



1	The new importance measures based on vector projection for
2	multivariate output: application on hydrological model
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### 28 Abstract:

29 Analyzing the effects of the inputs on the correlated multivariate output is important to assess 30 risk and make decisions in Hydrological processes. However, the existing methods, such as output decomposition approach and covariance decomposition approach, can't provide sufficient 31 32 information of the effects of the inputs on the multivariate output, since these methods only 33 measure the influence of input variables on the magnitudes of variances of the dimensionalities in 34 the multiple output space and ignore the effects on the dimensionality directions of output 35 variances. In this paper, a new kind of sensitivity indices based on vector projection for the 36 multivariate output is proposed. By the projection of the conditional vectors on the unconditional 37 vector in the dimensionless multiple output space, the new sensitivity indices measure the influence of the input variables on the magnitudes of variances and directions of the 38 39 dimensionalities simultaneously. The mathematical properties of the proposed index are discussed, 40 and its link with the Sobol indices is derived. And Polynomial Chaos Expansion (PCE) is used to estimate the proposed sensitivity indices. The results for two numerical examples and a 41 42 hydrological model indicate the validity and potential benefits of the vector projection index and 43 the efficiency of estimation approach.

44

### 45 Keywords:

46 Sensitivity analysis; Multivariate output; Vector projection; Dimension; HBV;

### 47 1. Introduction

Models with multivariate output are widely used in the field of engineer and science, and the 48 49 multivariate output is correlated in some degree. For example, output of multiple elicitation 50 surveys are applied to the cost of key low-carbon energy technology (Bosetti, Marangoni et al. 51 2015), and many dynamic models used to study risk assessment and decision support in ecology 52 and crop science generate time-dependent model predictions, with time being either discretized 53 in a finite number of time steps or considered as continuous(Lamboni, Monod et al. 2011). Traditional methods for Global Sensitivity Analysis (GSA), including the elementary effect method 54 55 (Campolongo, Cariboni et al. 2007, Campolongo, Saltelli et al. 2011), variance based method (Homma and Saltelli 1996, Sobol' 2001), derivative based method (Sobol' and Kucherenko 2009, 56 Sobol' and Kucherenko 2010) and moment dependent method (Borgonovo 2007, Cui, Lü et al. 2010, 57 Luyi, Zhenzhou et al. 2012), were designed for scalar output. And the direct way to perform 58 sensitivity analysis for models with multivariate output is to perform sensitivity analysis for each 59





60 output separately. However, this way is just a repetition of the traditional GSA and it ignores the 61 correlations among the multivariate output. Thus, it may be insufficient to perform sensitivity 62 analysis on each output separately or on a few context specific scalar functions of the output 63 (Lamboni, Monod et al. 2011). A high degree of redundant sensitivity indices can be obtained when 64 the correlation in the outputs is strong. In such a case, it is difficult to interpret the result (Garcia-Cabrejo and Valocchi 2014). Saltelli and Tarantola proposed to define a scalar index of interest to 65 66 apply the GSA to simplify the original problem (Saltelli, Tarantola et al. 2000). It is recommended to 67 apply sensitivity analysis to the multivariate output as a whole, and criteria and methods need to 68 be developed for the sensitivity analysis of multivariate output. 69 Campbell (Campbell, McKay et al. 2006) proposed the output decomposition method for 70 sensitivity analysis, which consists in (i) performing an orthogonal decomposition of the 71 multivariate output, and (ii) applying sensitivity analysis on most informative components 72 separately. This method gives more attention to a few components rather than the whole output. 73 To summarize the sensitivity over the whole output, Lamboni (Lamboni, Monod et al. 2011)

proposed a new synthetic sensitivity criterion and extended the criterion to the continuous case. Generalized Sobol' sensitivity indices for multivariate output based on the decomposition of covariance matrix of model outputs was defined by Gamboa et al (Gamboa, Janon et al. 2013), and it is more computational efficient since it doesn't need spectral decomposition compared to the output decomposition method (Lamboni, Monod et al. 2011).

79 These sensitivity analysis methods for multivariate output only considered the sum of variance of 80 each output, which implicitly assumes that the relationship between outputs is simple and additive. 81 However, there are different dimensions of measurement and orders of magnitude among outputs, 82 which make them not be directly used for the comprehensive analysis. Therefore, it is necessary to have 83 a dimensionless process for the outputs before the comprehensive analysis. Besides, for multivariate 84 output space, each output represents one dimensionality of the multivariate output space. The 85 variance of each output can represent the uncertainty of each dimensionality, which can be 86 regarded as the magnitude of each variance dimensionality. The covariance decomposition 87 method compares the importance of the model inputs by the influence of the inputs on the 88 variance of each output. For the output decomposition method, the original outputs are 89 transformed into a new set of outputs, which form a transformed space. Then, the influence of the 90 model inputs on the variance of the new outputs tells the importance of each input. The sensitivity 91 methods above can tell the influence of the model inputs on the variance of model outputs, which 92 can be regarded as an influence on the magnitude of all the variance dimensionalities. However, 93 they can't tell the influence of the model inputs on the directions of all the variance 94 dimensionalities, i.e., the direction of the variance vector of the output space, which can reflect 95 another character of the multivariate output uncertainty space. Thus, these methods are not





96 sufficient to tell the importance of model inputs.

97 In this work, we introduce a new sensitivity index based on vector projection which contains the 98 influence of the input uncertainties on the magnitudes and directions simultaneously of all the 99 multivariate output variance vector. Through dimensionless process, the influence of dimension of 100 outputs can be eliminated. Then the conditional variances and unconditional variances of each output 101 are set as vectors, the influence of the input uncertainties can be reflected by the similarity between 102 the conditional variances vector and the unconditional variances vector, which can be measured by the 103 vector projection. 104 The rest of this paper is organized as follows. The next section briefly reviews the global sensitivity 105 indices based on the variance for scalar output and multiple outputs, then the definition and properties 106 of the vector projection method. In Section 3, Polynomial Chaos Expansion (PCE) is applied to estimate 107 the new sensitivity index. In Section 4, the new sensitivity index is illustrated by two numerical examples

and HBV model, which gives the hydrological forecasts and predicts the potential climate changes orfloods. Conclusions come at the end of paper.

## 110 2. Methodology

#### 111 **2.1** The traditional importance measures

#### 112 2.1.1 Variance based method

The importance measure (IM) is defined as "the study of how uncertainty in the output of a model
(numerical or otherwise) can be apportioned to different sources of uncertainty in the model input"
(Saltelli, Tarantola et al. 2004), and Sobol decomposition is one of the main methodologies for IM.

116 Let  $\mathbf{Y} = (Y^{(1)}, ..., Y^{(m)})$  denote the m-dimensional model output vector, where 117  $Y^{(r)} = g^{(r)}(\mathbf{X}) \ (r = 1, ..., m)$ , and  $\mathbf{X} = (X_1, X_2, ..., X_n)^T$  is the vector of n-dimensional independent input 118 variables. In the case of scalar output r = 1, the Sobol decomposition of the function 119  $Y^{(1)} = g^{(1)}(X_1, X_2, ..., X_n)$  is given by

120 
$$Y^{(1)} = g_0^{(1)} + \sum_{i=1}^n g_i^{(1)} + \sum_{i_j=1}^n \sum_{i_2=1+i_1}^n g_{i_1,i_2}^{(1)} (X_{i_1}, X_{i_2}) + \dots + g_{1,2,\dots,n}^{(1)} (X_1, \dots, X_n)$$
(1)

121 where  $g_0^{(1)} = E(Y^{(1)}), g_i^{(1)} = E(Y^{(1)} | X_i) - g_0^{(1)}$  and  $g_{i_1, i_2}^{(1)} = E(Y^{(1)} | X_{i_1}, X_{i_2}) - g_{i_1}^{(1)} - g_{i_2}^{(1)} - g_0^{(1)}$ . It is

122 shown by Sobol [2] that  $g_i^{(1)}$  is the variation of  $Y^{(1)}$  due to change of  $X_i$  only when the mean  $g_0^{(1)}$ 123 has been considered, and similarly  $g_{i_1,i_2}^{(1)}$  is the variation of  $Y^{(1)}$  when  $X_{i_1}$  and  $X_{i_2}$  are interacting. 124 All the terms in Eq.(1) are orthogonal. Taking variances to both sides of Eq.(1),the following Eq.(2) can 125 be obtained:

126 
$$V^{Y^{(1)}} = \sum_{i=1}^{n} V_{X_{i}}^{Y^{(1)}} + \sum_{i_{1}=1}^{n} \sum_{i_{2}=1+i_{1}}^{n} V_{X_{i_{1}}X_{i_{2}}}^{Y^{(1)}} + \dots + V_{X_{1}X_{2}\dots X_{n}}^{Y^{(1)}}$$
(2)

127 where 
$$V^{Y^{(1)}} = \operatorname{var}(Y^{(1)}) = \int (g^{(1)}(\mathbf{x}))^2 f_{\mathbf{x}}(\mathbf{x}) d\mathbf{x} - (g_0^{(1)})^2$$
,  $V_{X_i}^{Y^{(1)}} = V(g_i^{(1)}) = V(E(Y^{(1)} \mid X_i))$  and

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128  $V_{X_{i_{1}}X_{i_{2}}}^{Y^{(1)}} = V(g_{i_{1},i_{2}}^{(1)}) = V(E(Y^{(1)} | X_{i_{1}}, X_{i_{2}})) - V_{X_{i_{1}}}^{Y^{(1)}} - V_{X_{i_{2}}}^{Y^{(1)}}$ . The first order partial variance  $V_{X_{i}}^{Y^{(1)}}$  can be 129 explained as the average reduction of model output variance resulting from fixing  $X_{i}$ , which measures 130 the individual contribution of  $X_{i}$  to the total variance  $V^{Y^{(1)}}$ . The second order partial variance  $V_{X_{i_{x}}X_{i_{2}}}^{Y^{(1)}}$ 131 represents the interaction effect between  $X_{i_{1}}$  and  $X_{i_{2}}$ . In the same way explanation can be given to 132 the higher order partial variances. And the total partial variance  $V_{T_{i}}^{Y^{(1)}}$  contributed by  $X_{i}$  is defined as 133 the summation of all terms in Eq. (2) with subscripts including i:

134 
$$V_{T_i}^{Y^{(1)}} = V_{X_i}^{Y^{(1)}} + \sum_{i_1 \neq i}^n V_{X_i X_{i_1}}^{Y^{(1)}} + \dots + V_{X_1 \dots X_n}^{Y^{(1)}}$$
(3)

135 So  $V_{T_i}^{Y^{(1)}}$  consists of the individual effect of  $X_i$  and its interaction effects with all the other n-1 input 136 variables  $\mathbf{X}_{-i} = (X_1, ..., X_{i-1}, X_{i+1}, ..., X_n)$ . The measure  $V_{T_i}^{Y^{(1)}} = V^{Y^{(1)}} - V(E(Y^{(1)} | \mathbf{X}_{-i}))$  is the average 137 residual variance of the model output when all the inputs but  $X_i$  are fixed over their full ranges.

138 Dividing  $V_{X_i}^{Y^{(1)}}$  and  $V_{T_i}^{Y^{(1)}}$  by the total variance  $V^{Y^{(1)}}$ , the main effect index  $S_i$  and total effect index  $S_{T_i}$ 139 for  $X_i$  on the first output can be obtained as follows.

140 
$$S_i^{Y^{(1)}} = \frac{V_{X_i}^{Y^{(1)}}}{V^{Y^{(1)}}}$$
(4)

141 and

152

142 
$$S_{T_{i}}^{Y^{(1)}} = \frac{V_{T_{i}}^{Y^{(1)}}}{V^{Y^{(1)}}} = \frac{V^{Y^{(1)}} - V(E(Y^{(1)} \mid \boldsymbol{X}_{-i}))}{V^{Y^{(1)}}}$$
(5)

143 2.1.2 Covariance decomposition approach

144 In the case of multivariate output r = m (m > 1), taking the covariance matrices for both sides

145 of Y, Gamboa (Garcia-Cabrejo and Valocchi 2014) obtained

146 
$$C(Y^{(1)},...,Y^{(m)}) = \sum_{i=1}^{n} C_{i}(Y^{(1)},...,Y^{(m)}) + \sum_{1 \le i \le j \le n} C_{i,j}(Y^{(1)},...,Y^{(m)}) + \sum_{1 \le i < j < k \le n} C_{i,j,k}(Y^{(1)},...,Y^{(m)}) + \cdots + C_{1,2,...,n}(Y^{(1)},...,Y^{(m)})$$
(6)

147 The expression implies that the covariance matrix 
$$C$$
 of the multivariate output can be partitioned  
148 into the sum of covariance matrices that comes from changes in single  $C_i$ , pairs  $C_{i,j}$ , triples  $C_{i,j,k}$ 

149 and so on of input variables.

150 When m = 1, Eq.(6) regresses to Eq.(2) the decomposition of the variance for the scalar output

151 Take the trace about the both sides of Eq.(6), Eq.(7) can be obtained,

$$Tr[\mathbf{C}(Y^{(1)},...,Y^{(m)})] = \sum_{i=1}^{n} Tr[\mathbf{C}_{i}(Y^{(1)},...,Y^{(m)})] + \sum_{1 \le i \le j \le n} Tr[\mathbf{C}_{i,j}(Y^{(1)},...,Y^{(m)})] + \sum_{1 \le i < j < k \le n} Tr[\mathbf{C}_{i,j,k}(Y^{(1)},...,Y^{(m)})] + \dots + Tr[\mathbf{C}_{1,2,..,n}(Y^{(1)},...,Y^{(m)})]$$

$$(7)$$





154

According to Eq.(7), the multivariate single effect index  $SI_i^M$  of the input variable  $X_i$  is given by

$$S1_{i}^{M}(Y^{(1)},...,Y^{(m)}) = \frac{Tr[\mathbf{C}_{i}]}{Tr[\mathbf{C}]}$$
(8)

155 While the multivariate total effect index  $ST_i^M$  can be defined as

156 
$$ST_{i}^{M}(Y^{(1)},...,Y^{(m)}) = \frac{Tr[\mathbf{C}_{i}] + \sum_{1 \le i \le j \le n} Tr[\mathbf{C}_{i,j}] + \sum_{1 \le i < j < k \le n} Tr[\mathbf{C}_{i,j,k}] + \dots + Tr[\mathbf{C}_{1,2,\dots,n}]}{Tr[\mathbf{C}]}$$
(9)

157 The trace  $Tr[\mathbf{C}]$  is the sum of the variances of all outputs  $Y^{(r)}(r=1,...,m)$ . The  $SI_i^M$  or  $ST_i^M$ can be interpreted as the sum of the variances associated with input variable  $X_i$  and  $X_{-i}$  of all 158 the outputs Y . Garcia-Cabrejo et al. (Garcia-Cabrejo and Valocchi 2014) pointed out that the 159 output decomposition method and the covariance decomposition method are equivalent if the 160 161 first K eigenvectors in the principle component decomposition preserve the original variance of 162 outputs. The output and covariance decomposition methods mainly focus on the sum of the 163 variances of the multivariate output. However, the comprehensive effect for the input variable on 164 the multiple output may not be equal to the sum of each input contribution to the scalar output. If the correlation is in the output, the traditional sensitivity measure for the multivariate output is 165 difficult to be interpreted. Furthermore, these methods ignore the influence of the dimension of 166 the output variable. If some outputs have higher order of magnitude than others, they will make 167 168 larger contribution improperly over the whole outputs (Szirtes and Rózsa 2007). To solve these 169 problems, an alternative measure has been proposed for the importance measure of the multivariate output. It is called the vector projection approach. 170

#### 171 **2.2** The Definitions and properties of the new importance measure for multivariate

### 172 output based on the vector projection

173 2.2.1 Preliminaries

178

174 Assume random input variables  $\mathbf{X} = (X_1, \dots, X_n)$  be independent defined on some probability

175 space  $(\Omega, P)$ , and  $Y^{(r)} = g^{(r)}(\mathbf{X})(r = 1, ..., m)$ .

176 2.2.2 Definition of Vector Projection approach

177 Transformed by Eq.(10), the output  $Y^{(r)}$  can be dimensionless

$$\hat{Y}^{(r)} = \frac{Y^{(r)}}{E(|Y^{(r)}|)} \tag{10}$$

179 where  $E(\cdot)$  is the expectation operator and  $|\cdot|$  is the absolute operator.

180 From Eq.(2), the variance decomposition of  $\hat{Y} = (\hat{Y}^{(1)}, ..., \hat{Y}^{(m)})$  can be obtained:

181 
$$\mathbf{V}^{\hat{\mathbf{Y}}} = \sum_{i=1}^{n} \mathbf{V}_{X_{i}}^{\hat{\mathbf{Y}}} + \sum_{i_{1}=1}^{n} \sum_{i_{2}=1+i_{1}}^{n} \mathbf{V}_{X_{i_{1}}X_{i_{2}}}^{\hat{\mathbf{Y}}} + \dots + \mathbf{V}_{X_{1}X_{2}\dots X_{n}}^{\hat{\mathbf{Y}}}$$
(11)





186

182 where *m* -dimension vectors,  $\mathbf{V}_{i_{1},i_{2},...,i_{r}} = [V_{X_{i_{1},i_{2}...,i_{r}}}^{\hat{y}^{(1)}}, V_{X_{i_{1},i_{2}...,i_{r}}}^{\hat{y}^{(2)}}, ..., V_{X_{i_{1},i_{2}...,i_{r}}}^{\hat{y}^{(m)}}]^{T}$ ,  $(1 \le i_{r}(r = 1,...,n) \le n)$  and 183  $\mathbf{V}^{\hat{\mathbf{Y}}} = [V^{\hat{y}^{(1)}}, V^{\hat{y}^{(2)}}, ..., V^{\hat{y}^{(m)}}]^{T}$  are the *r*th,  $(r \in (1, 2, ..., n))$  conditional variances and the unconditional 184 variances of the multivariate output respectively. The above equation can be simplified as following by 185 ignoring the superscript  $\hat{\mathbf{Y}}$ .

$$\mathbf{V} = \sum_{i=1}^{n} \mathbf{V}_{i} + \sum_{i_{1}=1}^{n} \sum_{i_{2}=1+i_{1}}^{n} \mathbf{V}_{i_{1},i_{2}} + \dots + \mathbf{V}_{i_{1},2,\dots,n}$$
(12)

187 The vector projection can be used to generalize the important measure. According to the definition of 188 inner product (Durier 1994), the vector projection  $Q_i$  of the vector  $\mathbf{V}_i$  on the vector  $\mathbf{V}$  can be given 189 by

190 
$$Q_{i} = \|\mathbf{V}_{i}\|\cos \theta_{i} = \frac{\langle \mathbf{V}_{i}, \mathbf{V} \rangle}{\|\mathbf{V}\|} = \frac{\sum_{k=1}^{m} V_{\chi_{i}}^{\hat{\mathbf{Y}}^{(k)}} V^{\hat{\mathbf{Y}}^{(k)}}}{\sqrt{\sum_{k=1}^{m} (V^{\hat{\mathbf{Y}}^{(k)}})^{2}}}$$
(13)

191 where  $\theta_i$  is the angle from the vector **V** to the vector  $\mathbf{V}_i$ ,  $\langle \cdot, \cdot \rangle$  represents the inner product of two 192 vectors, and  $\|\cdot\|$  represents the magnitude of a vector. Then, normalize the projection by dividing the 193 norm of vector **V** and the new main effect index  $P_i$  is defined as following:

194 
$$P_{i} = \frac{Q_{i}}{\|\mathbf{V}\|} = \frac{\sum_{k=1}^{m} V_{X_{i}}^{\hat{y}^{(k)}} V^{\hat{y}^{(k)}}}{\sum_{k=1}^{m} (V^{\hat{y}^{(k)}})^{2}}$$
(14)

195 Similarly, the vector projection  $Q_{i_1,i_2,...,i_r}((r \in 1,...,n), 1 \le i_r \le n)$  of the interaction effect is given by:

196 
$$Q_{i_{1},i_{2},...,i_{r}} = \left\| \mathbf{V}_{i_{1},i_{2},...,i_{r}} \right\| \cos \theta_{i_{1},i_{2},...,i_{r}} = \frac{\langle \mathbf{V}_{i_{1},i_{2},...,i_{r}}, \mathbf{V} \rangle}{\left\| \mathbf{V} \right\|} = \frac{\sum_{k=1}^{m} V_{x_{i_{1}} x_{i_{2}}...x_{i_{r}}}^{\hat{Y}^{(k)}} V^{\hat{Y}^{(k)}}}{\sqrt{\sum_{k=1}^{m} (V^{\hat{Y}^{(k)}})^{2}}}$$
(15)

197 where  $\theta_{i_1,i_2,...,i_r}$  is the angle from vector **V** to vector  $\mathbf{V}_{i_1,i_2,...,i_r}$ . And the interaction effect index is:

198 
$$P_{i_1,i_2,...,i_r} = \frac{Q_{i_1,i_2,...,i_r}}{\|\mathbf{V}\|} = \frac{\sum_{k=1}^m V_{X_{i_1}X_{i_2}...X_{i_r}}^{\hat{Y}^{(k)}} V^{\hat{Y}^{(k)}}}{\sum_{k=1}^m (V^{\hat{Y}^{(k)}})^2}$$
(16)

199 Like Eq.(3) the total effect can be expressed as Eq.(17):

200 
$$\mathbf{V}_{T_i} = \mathbf{V}_i + \sum_{i_1 \neq i}^n \mathbf{V}_{i,i_1} + \dots + \mathbf{V}_{1,\dots,i,\dots,n}$$
(17)

201  $\mathbf{V}_{T_i}$  includes the individual effect of  $X_i$  and its interaction effects with all the other n-1 input 202 variables  $X_{-i}$ . Let  $\mathbf{V}_{-i} = [V_{\mathbf{X}_{-i}}^{Y^{(1)}}, V_{\mathbf{X}_{-i}}^{Y^{(2)}}, ..., V_{\mathbf{X}_{-i}}^{Y^{(m)}}]^T$  and the vector  $\mathbf{V}_{T_i} = \mathbf{V} - \mathbf{V}_{-i}$  contains the average





203 remaining variances of all model outputs when all the inputs but  $X_i$  are fixed over their full ranges.

204 The vector projection of the total effect  $Q_{T_i}$  can be expressed as:

205 
$$Q_{T_{i}} = \frac{\mathbf{V}_{T_{i}}^{T} \cdot \mathbf{V}}{\|\mathbf{V}\|} = \|\mathbf{V}\| - \frac{\langle \mathbf{V}_{-i}, \mathbf{V} \rangle}{\|\mathbf{V}\|} = \sqrt{\sum_{k=1}^{m} (V^{\hat{Y}^{(k)}})^{2}} - \frac{\sum_{k=1}^{m} V^{\hat{Y}^{(k)}}_{\mathbf{X}_{-i}} V^{\hat{Y}^{(k)}}}{\sqrt{\sum_{k=1}^{m} (V^{\hat{Y}^{(k)}})^{2}}}$$
(18)

206

207 And the total effect index is:

208 
$$P_{T_i} = \frac{Q_{T_i}}{\|\mathbf{V}_n\|} = 1 - \frac{\sum_{k=1}^m V_{\mathbf{X}_{-i}}^{\hat{Y}^{(k)}} V^{\hat{Y}^{(k)}}}{\sum_{k=1}^m (V^{\hat{Y}^{(k)}})^2}$$
(19)

209 Lemma 2.2.1 The vector projection measures sum up to 1, i.e,

210

211 
$$\sum_{i=1}^{n} P_i + \sum_{i_1=1}^{n} \sum_{j_2=1+i_1}^{n} P_{i_1,i_2} + \dots + P_{1,2,\dots,n} = 1$$
(20)

212 Proof.

$$\begin{split} \sum_{i=1}^{n} P_{i} + \sum_{i_{1}=1}^{n} \sum_{i_{2}=1+i_{1}}^{n} P_{i_{1},i_{2}} + \dots + P_{1,2,\dots,n} = \frac{\sum_{i=1}^{n} Q_{i} + \sum_{i_{1}=1}^{n} \sum_{i_{2}=1+i_{1}}^{n} Q_{i_{1},i_{2}} + \dots + Q_{1,2,\dots,n}}{\|\mathbf{V}\|} \\ &= \frac{\sum_{i=1}^{n} \|\mathbf{V}_{i}\| \cos \theta_{i} + \sum_{i_{1}=1}^{n} \sum_{i_{2}=1+i_{1}}^{n} \|\mathbf{V}_{i_{1},i_{2}}\| \cos \theta_{i_{1},i_{2}} + \dots + \|\mathbf{V}_{1,2,\dots,n}\| \cos \theta_{1,2,\dots,n}}{\|\mathbf{V}\|} \\ &= \frac{\sum_{i=1}^{n} \sum_{k=1}^{m} V_{i_{1}}^{\hat{\gamma}^{(i)}} V^{\hat{\gamma}^{(i)}} + \sum_{i_{1}=1}^{n} \sum_{i_{2}=1+i_{1}}^{n} \sum_{k=1}^{m} V_{i_{1},i_{2}}^{\hat{\gamma}^{(i)}} + \dots + \sum_{k=1}^{m} V_{i_{1},i_{2},\dots,k}^{\hat{\gamma}^{(i)}} V^{\hat{\gamma}^{(i)}}}{\sum_{k=1}^{m} (V^{\hat{\gamma}^{(i)}})^{2}} \\ &= \frac{\sum_{k=1}^{m} V^{\hat{\gamma}^{(i)}} (\sum_{i=1}^{n} V_{i_{1}}^{\hat{\gamma}^{(i)}} + \sum_{i_{1}=1}^{n} \sum_{i_{2}=1+i_{1}}^{n} V_{i_{1},i_{2}}^{\hat{\gamma}^{(i)}} + \dots + V_{i_{1},i_{2},\dots,k}^{\hat{\gamma}^{(i)}})}{\sum_{k=1}^{m} (V^{\hat{\gamma}^{(i)}})^{2}} \\ &= \frac{\sum_{k=1}^{m} V^{\hat{\gamma}^{(i)}} V^{\hat{\gamma}^{(i)}}}{\sum_{k=1}^{m} (V^{\hat{\gamma}^{(i)}})^{2}} \\ &= \frac{\sum_{k=1}^{m} V^{\hat{\gamma}^{(i)}} V^{\hat{\gamma}^{(i)}}}{\sum_{k=1}^{m} (V^{\hat{\gamma}^{(i)}})^{2}} \end{split}$$

$$(21)$$

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215 **Proportion 2.2.1** For all input terms *i* the vector projection indices satisfy:

216 (i)  $0 \le \theta_i \le 2\pi, 0 \le P_i \le 1$ 





- 217 (ii) If  $X_i$  has no effect on Y, then  $P_i = 0$
- 218 (iii) If  $X_i$  has no effect on Y but  $X_j$  has effect on Y , then  $P_{i,j} = P_j$
- 219 (iv)  $P_i = \sum_{k=1}^m w_k S_i^{Y^{(k)}}, w_k = \frac{(V^{\hat{Y}^{(k)}})^2}{\sum_{k=1}^m (V^{\hat{Y}^{(k)}})^2}$

220 (v) 
$$P_i = \sum_{k=1}^m w_k corr(\hat{Y}^{(k)}, E(\hat{Y}^{(k)} | X_i))$$

- 221 where  $corr(\cdot, \cdot)$  is the correlation coefficient between two random variables.
- 222 Proof. Point(i):positivity is clear, as  $V_{X_i}^{\hat{y}^{(i)}}$  and  $V^{\hat{y}^{(i)}}$  are positive;  $P_i \leq 1$  follows from Eq.(19).Point(ii) and
- 223 point(iii) are easy to be proved by the definition. For (iv) and (v), more details are given in section 2.3.

### 224 2.3 The link between the vector projection index and the Sobol index

- A comparable definition of  $S_i$  proposed by Sobol' (Sobol 1996) is based on the correlation
- 226 between the *k*th output  $\hat{Y}^{(k)}$  and the conditional expectation  $E(\hat{Y}^{(k)} | X_i)$  of the *k*th output.

227 
$$S_i^{\hat{Y}^{(k)}} = corr(\hat{Y}^{(k)}, E(\hat{Y}^{(k)} | X_i))$$
 (21)

- 228
- 229
- 230 And  $P_i$  is given by

231
$$P_{i} = \frac{\sum_{k=1}^{m} V_{X_{i}}^{\hat{Y}^{(k)}} V^{\hat{Y}^{(k)}}}{\sum_{k=1}^{m} (V^{\hat{Y}^{(k)}})^{2}} = \frac{\sum_{k=1}^{m} \frac{V_{X_{i}}^{\hat{Y}^{(k)}}}{V^{\hat{Y}^{(k)}}} (V^{\hat{Y}^{(k)}})^{2}}{\sum_{k=1}^{m} (V^{\hat{Y}^{(k)}})^{2}} = \frac{\sum_{k=1}^{m} S_{i}^{\hat{Y}^{(k)}} (V^{\hat{Y}^{(k)}})^{2}}{\sum_{k=1}^{m} (V^{\hat{Y}^{(k)}})^{2}} = \sum_{k=1}^{m} S_{i}^{\hat{Y}^{(k)}} (V^{\hat{Y}^{(k)}})^{2} = \sum_{k=1}^{m$$

232 where 
$$w_k = \frac{(V^{Y^{(k)}})^2}{\sum_{k=1}^m (V^{\hat{Y}^{(k)}})^2}$$
 is the weight of the *k*th correlation coefficient of the output  $Y^{(k)}$  and the

conditional expectation  $E(\hat{Y}^{(k)} | X_i)$ . When m = 1, the weight  $w_k = 1$  and the index  $P_i$  degrades into the main effect index  $S_i$  of the scalar output. Similarly  $P_{Ti}$  is given by

235 
$$P_{T_{i}} = \frac{\sum_{k=1}^{m} S_{T_{i}}^{Y^{(k)}} (V^{\hat{Y}^{(k)}})^{2}}{\sum_{k=1}^{m} (V^{\hat{Y}^{(k)}})^{2}} = \sum_{k=1}^{m} w_{k} S_{T_{i}}^{Y^{(k)}} = \sum_{k=1}^{m} w_{k} corr(Y^{(k)}, E(Y^{(k)} \mid \boldsymbol{X}_{\sim i}))$$
(23)

And when m=1, the index  $P_{Ti}$  degrades into the total effect index  $S_{Ti}$  of the scalar output.

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238 239

Fig 1.The relationship among  $\mathbf{V}, \mathbf{V}_i, \mathbf{V}_{i_1, i_2}, \dots, \mathbf{V}_{i_1, \dots, n}$  for two outputs.

240

For the scalar output, the Sobol index measures the ratio of magnitude of the conditional variance 241 242 to the magnitude of the unconditional variance. For the multivariate output case, multiple parameters 243 can be expressed as a vector and the inner product can measure the similarity between the vectors. 244 The degree of the coincidence, between the vector  $\mathbf{V}_i$  included all conditional variances and the vector  ${f V}\,$  included all unconditional variances implies the main effect contribution of each input factor to the 245 multivariate variance of all the outputs. Fig.1 shows the geometric interpretation of the vector 246 247 projection measure for multivariate output (m=2). In Fig.1, we can see that the vector angle  $\theta_i$ 248 reflects the difference of the direction between two vectors, the smaller is, the closer the overlapping between vectors is. Except for vector angle, the magnitude of vector  $\mathbf{V}_i$  also influences the 249 250 coincidence degree. The new sensitivity index is the ratio of the vector projection that from the vectors  $\mathbf{V}_i$  to the vector  $\mathbf{V}$  to the norm of the unconditional variance vector. 251

252





## 253 **3. Estimation of the new sensitivity indices**

## 254 3.1 Polynomial Chaos Expansion

The Polynomial Chaos expansion (PCE) of 2-nd order random variable is a decomposition of the form (Wiener 1938, Ghanem and Spanos 1991)

257 
$$Y = \sum_{j=0}^{\infty} \alpha_j \Psi_j(\mathbf{x})$$
(24)

where  $\alpha_j$  is the *jth*  $(j = 1,...,\infty)$  coefficient,  $\Psi_j$   $(j = 1,...,\infty)$  are orthogonal to each other with respect the corresponding PDF (Xiu and Karniadakis 2002, Xiu 2010) and  $\mathbf{x} = (x_1, x_2, ..., x_n)$  are independent standard normal random variables. To be used in engineering models, Eq. (24) needs to be truncated. The order of the polynomials is M and the number of input variables is n, then the total number of terms P+1 with order less than or equal to M is given by

263 
$$P+1 = \frac{(M+n)!}{M!n!}$$
(25)

264 There are two approaches for the estimation of the coefficients: projection and regression. The projection can take advantage of the orthogonal nature of the polynomial  $\Psi$  and the coefficients 265 are estimated using multidimensional numerical integration (Ghanem and Spanos 1991), but it 266 267 requires a large number of the model evaluations to compute integration (Xiu 2010). In the 268 regression approach (Berveiller, Sudret et al. 2006, Sudret 2008), the coefficients are estimated by 269 minimizing the sum of squares of the difference between a set of model evaluations  $\mathbf{Y}_{\scriptscriptstyle N}$  . Assume a set of realizations to be  $\{\xi^{(1)},\xi^{(2)},...,\xi^{(N_0)}\}\$  for **X**, where  $N_0$  is the base number of model 270 realizations. Then  $\mathbf{Y}_{N} = \{y^{(1)}(\boldsymbol{\xi}^{(1)}), y^{(2)}(\boldsymbol{\xi}^{(2)}), ..., y^{(N_{0})}(\boldsymbol{\xi}^{(N_{0})})\}, \boldsymbol{\xi}^{(k)} = (\boldsymbol{\xi}_{1}^{(k)}, ..., \boldsymbol{\xi}_{n}^{(k)}), (k = 1, ..., N_{0}) \text{ and } \boldsymbol{\xi}^{(k)} = (\boldsymbol{\xi}_{1}^{(k)}, ..., \boldsymbol{\xi}_{n}^{(k)}), (k = 1, ..., N_{0})$ 271 we define  $\Psi$  the matrix whose coefficients are given by  $\Psi_{kj} = \Psi_j(\xi^{(k)}), k = 1, ..., N_0; j = 0, ..., P+1$ 272 with evaluation of the orthogonal polynomials at the collocation points  $\xi^{(k)}$  , from these we can 273 274 obtain the coefficients  $\alpha_i$  as

275

$$\boldsymbol{\alpha} = (\boldsymbol{\Psi}^{\mathrm{T}} \boldsymbol{\Psi})^{-1} \boldsymbol{\Psi}^{\mathrm{T}} \boldsymbol{Y}_{\mathrm{N}}$$
(26)

Due to the orthogonality of the basis, it is easy to show that the statistical moments of the random
variable *Y* such as the mean and variance respectively read:

$$Y = E[Y] = \alpha_0$$
  

$$\sigma_Y^2 = Var[Y] = \sum_{j=1}^{p} \alpha_j^2 E[\Psi_j^2]$$
(27)

279

278

## 280 3.2 Estimating the new sensitivity indices for multivariate output by the PCE

281 The Sobol decomposition of multivariate output  $\hat{Y}^{(k)}$  (k = 1,...,m) (see Eq.(2)) can be





282 expressed from a reorganization of its PCE (Sudret 2008) as

284  $\hat{Y}^{(k)} = \alpha_0^{(k)} + \sum_{i=1}^d \sum_{j \in I_i} \alpha_j^{(k)} \Psi_{k,j}(x_i) + \sum_{1 \le i_1 \le i_2 \le d} \sum_{j \in I_{\eta,2}} \alpha_j^{(k)} \Psi_j^{(k)}(x_{i_1}, x_{i_2}) + \cdots + \sum_{1 \le i_1 \le \cdots \le i_s \le d} \sum_{j \in I_{\eta, \dots, i_s}} \alpha_j^{(k)} \Psi_j^{(k)}(x_{i_1}, \dots, x_{i_s}) + \cdots$ (28)

285 where  $I_{i_1,...,i_s}$  is the set of multiple tuples and indices  $(i_1,...,i_s)$  are nonzero:

286 
$$I_{i_{1},...,i_{s}} = \begin{cases} a_{i}^{(k)} > 0 & \forall i \in \{i_{1},...,i_{s}\} \\ a_{i}^{(k)} = 0 & \forall i \notin \{i_{1},...,i_{s}\} \end{cases}$$
(29)

where  $a_i^{(k)} \ge 0$  and  $\sum_{i=1}^{M} a_i^{(k)} \le P$  is an integer set used to correspond each term in Eq.(24) to the orthogonal polynomials (Sudret 2008). The variance of  $\hat{Y}^{(k)}$  can be obtained using Eq.(27), and therefore the main effect of the new sensitivity index for an input variable  $X_i$  can be given by:

290 
$$\hat{P}_{i} = \frac{\sum_{k=1}^{m} (\sum_{j \in I_{i}} (\alpha_{j}^{(k)})^{2} E((\Psi_{j}^{(k)})^{2}) \sum_{i=1}^{p} (\alpha_{i}^{(k)})^{2} E((\Psi_{i}^{(k)})^{2}))}{\sum_{k=1}^{m} (\sum_{i=1}^{p} (\alpha_{i}^{(k)})^{2} E((\Psi_{i}^{(k)})^{2}))^{2}}$$
(30)

291 And the interaction effect of any group of input variables  $X_{i_1,...,i_r}$  can be estimated as follows by PCE

292 
$$\hat{P}_{i_1,\dots,i_s} = \frac{\sum_{k=1}^{m} (\sum_{j \in I_{i_1\dots,i_s}} (\alpha_j^{(k)})^2 E((\Psi_j^{(k)})^2) \sum_{i=1}^{P} (\alpha_i^{(k)})^2 E((\Psi_i^{(k)})^2)))}{\sum_{k=1}^{m} (\sum_{i=1}^{P} (\alpha_i^{(k)})^2 E((\Psi_i^{(k)})^2))^2}$$
(31)

293 Similarly, the total effect index of  $X_i$  can be compactly expressed as

294 
$$\hat{P}_{T_i} = \frac{\sum_{k=1}^{m} (\sum_{j \in I_{i^*}} (\alpha_j^{(k)})^2 E((\Psi_j^{(k)})^2) \sum_{i=1}^{p} (\alpha_i^{(k)})^2 E((\Psi_i^{(k)})^2))}{\sum_{k=1}^{m} (\sum_{i=1}^{p} (\alpha_i^{(k)})^2 E((\Psi_i^{(k)})^2))^2}$$
(32)

295 where  $I_{i+} = I_i + \sum_{i_i \neq i}^n I_{i,i_i} + I_{1,...,i_n}$ .

Therefore, the proposed new sensitivity indices for the multivariate output have analytical expressions which are estimated from the coefficients of the PCE of the output variables. There is no additional cost for obtaining the new sensitivity indices once the coefficients of the PCE are available.

## 300 **4. Example**

301 In this section the new sensitivity index is applied to two numerical examples and a 302 hydrological model to analyze the influence of the input variables on the multivariate output. And 303 the results of the new sensitivity index based on the vector projection index will be compared with





304	the sensitivity index based on the covariance decomposition method. To ensure the convergence
305	of the computational results, the sample size of Monte Carlo Simulation (MCS) for all the sensitivity
306	indices is taken as $N{=}100000$ . The results of the PCE in different orders ( $M$ ) to estimate the new
307	sensitivity indices are compared with the results of the MCS to verify the effectiveness of the PCE
308	based method.

309

310

# 311 4.1 Numerical examples

312 Example 4.1 Consider a linear model with multivariate output

313  

$$\begin{cases}
y^{(1)} = x_1 + 9 \times x_2 + x_3 + x_4 \\
y^{(2)} = 100 \times (x_1 + x_2 + 5 \times x_3 + x_4) \\
x_1 \sim N(0, 1), x_2 \sim N(0, 1), x_3 \sim N(0, 1), x_4 \sim N(0, 1)
\end{cases}$$
(33)

314	The sensitivity results obtained by the Sobol index $S_i$ for each output, the covariance
315	decomposition method $S1^M_i$ and the proposed index $P_i$ are listed in Table 1. For the above
316	equations, we magnify the second function $y_2$ 100 times to simulate the influence of dimension.
317	Since the input variables are standardized normal random variables, it is straightforward to find
318	the important measure ranking is $X_2 > X_3 > X_1 = X_4$ through qualitative analysis.

319

#### 320 Table 1 Sensitivity indices for Example 1

	Function						
Indices	evaluation	$X_1$	$X_{2}$	$X_{3}$	$X_4$	Time	
	number						
5 x <sup>(1)</sup> MC5	$(4 + 2) \times 10^6$	0.0134	0.9643	0.0132	0.0129	2 21E9c	
$S_i - y - MCS$	$(4+2) \times 10$	(3)	(2)	(1)	(4)	2.21585	
$S_i$ - $y^{(2)}$ -MCS	$(4+2) \times 10^{6}$	0.0355(3)	0.0357(2)	0.8930(1)	0.0354(4)	2.2158s	
$S1_i^M$ -MCS	$(4+2) \times 10^{6}$	0.0360(3)	0.0365(2)	0.8925(1)	0.0359(4)	2.2158s	
D MCC	(4 . 0) 100	0.0231(3)	0.4999	0.4517	0.0229	2.1460s	
$P_{\rm i}$ -MCS	$(4+2) \times 10^{3}$		(2)	(1)	(4)		
P DCE	45(14-2)	0 0220(4)	0.5221	0.4314	0.0241	0.06226	
I <sub>i</sub> -ICE	43(101-2)	0.0239(4)	(1)	(2)	(3)	0.00323	
P DCE	105(M-2)	0.0238(4)	0.4997	0.4526	0.0238	0.06626	
I <sub>i</sub> -ICE	105(101=5)		(1)	(2)	(3)	0.00023	
P DCE	240(04.4)	0.0222(4)	0.5001	0.4519	0.0228	0.0721c	
I <sub>i</sub> -FCE	210(IVI=4)	0.0233(4)	(1)	(2)	(3)	0.07315	





321 322 Since there are no interaction term in this example, just the main sensitivity index of the 323 original sensitivity indices is calculated. From Table 1, it can be observed the following aspects. Firstly, the importance rankings and the sensitivity values obtained by  $S_i$  for  $\mathbf{y}^{(2)}$  and  $S\mathbf{1}_i^M$ 324 are the same. This is easy to explain by the fact that  $S1_i^M$  is influenced by the high order of 325 magnitude of dimension of the second function  $y^{(2)}$  .Therefore,  $S1_i^M$  can't describe output 326 327 variability comprehensively during the dimensions of outputs are different, and the magnitude orders of the  $y^{(1)}$  and  $y^{(2)}$  have too big discrepancy. Secondly, the ranking result of the vector 328 329 projection index from the quantitative analysis is equal to the ranking of qualitative analysis, which 330 denotes that the importance measure based on the new sensitivity index is more applicable than the traditional indices for the multivariate output. Thirdly, there is less computational cost for PCE 331 to obtain the convergent values. So the accuracy and efficiency for estimating the new sensitivity 332 333 index can be improved by PCE based method.

334

335 **Example 4.2** Consider the following nonlinear model used in (Luyi, Zhenzhou et al. 2016)

336

$$g^{(1)}(\boldsymbol{X}) = 0.03 - \frac{1.905X_1X_2^2}{X_3X_7} - \frac{0.565X_1X_2^2}{X_4X_8}$$
337
$$g^{(2)}(\boldsymbol{X}) = X_5X_3 - 1.185X_1X_2$$

$$g^{(3)}(\boldsymbol{X}) = X_6X_4 - 0.75X_1X_2$$
(34)

The input variables follow normal distribution, and their distribution parameters are shown in Table 2. The sensitivity results are listed in Table 3. Since this example has interaction terms, the main effect indexes and the total effect indexes based on the covariance decomposition and the vector projection are both presented in Table 3. To compare other differency between the new indices with the traditional method for multivariate output expect dimension, we calculate the results of  $\hat{S}1_i^M$  and  $\hat{S}T_i^M$  which the influence of the dimension of the outputs is eliminated.

344

345	Table 2 the distribution parameters of Example 2
-----	--

	Variables	$X_1$	$X_{2}$	$X_{3}$	$X_4$	$X_5$	$X_{6}$	$X_7$	$X_8$
	Mean	20000	12	0.04	9.82×10 <sup>-4</sup>	1.34×10 <sup>7</sup>	3.35×10 <sup>8</sup>	2×10 <sup>10</sup>	1×10 <sup>11</sup>
	Standard deviation	1400	0.12	0.0048	5.892×10 <sup>-</sup> 5	2.412×10 <sup>6</sup>	4.02×10 <sup>7</sup>	1.2×10 <sup>9</sup>	6×10 <sup>9</sup>
46	Table 3 Sensitivit	ty indices f	for Exar	nple 2					
indices Function									





	evaluation	$X_1$	$X_{2}$	$X_{3}$	$X_4$	$X_5$	$X_{6}$	$X_7$	$X_8$	Time
	number									
$S1_i^M$ -MCS	$(8+2) \times 10^{6}$	0.0333	0.0003	0.2558	0.0230	0.5788	0.0959	0	0	5.4545s
		(4)	(6)	(2)	(5)	(1)	(3)	(7)	(8)	
ST <sup>M</sup> MCS	$(8+2) \times 10^{6}$	0.0338	0.0003	0.2653	0.0241	0.5874	0.0963	0	0	E AEAEc
$SI_i$ -MCS		(4)	(6)	(2)	(5)	(1)	(3)	(7)	(8)	5.4545S
Ê1 <sup>M</sup> MCS	$(8 + 2) \times 10^6$	0.1758	0.0122	0.1807	0.0920	0.3147	0.1506	0.0092	0.0547	E E622c
51 <sub>i</sub> -MCS	$(8+2) \times 10$	(3)	(7)	(2)	(5)	(1)	(4)	(8)	(6)	5.50525
ŜT <sup>M</sup> MCS	$(8 + 2) \times 10^6$	0.1775	0.0130	0.1870	0.0940	0.3193	0.1521	0.0100	0.0553	5 56226
$SI_i$ -MCS	$(0+2) \times 10$	(3)	(7)	(2)	(5)	(1)	(4)	(8)	(6)	5.50525
P-MCS	$(8 + 2) \times 10^6$	0.1535	0.0105	0.2149	0.0690	0.4034	0.0836	0.0079	0.0474	5.4323s
I <sub>i</sub> -mes	$(8+2) \times 10^{-10}$	(3)	(7)	(2)	(5)	(1)	(4)	(8)	(6)	
P MCS	$(9 + 2) + 10^6$	0.1535	0.0105	0.2149	0.0696	0.4034	0.0836	0.0079	0.0474	E 4222c
T <sub>Ti</sub> -MCS	$(0+2) \times 10$	(3)	(7)	(2)	(5)	(1)	(4)	(8)	(6)	J.4JZJS
P PCF	315	0.1531	0.0109	0.2148	0.0687	0.4043	0.0852	0.0083	0.0485	0.06946
I <sub>i</sub> -I CL	M=2	(3)	(7)	(2)	(5)	(1)	(4)	(8)	(6)	0.00945
P_PCF	315	0.1537	0.0111	0.2209	0.0695	0.4101	0.0855	0.0085	0.0479	0.06046
T <sub>Ti</sub> TCL	M=2	(3)	(7)	(2)	(5)	(1)	(4)	(8)	(6)	0.06945
P_PCF	1155	0.1542	0.0111	0.2151	0.0691	0.4026	0.0845	0.0084	0.0479	0 1/58c
I <sub>i</sub> -I CL	M=3	(3)	(7)	(2)	(5)	(1)	(4)	(8)	(6)	0.14585
	1155	0.1550	0.0112	0.2212	0.0698	0.4084	0.0848	0.0085	0.0483	0 14596
T <sub>Ti</sub> -TCL	M=3	(3)	(7)	(2)	(5)	(1)	(4)	(8)	(6)	U.1458S
P_PCF	3465	0.1539	0.0110	0.2153	0.0688	0.4035	0.0841	0.0084	0.0478	0 7/12c
I <sub>i</sub> -I CL	M=4	(3)	(7)	(2)	(5)	(1)	(4)	(8)	(6)	0.74125
P -PCF	3465	0.1546	0.0111	0.2215	0.0696	0.4093	0.0844	0.0086	0.0473	0 7/12c
Ti TI CL	M=4	(3)	(7)	(2)	(5)	(1)	(4)	(8)	(6)	0.7412s

We note from Table 3 that the importance rankings of the nonlinear model of the input variables 347 obtained by  $P_i$  and  $P_{T_i}$  are same with the rankings obtained by  $\hat{S}1_i^M$  and  $\hat{S}T_i^M$ , but the values of 348 the importance measure of them are different. That is because that  $\hat{S}1_i^M$  and  $\hat{S}T_i^M$  only contain 349 the magnitudes of the variances in the multiple output space, whereas  $P_{i}$  and  $P_{Ti}$  include the 350 351 magnitudes of variances and the directions in the multiple output space. This indicates that the importance measures based on the vector projection are more comprehensive than the 352 generalized Sobol indexes. In addition, although the results of  $P_{i}$  and  $P_{Ti}$  estimated by MCS and 353 354 PCE are approximately equal, the computation cost of PCE is much less than that of MCS. Once the 355 coefficients of the PCE are estimated, the multivariate sensitivity indices can be obtained without additional computational cost shown in Eqs.(30)-(32). Therefore, the proposed measure  $P_i$ 356





- 357 provides an efficient alternative for the sensitivity analysis for multivariate output space by taking
- 358 both of its dimension, magnitudes and directions of the multivariate variances into account
- 359 simultaneously.
- 360

### 361 4.2 The hydrological model: HBV model

- 362 The HBV model is a conceptual model for rainfall-runoff simulation and takes the precipitation,
- 363 temperature and potential evaporation as the inputs. The model consists of a degree-day snow
- 364 model, soil-moisture accounting model and a runoff response model (Kollat, Reed et al. 2012). A
- 365 sketch map of the HBV model is shown in Fig 2.





Fig.2 Sketch map of the HBV model

There are 13 parameters that should be calibrated for the HBV model. The parameters and the corresponding ranges are shown in Table 1 (the first four parameters are related to degree-day snow module, next three parameters are related to soil-moisture accounting model, and the last six ones are related to the runoff response model). The ranges of the parameters are based on prior studies (Kollat, Reed et al. 2012).

373





Parameters	Meaning	Units	Ranges	
Ts	Threshold temperature	°C	[-3.0,3.0]	
CFMAX	Degree day factor	$mm \cdot {}^{\mathrm{o}}C^{^{-1}} \cdot d^{^{-1}}$	[0.0,20.0]	
CFR	Refreezing factor	-	[0.0,1.0]	
CWH	Water holding capacity factor of snow	-	[0.0,0.8]	
BETA	Shape parameter	-	[0.0,7.0]	
I D	limiting soil moisture at which potential	_	[0 3 1 0]	
LF	evaporation occurs		[0.5,1.0]	
FC	Maximum soil moisture content	mm	[0.0,2000.0]	
PERC	percolation rate into deep layer	$mm \cdot d^{-1}$	[0.0,100.0]	
$K_{0}$	near-surface flow recession coefficient	$d^{-1}$	[0.05,2]	
$K_1$	interflow recession coefficient	$d^{-1}$	[0.01,1]	
$K_{2}$	base flow recession coefficient	$\mathbf{d}^{-1}$	[0.05,0.1]	
UZL	Near surface flow threshold	mm	[0.0,100.0]	
MAXBAS	Base length for transformation	d	[1,6]	

374 Table 4 The parameters of HBV model and the corresponding ranges

There are a variety of criterions for the calibration of HBV model (Diskin and Simon 1977, van Werkhoven, Wagener et al. 2009). Here we consider three metrics, which are Nash-Sutcliffe efficiency (NSE) (Nash and Sutcliffe 1970, Kollat, Reed et al. 2012), Transformed Root-Mean Square Error (TRMSE) (Kollat, Reed et al. 2012) and Slope of the Flow Duration Curve (SDFCE). Jan suggested that the combination of different functions is suitable to judge different parameter sets which may perform more or less similarly well (Seibert 1997).

381 Nash Sutcliffe Efficiency(NSE )

The first objective emphasizes peak flow errors using the Nash-Sutcliffe Efficiency as shown in
 Eq.(34),

384

$$NSE = 1 - \frac{\sum_{t=1}^{N} (Q_{s,t} - Q_{o,t})^{2}}{\sum_{t=1}^{N} (Q_{o,t} - \overline{Q_{o}})^{2}}$$

(34)

385

where  $Q_{s,t}$  is the simulated runoff at time t,  $Q_{o,t}$  is the observed runoff at time t, and  $\overline{Q_o}$  is the mean observed flow over the calibration period. N is the summation, which performs over t = 1through the number of time steps on the calibration period.NSE is most often used as a hydrologic model calibration objective, which ranges from 1 to  $-\infty$ Transformed Root-mean-square-error (RMSE)

391 The second objective emphasizes low flow errors using the Box-Cox transformed root-mean-





- 392 square-error as shown in Eq.(35)
- 393

394 
$$RMSE = \sqrt{\frac{1}{N} \sum_{t=1}^{N} (Q_{s,t} - Q_{o,t})^2}$$
(35)

395

- 396 Slope of the Flow Duration Curve(SDFCE)
- 397
   398
   398 simulating the slope of the flow duration curve(SFDCE) as shown in Eq.(35)

399 
$$SFDCE = \left| \frac{Q_{s,67\%} - Q_{s,33\%}}{Q_{o,67\%} - Q_{o,33\%}} - 1 \right| \times 100\%$$
(35)

400 About the three response outputs, they have different dimensions and the third function's



401 dimension has the largest orders of magnitude.













408 409

Fig.6.The total effect indices of multivariate output of the HBV model

In Figs.3 and 4, the results of the Sobol index  $S_i$  and  $ST_i$  of three outputs are presented respectively. And the sensitivity analysis results of the multivariate output of the HBV model, which are obtained by the vector projection indices  $P_i$  and  $P_{Ti}$  and the covariance decomposition method  $SI_i^M$  and  $ST_i^M$ , are shown in Figs.5 and 6. The MCS with  $(13+2)\times10^5$  model evaluations and the PCE with 6720 model evaluations (M = 3) are used to get the convergent results, which verifies the efficiency of the PCE.

As for this hydrological model, we can find For SFDCE, it can be found that the ranking 416 obtained by  $S_i$  shown in Fig.3 is same as that by  $S_i^M$  shown in Fig.5, and the ranking obtained by 417  $S_{T}$  shown in Fig.4 is also same as that by  $S_{T}^{M}$  shown in Fig.6, which is caused by the influence of 418 419 dimension of SFDCE. This suggests that in multivariate output case, the magnitude orders of the 420 dimension has great impact on ranking results. For the main effect, Fig.5 shows that although both  $P_i$  and  $SI_i^M$  identify the same important variables BATE and FC, the rankings they are obtained 421 422 are not same. P<sub>i</sub> indicates that FC is more important than BATE based on the vector projection, 423 while  $S1_{i}^{M}$  indicates BATE has the largest importance for the multivariate output, followed by FC. For the total effect, Fig6 shows that the rankings obtained by  $PT_i$  and  $ST_i^M$  are totally different, 424 and  $PT_{i}$  considers more interaction effect between the input variables, since  $PT_{i}$  which includes 425 magnitudes of the variances and the directions in the dimensionless multiple output space, but 426 427 the traditional sensitivity index just includes magnitudes of variances in the multiple output space. In addition, Fig.5 and 6 show that results of PCE are similar to those of MSC. The PCE is able to 428 429 evaluate the proposed index, with  $6720 \mod e$  valuations (M = 3) which is much lower than





### 430 MCS with $(13+2) \times 10^5$ model evaluations.

Based on the above results, it can be concluded that the parameters BETA and FC have much more importance for 3 outputs represented by NSE, TRMSE and SFDCE among 13 inputs, the following importance inputs are the parameters CFMAX, TS,CWH,K1,UZL,MAXBAS since they have large interaction effects. For the rest parameters CFR, LP, PERC, K0 and K2, they have less contribution to the multivariate output.

### 436 5. Conclusions

437 The vector projection importance measure is proposed in this paper to evaluate the comprehensive effect of the inputs on the magnitudes of variances and directions of the multiple 438 439 output space. The mathematical properties of the new sensitivity index are derived and its 440 geometric significance is discussed. Two numerical examples and a hydrological model are employed to verify the effectiveness of the proposed method. Comparison with the covariance 441 decomposition method shows that the new sensitivity index based on the vector projection can 442 measure the effect of the inputs on the whole uncertainty of the multivariate output synthetically. 443 444 The rankings of the input variables obtained by the generalized sensitivity indices are not 445 necessarily the same with the proposed index. This is easy to understand by the fact that the vector 446 projection based method additionally considers the effects on the dimension and directions which 447 are ignored by traditional indices. Thus, only measuring the effects of the input variables on the 448 magnitudes of variances is not enough to reflect the relative importance of the input variables 449 comprehensively. In addition, the Polynomial Chaos Expansion method is used to estimate the new 450 sensitivity indices for the multivariate output, and the main computational cost of the PCE based 451 method is the estimation of the coefficients of the expansions. Thus the PCE based method for 452 estimating the new sensitivity index is efficient compared with the Monte Carlo Simulation.

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