum_{h_{\mathrm{k}}=1}^{2}(Y^{g(h_1,j_1),g(h_2,j_2)\cdots g(h_{\mathrm{k}},j_{\mathrm{k}})} - Y^{g(o,j_1),g(o,j_2),\cdots g(o,j_{\mathrm{k}})})^2 \tag{21}$$

Then, for each effect, the variance fraction η^2 is derived as follows:

$$\eta_i^{\ 2} = \frac{1}{J}\sum_{j=1}^{J}\frac{SS_i^{\ j}}{SST^{\ j}} \tag{22}$$

$$\eta_I^{\ 2} = 1 - \sum_{i=1}^{k}\eta_i^{\ 2} \tag{23}$$

To evaluate the performance of the above different subsampling ANOVA approaches, two test cases are applied in the following.

3、 Analytical case

3.1. Problem statement

A simple model with three unknown parameters is employed to illustrate the proposed subsampling ANOVA approaches, which is expressed as follows:

$$F_3(X_1, X_2, X_3) = X_1 * X_3 + X_1 * \sin(\frac{\pi}{2} * X_2) + X_2 * e^{|X_3|} + X_1 * X_2 * X_3 \tag{24}$$

where X_1, X_2 and X_3 are independent variables uniformly distributed within [0, 1]. This simplified model is proposed by (Chen et al., 2019). The purpose of this model is to explore the sensitivity indices change of model parameters with different subsampling methods in the ANOVA-based sensitivity analysis. In our study, we define “5” as the five levels are selected equidistantly within the initial parameter range firstly. Then the five levels are subsampled (see section 2.1), and totally 10 ($C_5^2 = \frac{5*4}{2*1} = 10$) combinations of different level pairs are obtained for two-level ANOVA. Similarly, “2” represents only two levels (maximum and minimum values) of the parameter were selected from the range, without subsampling. For example, “522” means that five levels of X_1 are selected with equidistantly from the range before subsampling, meanwhile only two levels of the X_2 and X_3 are selected from the range. In turn, we define 252, 225, 552, 525, 255, 222, 333, 444 and 555 for different ANOVA approaches. For 522, 252 and 225, only one of the three parameters is subsampled, which represent single-subsampling ANOVA. For 552, 525 and 255, two of the three parameters are subsampled, which represent multiple-subsampling ANOVA scheme. Similarly, 222,333,444 and 555 represent full-subsampling ANOVA with different parameters levels.

3.2 Influence of subsampled parameter

Figure 1. presents sensitivity indices of individual and interactions of the three parameters under different subsampling ANOVA approaches. Figure 1(a) represents single-subsampling ANOVA and Figure 1(b) represents multiple-subsampling ANOVA. Firstly, it can be found that the parameter’s sensitivity varies with each other. In detail, the sensitivity range of X_1,X_2,X_3 and interactions are 4.1%-41.2%, 25.1%-78.5%, 7.5%-47.3% and 7.0%-15%, respectively. In most cases, X_2 is the most sensitive parameter. Secondly, the parameter’s individual sensitivity varied significantly with different subsampling scheme. For single-subsampling ANOVA, the minimum value (the red bar) of X_1’s sensitivity is obtained in 522 where only X_1 is subsampled. Similarly, the minimum values (the red bar) of X_2’s and X_3’s sensitivities are obtained

in 252 and 225, respectively. The results indicate that the individual sensitivity of the parameter will reduce sharply when the parameter is subsampled in single-subsampling ANOVA. As for multiple-subsampling ANOVA in Figure 1(b), the maximum value (blue bar) of X_1's sensitivity is obtained in 255 where only X_1 is non-subsampled. Similarly, the maximum values of X_2's and X_3's sensitivities are obtained in 525 and 552, which indicate that in multiple-subsampling ANOVA, the individual sensitivity will increase for the non-subsampled parameter. Thirdly, the black bars in Figure 1 represent sensitivity indices of individual and interactions for the three parameters obtained by Sobol's. Compared with sobol's results, the subsampling process will reduce the subsampled parameter's individual sensitivity and increase the non-subsampled parameter's individual sensitivity. Lastly the subsampling process not only change the value of parameter sensitivities but also change the ordering of the parameter sensitivities (as shown in supporting masteries Figure S1-S3). For example, the order of sensitivity for the case by the 522 method is parameter x2 > x3 > interaction > x1 while 252 values yield a slightly different order: x3 > x1 > x2 > interaction. This also indicates that the results of either single- or multiple-subsampling schemes are biased. Consequently, the full-subsampling ANOVA approach is expected to employ in the following part aims to diminish the deviation.

3.3 Influence of parameter levels

In the full-subsampling ANOVA approach, different levels can be chosen for each parameter from its variation range. In this study, four scenarios would be tested with each parameter having 2, 3, 4 or 5 levels (i.e. 222, 333, 444 and 555) respectively. Figure 2 shows the influence of parameters levels on individual and interactions sensitivity. The sensitivities of three parameters change with the parameters levels change. As the parameters levels increase from 222 to 555, the individual sensitivity of X_1 and X_3 gradually increase from 11.7% and 19.4% to 19.1% and 24.1%, respectively. At the same time, the interactive parameter sensitivity gradually decrease from 18.1% to 5.5%. The individual sensitivity of X_2 which has the biggest contribution keeps relatively stable, ranging from 50.9% to 52.2%. The results show that for full–subsampling ANOVA method, the individual and interactive parameters sensitivities are affected by the subsampled parameters levels. The increased parameters levels increase the sensitivity value slightly for the low sensitive parameter and decrease the interactive sensitivity. Another thing to watch out is that the order of parameters sensitivities would change when the parameter level increases from 2 to 3. While when the 3 or more parameter levels are chosen, the variation of the obtained results is relatively small and the order of parameters sensitivities remained consistent with that of sobol's. As a whole, the full-subsampling ANOVA approach with more than 3 levels is suggested to diminish the deviation.

3.4 Comparison with sobol's method

To evaluate the accuracy of different subsampling ANOVA approaches, the sobol's method is used as a benchmark method, which is widely used in hydrological models (Zhang et al., 2013, Wang et al., 2018, Song et al., 2015, Sobol', 2010) as an effective approach to globally characterize single- and multiple-parameter interactive sensitivities (Tang et al., 2007). In this study, take sensitivity indices calculated by sobol's method as base values, the deviation between subsampling ANOVA and sobol's can be evaluated as $\sum_{i=1}^{I}(\eta_i^{*}-\eta_i^{sobol's})^2$, where η_i^{*} is the sensitivity indices calculated by the subsampling ANOVA approaches, $\eta_i^{sobol's}$ is the sensitivity indices calculated by sobol's method. All the sensitivity indices calculated by subsampling ANOVA and sobol's are available in supporting material and the deviations between subsampling ANOVA and sobol's methods are presented in Figure 3.

The deviations between results of subsampling ANOVA and sobol's vary (0.0008-0.114) with different subsampling schemes and parameters levels. The lower deviation indicates the individual and interactions sensitivity calculated are more accurate. For single-subsampling ANOVA and multiple-subsampling ANOVA approaches, the corresponding deviations range from 0.024 to 0.114. As expected, significantly better performances (the corresponding deviations range from 0.001 to 0.016) are obtained in full-subsampling ANOVA method. Moreover, the deviations are lower than 0.002 if 3 or more parameter levels are chosen in the full-subsampling ANOVA. Such deviations indicate that biased/inaccurate sensitivity indices obtained through the single/multiple-subsampling ANOVA methods. The negligible bias in full-subsampling ANOVA method show that the parameters sensitivities are very close to the “true value” when the subsampled parameter level is 3 or more. Therefore, in order to get more reliable parameter sensitivity results, the full-subsampling scheme with 3 or more parameter levels is necessary for the application of subsampling ANOVA methods.

Many researches point that sobol's method is computationally expensive (Tang et al., 2008, Tian, 2013, Reusser et al., 2011). Here, to illustrate the computational advantages of the subsampling ANOVA methods, the number of model running and the number of calculations of variance required by subsampling ANOVA methods and sobol’s are presented in Table 1. Generally speaking, N*(M+2) model evaluations are required for the application of sobol’s, where N is the random sample size and M is the number of parameters, for more details about sobol’s method, please refer to (Sobol', 1990, Nossent et al., 2011). In this case study, in order to get a stable result of the sensitivity analysis, different set of N samples are applied in the sobol’s. We found that the sensitivity analysis remained relatively stable when N was larger than 2000. So in this simple three-parameter model, the number of running the model is 2000*(3+2), which is a barely acceptable computing requirement.

Fortunately the subsampling ANOVA methods can significantly reduce the calculation requirements while sobol's calculation accuracy is achieved. For example, in full-sampling "444", the model needs to run only 64 times (64=4*4*4). It should be noted that after running the model 64 times, the 64 sets of model responses can be obtained. Through resampling process, 216 sets (216=$C_4^2 * C_4^2 * C_4^2$, where $C_4^2 = \frac{4*3}{2*1} = 6$) of 2*2*2 combination can be obtained, and each combination can calculate a set of variance results. Thus, 216 sets of variance results can be obtained. The final sensitivity results can be obtained by averaging and homogenizing the 216 sets of variance. The number of running the model decides the computing requirements. Through reducing the number of model runs, the subsampling ANOVA methods are effective and feasible sensitivity analysis methods with relatively low computational requirements. Reduction of model running times requirement is very important, especially for those models with limited parameters but extensive computational demand.

4、Practical case study

4.1 Problem statement

To further illustrate the applicability of the subsampling ANOVA methods, the proposed approaches are applied for parameter sensitivity analyses in hydrological simulation through the conceptual model GR4J, as shown in Figure 4. The study area is Zengjiang River which is one tributary of Dongjiang River located in the Pear River Delta, China as shown in Figure 5. The meteorological data (daily evaporation and daily precipitation) are collected from Qilinzui Hydrological Station (as shown in Figure 5) during the period of 2009-2015 which were obtained from Hydrological Data of Pearl River Basin, Annual Hydrology Report, P. R. China. The total drainage area above the Qilinzui Hydrological Station is 2866 km^2, accounting for 91% of the Zengjiang River basin (3160 km^2). The mean annual temperature and precipitation are 21.6°C and 2188 mm, respectively. More details about Zengjiang River basin can be found in (Tao et al., 2011).

GR4J model is a rainfall-runoff model which is based on four free parameters from daily rainfall data. In GR4J, the production components include an interception of raw rainfall and potential evapotranspiration by an interception reservoir of null capacity, a soil moisture accounting procedure to calculate effective rainfall and a water exchange term to model water losses to or gains from deep aquifers. Its routing module includes two flow components with constant volumetric split (10–90%), two unit hydrographs, and a non-linear routing store (as shown in Figure 4). The descriptions and initial fluctuating ranges of GR4J model parameters are presented in Table 1. For more details of GR4J model, please refer to the literature (Perrin et al., 2003). The initial fluctuating ranges of GR4J model parameters are wide considering the structure varies in different basins. However, for a specific watershed, the appropriate parameter range should be obtained through the calibration process that produce an acceptable level of model performance (Freer et al., 1996, Pianosi et al., 2016, Shin et al., 2013). It's reported that the parameters sensitivities were strongly influenced by the range of parameter values used (Shin et al., 2013, Wang et al., 2013), therefore it is important to obtain an appropriate parameter range corresponding to considered model performance before SA (Shin et al., 2013, Saltelli et al., 2019). Therefore, in this study, the model calibration based on the MH algorithm is used prior to SA in order to constraint the input variability space. The details about MH algorithm are presented in supporting materials. Nash–Sutcliffe model efficiency (NSE) is used to assess the predictive power of model results which involves standardization of the residual variance. Here, the objective functions adopted can be represented as follows (Nash and Sutcliffe, 1970, Legates and Jr, 1999):

$$NSE = 1 - \frac{\sum_{i=1}^{n}\left(Q_{obs,i} - Q_{sim,i}\right)^2}{\sum_{i=1}^{n}\left(Q_{obs,i} - \overline{Q_{obs}}\right)^2} \tag{25}$$

where Q_{sim} is the simulated runoff, Q_{obs} is the observed runoff, $\overline{Q_{obs}}$ is the mean value of the observed runoff and n is the sample size.

For the MH algorithm parameterization, the markov chain with 10,000 iterations for each parameter are examined and the model performance of each iteration are presented in Figure 6. The NSE is greater than 0.74 and remained stable after a number of iterations. In this study, the first 50% of the samples in markov chain are ruled out as a warm-up period. The last 50% of the samples passed the Heidelberger and Welch Convergence Diagnostics (Heidelberger and Welch, 1983). The posterior distributions are obtained from the last 5000 parameter sets and the posterior PDFs of each parameter are presented in Figure 7. All parameters ranges appear in a relatively small interval which is different from their initial value. The posterior PDFs of four parameters are approximately normal distribution characteristics, indicating that the parameters in GR4J are well identified after a number of iterations even with a wide range of prior densities. The predictive intervals of stream obtained by the last 5000 parameter sets are presented in Figure 8. It can be observed that the obtained predictive intervals can generally match the observations, except for some overestimations in high-flow periods. With the appropriate parameter range, the next work is to evaluate how much each parameter contributes to the stream uncertainty. Sensitivities of parameters in a rainfall–runoff model structure are specific to a site, and cannot be assumed from previous work in other catchments (Van Griensven et al., 2006, Shin et al., 2013). In this study, the proposed subsampling ANOVA methods are applied for analyzing parameters sensitivities of GR4J model in Zengjiang River basin. Based on the calibration of GR4J, the ranges of the four parameters are determined as presented in Table 2. Similar to Section 3.1, different subsampling ANOVA approaches, including single-subsampling ANOVA (5222, 2522, 2252 and 2225), multiple-subsampling ANOVA (5522, 5252, 5225, 2552, 2525, 2255, 5552, 5525, 5255 and 2555), and full-subsampling ANOVA with different parameters level (2222, 3333, 4444 and 5555) are defined and applied here.

4.2 Influence of subsampled parameter

With only one parameter subsampling, the contributions of individual and interactive effects for the four parameters in GR4J model are shown in Figure 9. There are several findings as follows. Firstly, taking sobol's results as the reference results, X_1 makes the largest independent contribution to GR4J model uncertainty in Zenjiang River and followed by the interactive effects of the four parameters. X_1(the first parameter) represents the maximum capacity of the production store. The high sensitivity of parameter X_1 indicates that runoff generation in Zengjiang basin is highly affected by the maximum capacity of the production store. The maximum capacity of the production store (X_1) increases to handle with an overestimation of rainfall and decreases to handle with underestimation, thus adapting its capacity to hold and evaporate different amounts of water (Oudin et al., 2006). Secondly, the parameters sensitivities obtained change significantly with different subsampling scheme. For example, the contributions of X_1 are 0.109, 0.230, 0.275 and 0.205 for the four single-subsampling schemes (where X_1, X_2, X_3, and X_4 are subsampled separately). The lowest sensitivity value for X_1 obtained in 5222, which X_1 decomposed into five levels and take subsampling. The other three parameters have the same basic behaviors as the X_1. Therefore, similar with section 3.2, the subsampling procedure also lead to a lower sensitivity value for one parameter which is subsampled in. Thirdly, the ranking of parameter sensitivity is influenced by different single-subsampling schemes. In order to check if hierarchy is kept by the methods more clearly, the bar plots which is close to Figure 9， but grouped by simulations and not by parameter are presented in supplementary materials Figure S4-S6. For instance, the sensitivity order is

Interactions >X_3 > X_4 > X_1 > X_2 in 5222 scheme, while in 2252 scheme, the sensitivity order is Interactions >X_1 > X_3 > X_4 > X_2. Such results indicate that the single-subsampling ANOVA approach generate unreliable sensitivity values, which are highly influenced by the parameter to be subsampled. In multiple-subsampling ANOVA, more than one parameters in GR4J model are subsampled. The contributions of individual and interactive effects for GR4J model parameters under different multiple-subsampling schemes are presented in Figure 10.

It can be found that, for each parameters, the red bar values are significantly lower than the blue bar values. The mean values of the red bars for X_1, X_2, X_3 and X_4 are 0.184, 0.033, 0.124 and 0.078, respectively. Meanwhile the mean values for the blue bars for X_1, X_2, X_3 and X_4 are 0.306, 0.098, 0.264 and 0.225, respectively. For each parameter, the mean value without subsampling (blue bars) is more than twice as much as the mean value with subsampling (red bars). This indicates that, similar with the single-subsampling scheme, the multiple-subsampling ANOVA approaches also generate unreliable results, and the subsampling-procedure would significantly reduce the resulting individual sensitivity value. In other words, the difference of sampling densities among parameters has great influence on quantification of parametric sensitivities in hydrologic modeling.

4.3 Influence of subsampled parameter level in full-subsampling

In the full-subsampling ANOVA approach, all the four parameters in GR4J model are subsampled. However, different levels for each parameter can be chosen before the subsampling procedure. Similar with the analytic case in section 3, four levels (2 to 5) are going to be chosen for each parameter in GR4J. The contributions of individual and interactions for GR4J model parameters under different parameter levels in full-subsampling ANOVA are presented in Figure 11. As the parameter levels increase from 2222 to 5555, the sensitivity of X_1, X_2 and X_4 gradually increase from 20.1%, 3.7% and 4.7% to 31.0%, 7.6% and 15.8%, respectively. At the same time, the contribution of X_3 and the interaction gradually decrease from 21.7% to 17.8% and 48.9% to 25.9%. The results indicate that the parameters levels will affect the individual and interactive sensitivities in the full-subsampling ANOVA approach. In details, the sensitivity of the most sensitive parameter and interaction generally decrease, while that of the other parameters increase with the parameter level increased. The obtained results would vary most significantly when the parameter level increases from 2 to 3. At the same time, the variation of the obtained results is relatively small and the order of parameters sensitivity would not change when the parameter levels are higher than three.

4.4 Compared with sobol's

The sensitivity values for the four parameters in GR4J model from the subsampling ANOVA (i.e. single-subsampling, multiple-subsampling and full-subsampling) and sobol's are discussed above. To compare the subsampling ANOVA and sobol's methods further, the deviations for parameter sensitivity values and the calculation cost are presented in Figure 12 and Table 3. There are significant differences between the deviations obtained with different subsampling ANOVA methods. The large deviations (> 0.08) are obtained with 2225, 2255 and 2525, meanwhile small deviations (< 0.01) are obtained with 3333, 4444, and 5555. Except for 2222, other full-subsampling schemes perform very well in the sensitivity analysis of GR4J model parameters. Therefore, in order to get reliable parameter sensitivity results, the three or more parameter levels in the full-subsampling ANOVA approach are recommended.

In this GR4J model study, 3 million random samples are applied in sobol's in order to get a stable result of the parameters sensitivities. So totally, the GR4J model need to run 3000000*(5+2) times, which is a very large computational requirement. However, the subsampling ANOVA methods can significantly reduce the calculation requirements while achieve similar calculation accuracy in GR4J model. For example, in full-sampling "4444" where the deviation is only 0.0006, the model only need to run 256 times (256=4*4*4*4). Similar with section 3.4, for the four parameters conceptual model, 1296 sets variance results can be obtained through subsampling process where $1296 = C_4^2 * C_4^2 * C_4^2 * C_4^2$ and $C_4^2 = \frac{4*3}{2*1} = 6$. The final sensitivity results obtained by averaging and homogenizing the 1296 sets of variance. Through reducing the number of model runs, the subsampling ANOVA methods are effective and feasible sensitivity analysis methods with relatively low computational requirements.

6、Conclusions and discussions.

Three kinds of subsampling-ANOVA schemes (single-, multiple- and full-subsampling) have been proposed and analyzed in this study. The applicability of different subsampling ANOVA schemes are illustrated through one simplified model and a rainfall-runoff conceptual model. To evaluate the performance of different subsampling ANOVA schemes, the traditional sobol's method is also used as benchmark in the study. The main purpose is to investigate the influence of different subsampling ANOVA schemes on sensitivity analyses results. Based on the case studies, some findings can be concluded:

1) The subsampling effectively diminishes the bias introduced by the biased variance estimator. In the application of subsampling ANOVA method, the parameter's individual sensitivity is related to the subsampling scheme. The subsampling process will reduce the subsampled parameter's individual sensitivity and increase the non-subsampled parameter's individual sensitivity. In other words, the difference of

sampling densities among parameters has great influence on quantification of parametric sensitivities in hydrologic modeling.

2) For full–subsampling ANOVA method, the deviation decreased with the parameters levels increased. The variation of the obtained parameters sensitivities is small and the order of parameters influences (i.e. sensitivity) would not change for three 3 or more parameter levels.

3) Compared with sobol's method, the subsampling ANOVA methods can significantly reduce the calculation requirements while achieve similar calculation accuracy. Particularly, in order to get reliable parameter sensitivity results, the full-subsampling scheme is necessary, and the 3 or more parameter levels are recommended.

In this study, the sobol's method is considered as the benchmark to evaluate the performance of the developed subsampling ANOVA approaches. Even though the subsampling ANOVA approaches may not produce better results than the sobol's method, the proposed subsampling ANOVA approaches, especially for the full-subsampling ANOVA method, have their own essential strengths. Firstly, the sobol's algorithm has high computational cost and the number of model evaluations required for the sobol's indices to converge increases rapidly with the number of parameters, making its efficiency questionable for complex hydrological models (Herman et al., 2013, Zhang et al., 2013, Khorashadi Zadeh et al., 2017, Shin et al., 2013). In comparison, the subsampling ANOVA approaches can effectively reduce the computational demands and generate reliable results (as shown in Table 1 and Table 3). The number of model evaluations is equal to the number of combinations with all the parameter levels. However, as indicated in this paper, the full-subsampling ANOVA approach can generate acceptable results with three or four levels for each parameter. Thus, the computational cost would be reduced greatly. Secondly, besides sensitivity analysis for parameters with continuous values (Qi et al., 2016c), the single-subsampling ANOVA algorithms has already been applied to analyze the sensitivity of discrete or non-numeric elements such as the statistical post processing scheme, precipitation products and the hydrological model (Bosshard et al., 2013, Qi et al., 2016a, Qi et al., 2016b). Consequently, the developed multiple-/full-subsampling ANOVA approaches can also handle with sensitivity analysis for both numeric and non-numeric variables. However, the sobol's approach can only deal with numeric variables.

The approaches proposed in this study just serve as a first basis for the application of subsampling ANOVA in hydrological model sensitivity analysis under multiple uncertainties. The number of levels would probably be higher to ensure robustness with a more complex model. The subsampling ANOVA algorithms can not only reduce the computing cost greatly, but also analyze the sensitivity of discrete or non-numeric elements. Further research is encouraged to examine the applicability of the subsampling ANOVA approaches in other non-numeric elements sensitivity analysis.

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Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Conflict of Interest

The authors have no conflict of interest to declare.

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