Sobol' Matrices For Multi-Output Models With Quantified Uncertainty[*]

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Abstract. Variance based global sensitivity analysis measures the relevance of inputs to a single output using Sobol' indices. This paper extends the definition in a natural way to multiple outputs, directly measuring the relevance of inputs to the linkages between outputs in a correlation-like matrix of indices. The usual Sobol' indices constitute the diagonal of this matrix. Existence, uniqueness and uncertainty quantification are established by developing the indices from a putative multi-output model with quantified uncertainty. Sobol' matrices and their standard errors are related to the moments of the multi-output model, to enable calculation. These are benchmarked numerically against test functions (with added noise) whose Sobol' matrices are calculated analytically.

Key words. Global Sensitivity Analysis, Sobol' Index, Surrogate Model, Multi-Output, Gaussian Process, Uncertainty Quantification

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1. Introduction.

This paper is concerned with analyzing the results of experiments or computer simulations in a design matrix of $M \geq 1$ input axes (columns) and $L \geq 1$ output axes (columns) over N samples (rows). Global Sensitivity Analysis (GSA) [33] examines the relevance of the various inputs to the various outputs. When pursued via ANOVA decomposition of a single output, this leads naturally to the well known Sobol' indices, which have by now been applied across most fields of science and engineering [36, 19]. This paper extends the definition in a natural way to multiple outputs $L \geq 1$.

Sobol' indices apportion the variance of a scalar output to the influence of various inputs. There is no generally accepted extension of Sobol' indices to multi-outputs $L > 1$. The Sobol' matrices developed in the present article apportion the correlation matrix of outputs – rather than the variance of a single output – to the influence of various inputs. The diagonal elements are identically the classical Sobol' indices, expressing the relevance of inputs to the output variables themselves. The off-diagonal elements express the relevance of inputs to the correlation between outputs. This may be of vital interest when outputs are, for example, yield and purity of a product, cost and efficacy of a process, or perhaps a single output measured at various times. The Sobol matrices reveal (amongst other things) which inputs it is worthwhile varying in an effort to alter the linkage between outputs.

Prior work on Sobol' indices with multiple outputs [17, 18, 49, 13] has settled ultimately on just the diagonal elements of the covariance matrix, so covariance between outputs re-

mains unexamined. Output covariance has been tackled in previous studies by performing principal component analysis (PCA) on outputs prior to performing GSA on the resulting diagonal covariance matrix of outputs [10]. This has been used in particular to study synthetic multi-outputs which are actually the dynamic response of a single output over time [26, 53]. Hierarchical sensitivity analysis [52] employs prior mapping to independent subsystems. In all these cases, output covariance is essentially removed prior to GSA. Only very recently has GSA attempted to incorporate output covariance at all [28], as an ingredient in a total fluctuation. The present article is the first to attempt GSA directly on output covariance itself. This direct approach is deliberately and explicitly motivated by the straightforward desire to examine the influence of inputs on the correlation between outputs.

Accurate calculation of Sobol' indices for a single output is computationally expensive and may require 10,000+ samples [27, 31]. A (sometimes) more efficient approach is calculation via a surrogate model, such as a Gaussian Process (GP) [35, 32], Polynomial Chaos Expansion (PCE) [20, 51, 50], low-rank tensor approximation [14, 25], or support vector regression [16, 13]. Semi-analytic expressions for Sobol' indices are available for scalar PCEs [44], and the diagonal elements of multi-output PCEs [18]. Semi-analytic expressions for Sobol' indices of GPs have been provided in integral form by [31] and alternatively by [12]. These approaches are implemented, examined and compared in [29, 43]. Both [31, 29] estimate the errors on Sobol' indices in semi-analytic, integral form. Fully analytic, closed form expressions have been derived without error estimates for uniformly distributed inputs [48] using a GP with a radial basis function kernel.

In this paper we develop Sobol' matrices and their error estimates in a general setting, then relate these to the moments of a surrogate model. This is to facilitate efficient calculation with limited data, when some form of surrogate is really indispensable. The resulting analytic formulae have been implemented for a multi-output Gaussian process (MOGP), allowing us to benchmark implementation against test functions with known Sobol' matrices. This is important, because practitioners are rarely privileged with an exact and reliable exogenous model linking outputs to inputs. Rather, GSA is a preliminary stage in reducing empirical observations to a tractable, analyzable representation. For example, it is frequently used to guide model reduction and the design of experiments, as well as or as part of optimization and risk assessment. Under these circumstances, the GSA itself must be robust and reliable, providing well benchmarked measures of its own uncertainty and domain of validity.

The contents of this paper are as follows. The next section introduces multi-output models with quantified uncertainty (MQUs) as a context which embraces any explicit or black-box function (simulation, experiment), surrogate (emulator, response surface, meta-model) or regression which supplies a probability distribution on its outputs. This encompasses multi-output models with no uncertainty (MNUs) as MQUs with zero variance. Sections 3 and 4 define Sobol' indices for MQUs, then extend them to Sobol' matrices. The development is leisurely and deliberate in order to make our viewpoint clear. In particular we seek to emphasise that this work is the natural – arguably unique – extension of the *definition* of a Sobol' index. Otherwise it may seem that the classical Sobol' indices occupying the diagonal could be extended to a full correlation matrix in a multitude of arbitrary ways. Sections 5 and 6 derive mean and standard error estimates on the Sobol' matrices of an MQU, then expresses them via the moments of the MQU. The latter is the key step towards implementation.

78 The perspective throughout is essentially Bayesian, regarding uncertainty as undetermined or
79 unobserved input(s).
80   Section 7 introduces a $L = 9$ output MNU composed of known test functions, and examines
81 its Sobol' matrices. Test MQUs consisting of the test MNU plus Gaussian noise are used
82 to benchmark a GP implementation of Sobol' matrices in section 8. This highlights some
83 advantages and limitations of the GP implementation. Conclusions are drawn in section 9.

84   **2. Multi-output models with quantified uncertainty.** The purpose of this Section is to
85 set the scene for this study, serve as a glossary of notation, and prove the formal founda-
86 tion of the construction to follow. Our notation is not quite standard, but is preferred for
87 lightness and fluency once grasped. Regarding notation and other topics, the intention is to
88 facilitate computation by combining efficient, tensorized operations such as `einsum` [1, 3, 4]
89 into numerically stable calculations. As such, the devices employed herein should be familiar
90 to practitioners of machine learning.
91   The preference throughout this paper is for uppercase constants and lowercase variables.
92 Square bracketed quantities such as $[u]_{\mathbf{M} \times \mathbf{N}}$ are tensors subscripted by (the cartesian product
93 of) their ranks, for bookkeeping. Each rank is expressed as an ordinal of axes, a tuple which
94 is conveniently also a naive set and may be subtracted from others as such

95
$$\mathbf{0} := () \subseteq \mathbf{m} := (0, \ldots, m - 1) \subseteq \mathbf{M} := (0, \ldots, M - 1)$$
$$\mathbf{M} - \mathbf{m} := \left\{ m' \in \mathbf{M} \,\middle|\, m' \notin \mathbf{m} \right\} = (m, \ldots, M - 1)$$

96 GSA decomposes input space by families of axes, and this notation facilitates that. It does
97 assume that input axes are expediently ordered already, which might impair convenience but
98 not generality. Conventional indexing of components is permitted under this scheme, by
99 allowing singleton axes to be written in italic without parentheses.
100   From a Bayesian perspective a determined tensor is a function of determined input(s),
101 a random variable (RV) a function of undetermined input, and a stochastic process (SP) a
102 function of both determined and undetermined inputs. In any case, all sources of (sans-serif)
103 uncertainty may be gathered in a single input $[\mathsf{u}]_M$, final to the definition of input space:

104 (2.1)
$$\mathbf{M} := (0, \ldots, M - 1) \quad \text{determined inputs on the unit interval} \quad\quad [u]_{\mathbf{M}} \in [0, 1]^M$$
$$M =: \mathbf{M} + \mathbf{1} - \mathbf{M} \quad\quad \text{an undetermined input on the unit interval} \quad\quad [\mathsf{u}]_M \sim \mathrm{U}(0, 1)$$

105 Exponentiation is always categorical – repeated cartesian $\times$ or tensor $\otimes$ – unless stated oth-
106 erwise. It is crucial to this work that all $\mathbf{M} + \mathbf{1}$ inputs vary completely independently of each
107 other – they are in no way codependent or correlated. Uncertainty is distributed uniformly
108 $[\mathsf{u}]_M \sim \mathrm{U}(0, 1)$ to exploit the "universality of the uniform" [9, pp.224], better known as the
109 inverse probability integral transform [7]. This explicitly provides a bijective mapping to
110 any RV $[\mathsf{x}]_M$ by inverting its cumulative distribution function (CDF) $\mathrm{P} \colon [\mathsf{x}]_M \mapsto [\mathsf{u}]_M$ in the
111 generalized sense

112
$$\mathrm{P}^{-1}([u]_M) := \inf \left\{ [x]_M \,\middle|\, \mathrm{P}([x]_M) \geq [u]_M \right\}$$

113 This mapping $\mathrm{P}^{-1} \colon [\mathsf{u}]_M \mapsto [\mathsf{x}]_M$ is the quantile function of $[\mathsf{x}]_M$ on $[0, 1]$, and embedding it
114 in an output model y can express any continuous RV at a given determined input $[u]_{\mathbf{M}}$. In

other words, the output model could be any continuous SP. The amenity of definition (2.1) is that each input $[u]_m$ is automatically a probability measure, for any $m \in \mathbf{M}$.

Throughout this work, expectations are subscripted by the input axes marginalized

$$\mathbb{E}_\#[\bullet] := \int_{[0]_\#}^{[1]_\#} [\bullet] \, \mathrm{d}\,[u]_\# \qquad \forall \# \subseteq \mathbf{M+1} \text{ or } \# \in \mathbf{M+1}$$

Covariances invoke the tensor product (summing the ranks of the arguments), and carry the subscript of their underlying expectation

$$\mathbb{V}_\#[[\bullet], [*]] := \mathbb{E}_\#[[\bullet] \otimes [*]] - \mathbb{E}_\#[\bullet] \otimes \mathbb{E}_\#[*] \qquad \forall \# \subseteq \mathbf{M+1} \text{ or } \# \in \mathbf{M+1}$$

The covariance of anything with itself is expressed with a single argument $\mathbb{V}_\#[\bullet] := \mathbb{V}_\#[\bullet, \bullet]$, as is customary.

A multi-output model with quantified uncertainty (MQU) is defined as any Lebesgue integrable function of input space (2.1) obeying

$$(2.2) \qquad \begin{aligned} y\colon [0,1]^{M+1} \to \mathbb{R}^L \quad \text{such that} \\ \mathbb{V}_\mathbf{M}\mathbb{E}_M\left[y([u]_{\mathbf{M+1}})\right]_l > \mathbb{E}_\mathbf{M}\mathbb{E}_M\left[y([u]_{\mathbf{M+1}})\right]_l = 0 \quad \forall l \in \mathbf{L} \end{aligned}$$

This forces every output component $l \in \mathbf{L}$ to depend on at least one determined input: constant functions and pure noise are not allowed, to avoid division by zero in GSA. Without loss of generality we have also offset the model to have zero mean $[0]_\mathbf{L}$. This is formally unnecessary, but it can be crucial to the numerical accuracy of computations.

Our notation will reflect machine learning practice [1, 3, 4] which facilitates parallel computation by tensorizing function application over batch dimensions such as $\mathbf{N}$ according to

$$\left[y([u]_{\mathbf{M+1}\times\mathbf{N}})\right]_{\mathbf{L}\times n} := y([u]_{\mathbf{M+1}\times n}) \qquad \forall n \in \mathbf{N}$$

To elucidate the meaning and purpose of an MQU, and set the stage for GSA, consider a design matrix of $[u]_{\mathbf{M}\times\mathbf{N}}$ inputs alongside $[Y]_{\mathbf{L}\times\mathbf{N}}$ outputs:

$$\begin{matrix} [u]_{0\times 0} & \cdots & [u]_{M-1\times 0} & [Y]_{0\times 0} & \cdots & [Y]_{L-1\times 0} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ [u]_{0\times N-1} & \cdots & [u]_{M-1\times N-1} & [Y]_{0\times N-1} & \cdots & [Y]_{L-1\times N-1} \end{matrix}$$

The sole purpose of an MQU is actually to provide a single number for any such design matrix of $N \in \mathbb{Z}^+$ samples (rows): namely, the probability that the output samples result from the input samples, to within any given uncertainty $[E]_{\mathbf{L}\times\mathbf{N}} \geq [0]_{\mathbf{L}\times\mathbf{N}}$

$$\mathbb{P}\left[[E]_{\mathbf{L}\times\mathbf{N}} \geq y([u]_{\mathbf{M+1}\times\mathbf{N}}) - [Y]_{\mathbf{L}\times\mathbf{N}} \geq -[E]_{\mathbf{L}\times\mathbf{N}} \mid [u]_{\mathbf{M}\times\mathbf{N}} = [u]_{\mathbf{M}\times\mathbf{N}}\right]$$

This is what it means to generate L quantifiably uncertain outputs from M determined inputs. Following the Kolmogorov extension theorem [34, pp.124], the meaning of an MQU is nothing other than an SP. This includes zero variance SPs – fully determined multi-output models

of no uncertainty (MNUs) – as MQUs $y([u]_{M+1})$ which do not depend on the final, undetermined input $[u]_M$. Kolmogorov's extension theorem formally identifies an SP – a collection $y([u]_{M+1}) = \{y([u]_{M+1}) \mid [u]_M = [u]_M\}$ of RVs indexed by determined inputs $[u]_M$ – with all its finite dimensional distributions $\{y([u]_{M+1\times N}) \mid [u]_{M\times N} = [u]_{M\times N}\}$. The latter viewpoint is the formal version of the random field [24] or random function interpretation of SPs [39, pp.42] frequently alluded to in machine learning [32]. It can be a helpful perspective on the objects appearing in this work.

In conception MQUs include any simulation, surrogate or regression which supplies a probability distribution (even a zero variance one) on its outputs. In practice, such an MQU is usually inferred from a design of experiments (DoE) which samples the determined inputs $[u]_M$ from $U(0,1)^M$. This is not restrictive, a preferred set of determined inputs $[x]_M$ may have any sampling distribution whatsoever, so long as it is continuous and its M axes mutually independent. Simply take the CDF $[u]_M = P([x]_M)$ before beginning, and apply the quantile function $[x]_M = P^{-1}([u]_M)$ described above and in [7] after finishing. In general and in summary, simply treat any $\tilde{y}([x]_{M+1})$ as the pullback of an MQU by the CDF of $[x]_{M+1}$.

To close this Section we shall formally secure the construction which follows. An MQU y is Lebesgue integrable by definition (2.2), so it must be measurable. All measures throughout this work are finite (probability measures, in fact), so integrability of y implies integrability of y^n for all $n \in \mathbb{Z}^+$ [45]. Therefore, Fubini's theorem [47, pp.77] allows all expectations to be taken in any order, which will be crucial later. We can thus safely construct any SP which is polynomial in y and its marginals; and freely extract finite dimensional distributions from it by the Kolmogorov extension theorem [34, pp.124]. This guarantees existence and uniqueness of every device in this paper.

3. Sobol' indices. This Section recapitulates the definition of classical Sobol' indices in the context of an MQU, to prepare the way for easy generalization to Sobol' matrices in the next Section. Sobol' indices are classically constructed [41] from a High Dimensional Model Representation (HDMR or Hoeffding-Sobol' decomposition [11]). This is enlightening, but not strictly necessary. Instead, we shall swiftly construct the indices from an MQU. Later, this will allow us to derive standard errors on the Sobol' indices.

In essence, GSA is performed by marginalizing (obscuring) determined input axes selectively. A reduced model (mQU) is an SP defined as

$$(3.1) \qquad [y_m]_L := \mathbb{E}_{M-m}[y([u]_{M+1})]_L \qquad \forall m \subseteq M$$

When $M - m = 0$, nothing is marginalized and y_M is called the full model (MQU). The undetermined input $[u]_M$ is never marginalized, and each mQU depends on m determined inputs $[u]_m$ alongside $[u]_M$. Any distributional assumption about inputs simply pulls back (factors through) expectations here with no impact whatsoever: $U(0,1)$ is no more than a proxy for the CDF of any continuous distribution.

An mQU $[y_m]_L$ is *not* automatically converted to a new MQU over $[u]_{m+1}$ by re-indexing $[u]_M$ to $[u]_m$. This would *not* be the same as simply hiding columns $M - m$ in the design matrix of the previous Section. In general the new MQU would *not* adequately reflect the original full model, because any output variation due to marginalized inputs $[u]_{M-m}$ has simply been lost: it cannot be re-allocated to the new undetermined input $[u]_m$. This gets

186 to the heart of GSA: assessing the degree to which a reduced model mQU mimics its full
187 model. Which is a matter of assessing how much output variation has been lost through
188 marginalization.
189   The marginal variance of an mQU is a tensor-valued RV (function of $[u]_M$) defined as

190 (3.2) $$\mathbb{V}_{\mathbf{m}}[\mathbf{y_m}]_{\mathbf{L} \times \mathbf{L}} := \mathbb{V}_{\mathbf{m}}[[\mathbf{y_m}]_{\mathbf{L}}]$$

191 It is – for all realizations $[u]_M = [u]_M$ – a symmetric tensor by definition and positive semi-
192 definite by Jensen's inequality. We may therefore define a vector RV which is the square root
193 of its diagonal, namely the standard deviation $\mathbb{D}_{\mathbf{m}}[\mathbf{y_m}]_{\mathbf{L}}$

194 (3.3) $$\mathbb{D}_{\mathbf{m}}[\mathbf{y_m}]_l := \sqrt{\mathbb{V}_{\mathbf{m}}[\mathbf{y_m}]_{lxl}} \quad > 0 \qquad \forall l \in \mathbf{L}$$

195 This is positive definite due to the positive variance clause in the definition (2.2) of an MQU.
196   The closed Sobol' index of scalar output $[y([u]_{\mathbf{M+1}})]_l$ with respect to input axes $\mathbf{m}$ is
197 defined as an RV

198 (3.4) $$[\mathsf{S_m}]_l := \frac{\mathbb{V}_{\mathbf{m}}[\mathbf{y_m}]_{l \times l}}{\mathbb{V}_{\mathbf{M}}[\mathbf{y_M}]_{l \times l}}$$

199 The definition originated [40] for fully determined functions (y independent of $[u]_M$). It was
200 later extended to random inputs [42] and GPs [31, 29]. The latter work introduced the Sobol'
201 index as an RV constructed from an important category of SP.
202   The complement of a closed index is called a total index [21]

203 (3.5) $$\left[\mathsf{S}^T_{\mathbf{M-m}}\right]_l := 1 - [\mathsf{S_m}]_l$$

204   Sobol' indices are readily interpreted, given that codependent inputs (reviewed in [46])
205 are beyond the scope of this work. By Definition (3.4) a closed index $S_{\mathbf{m}} \in [0,1]$ measures
206 the proportion of output variance captured by the reduced model $\mathbf{y_m}$. This, in turn, indicates
207 the influence or relevance of input axes $\mathbf{m}$. The full model $\mathbf{y_M}$ explains everything explicable,
208 so its Sobol' index is $[\mathsf{S_M}]_l = [\mathsf{S}^T_{\mathbf{M}}]_l = 1$. The void model $\mathbf{y_0}$ is just the mean output – an RV
209 depending only on undetermined noise $[u]_M$ – which explains nothing, so its Sobol' index is
210 $[\mathsf{S_0}]_l = [\mathsf{S}^T_{\mathbf{0}}]_l = 0$.
211   The closed index with respect to a single input axis $m \in \mathbf{M}$ is called a first-order index

212 (3.6) $$[\mathsf{S}_m]_l := [\mathsf{S_{m+1-m}}]_l$$

213 Because inputs may cooperate to affect the output, a closed index often exceeds the sum of
214 its first-order contributions, obeying (for any realization $[u]_M = [u]_M$)

215 (3.7) $$\sum_{\dot{m} \in \mathbf{m}} [\mathsf{S}_{\dot{m}}]_l \leq [\mathsf{S_m}]_l \leq \left[\mathsf{S}^T_{\mathbf{m}}\right]_l$$

216 The final inequality observes that a closed index only includes cooperation of input axes $\mathbf{m}$
217 with each other, whereas a total index also includes cooperation between $\mathbf{m}$ and $\mathbf{M-m}$

218 (but excludes cooperation of input axes $\mathbf{M} - \mathbf{m}$ with each other). This is the only difference
219 between closed and total indices, but it is an important one.
220   Regarding the covariance between any reduced model and its full model, Fubini's theorem
221 and the law of iterated expectations safeguard the intuitive identity

$$
\begin{aligned}
\mathbb{V}_{\mathbf{M}}[\mathsf{y}_{\mathbf{m}}, \mathsf{y}_{\mathbf{M}}]_{\mathbf{L} \times \mathbf{L}} &:= \mathbb{E}_{\mathbf{M}}[[\mathsf{y}_{\mathbf{m}}]_{\mathbf{L}} \otimes [\mathsf{y}_{\mathbf{M}}]_{\mathbf{L}}] - \mathbb{E}_{\mathbf{M}}[\mathsf{y}_{\mathbf{m}}]_{\mathbf{L}} \otimes \mathbb{E}_{\mathbf{M}}[\mathsf{y}_{\mathbf{M}}]_{\mathbf{L}} \\
&= \mathbb{E}_{\mathbf{m}}[[\mathsf{y}_{\mathbf{m}}]_{\mathbf{L}} \otimes [\mathsf{y}_{\mathbf{m}}]_{\mathbf{L}}] - [\mathsf{y}_{\mathbf{o}}]_{\mathbf{L}} \otimes [\mathsf{y}_{\mathbf{o}}]_{\mathbf{L}} \\
&=: \mathbb{V}_{\mathbf{m}}[\mathsf{y}_{\mathbf{m}}]_{\mathbf{L} \times \mathbf{L}}
\end{aligned}
$$

222 (3.8)

223 Using this, the correlation between (the scalar output predicted by) an mQU and its parent
224 MQU is an RV

225 (3.9)
$$
[\mathsf{R}_{\mathbf{mM}}]_l := \frac{\mathbb{V}_{\mathbf{M}}[\mathsf{y}_{\mathbf{m}}, \mathsf{y}_{\mathbf{M}}]_{l \times l}}{\mathbb{D}_{\mathbf{m}}[\mathsf{y}_{\mathbf{m}}]_l \, \mathbb{D}_{\mathbf{M}}[\mathsf{y}_{\mathbf{M}}]_l} = \frac{\mathbb{D}_{\mathbf{m}}[\mathsf{y}_{\mathbf{m}}]_l}{\mathbb{D}_{\mathbf{M}}[\mathsf{y}_{\mathbf{M}}]_l}
$$

226 The square of the correlation is a discerning measure of the quality of prediction [15] called
227 the coefficient of determination. Which is now clearly identical to the closed Sobol' index

228 (3.10)
$$
[\mathsf{R}_{\mathbf{mM}}]_l^2 = \frac{\mathbb{V}_{\mathbf{m}}[\mathsf{y}_{\mathbf{m}}]_{l \times l}}{\mathbb{D}_{\mathbf{M}}[\mathsf{y}_{\mathbf{M}}]_l \, \mathbb{D}_{\mathbf{M}}[\mathsf{y}_{\mathbf{M}}]_l} =: [\mathsf{S}_{\mathbf{m}}]_l
$$

229 Sobol' indices may be used to identify reduced models $[\mathsf{y}_{\mathbf{m}}]_l$ which adequately mimic the full
230 model $[\mathsf{y}_{\mathbf{M}}]_l$. A closed index close to 1 confirms that the two models make nearly identical
231 predictions. Simplicity and economy (not least of calculation) motivate the adoption of a
232 reduced model, a closed Sobol' index close to 1 is what justifies it. This is precisely equivalent
233 to screening out (obscuring) $\mathbf{M} - \mathbf{m}$ input axes on the grounds that their influence on $[\mathsf{y}_{\mathbf{M}}]_l$
234 – measured by their total index $\left[S_{\mathbf{M}-\mathbf{m}}^T\right]_l$ – is close to 0.

235   **4. Sobol' matrices.** This Section introduces a tensor RV called the Sobol' matrix of an
236 mQU. This is defined by tensorizing the definitions of the previous Section, replacing l for a
237 scalar output with $\mathbf{L} \times \mathbf{L}$ for a vector output. All division is performed elementwise, inverting
238 Hadamard multiplication $\circ$

239 (4.1) $[*]_\square = \dfrac{[\bullet]_\square}{[\star]_\square} \quad \Longleftrightarrow \quad [*]_\square \circ [\star]_\square = [\bullet]_\square \quad \Longleftrightarrow \quad [*]_\# [\star]_\# = [\bullet]_\# \quad \forall \# \in \square$

240   The tensorization of definition (3.4) is problematic, as it may invoke division by zero.
241 Instead, we shall tensorize the alternative definition (3.10) of a closed Sobol' index as a
242 coefficient of determination. We shall then compare the two definitions in the light of a toy
243 example.
244   The closed Sobol' matrix of vector output $[y([\mathsf{u}]_{\mathbf{M}+\mathbf{1}})]_{\mathbf{L}}$ with respect to input axes $\mathbf{m}$ is
245 defined as the tensor RV

246 (4.2)
$$
[\mathsf{S}_{\mathbf{m}}]_{\mathbf{L} \times \mathbf{L}} := \frac{\mathbb{V}_{\mathbf{m}}[\mathsf{y}_{\mathbf{m}}]_{\mathbf{L} \times \mathbf{L}}}{\mathbb{D}_{\mathbf{M}}[\mathsf{y}_{\mathbf{M}}]_{\mathbf{L}} \otimes \mathbb{D}_{\mathbf{M}}[\mathsf{y}_{\mathbf{M}}]_{\mathbf{L}}}
$$

247 The complement of a closed Sobol' matrix is called a total Sobol' matrix

248 (4.3)
$$
\left[\mathsf{S}_{\mathbf{M}-\mathbf{m}}^T\right]_{\mathbf{L} \times \mathbf{L}} := [\mathsf{S}_{\mathbf{M}}]_{\mathbf{L} \times \mathbf{L}} - [\mathsf{S}_{\mathbf{m}}]_{\mathbf{L} \times \mathbf{L}}
$$

Let us emphasise that these definitions are equivalent to the Sobol' index definitions (3.4) and (3.5) on the Sobol' matrix diagonal

$$[\mathsf{S_m}]_{l\times l} = [\mathsf{S_m}]_l \quad \text{and} \quad \left[\mathsf{S_m}^T\right]_{l\times l} = \left[\mathsf{S_m}^T\right]_l \qquad \forall l \in \mathbf{L}$$

Just as a Sobol' index is a proportion of output variance, each element of a Sobol' matrix is a component of output correlation. Unlike the former, the latter can be negative. It is still sometimes useful to examine the first-order matrix for a single input axis m

$$(4.4) \qquad\qquad [\mathsf{S}_m]_{\mathbf{L}\times\mathbf{L}} := [\mathsf{S_{m+1-m}}]_{\mathbf{L}\times\mathbf{L}}$$

However, there is no ordering analagous to (3.7) as contributions of opposing sign may offset each other.

Closed Sobol' matrices are related to the marginalized correlation matrices defined by tensorizing definition (3.9)

$$(4.5) \qquad\qquad [\mathsf{R_{mm'}}]_{\mathbf{L}\times\mathbf{L'}} := \frac{\mathbb{V}_{\mathbf{m}}[\mathsf{y_m}, \mathsf{y_{m'}}]_{\mathbf{L}\times\mathbf{L'}}}{\mathbb{D}_{\mathbf{m}}[\mathsf{y_m}]_{\mathbf{L}} \otimes \mathbb{D}_{\mathbf{m'}}[\mathsf{y_{m'}}]_{\mathbf{L'}}} \qquad \forall \mathbf{m}, \mathbf{m'} \in \mathbf{M}$$

In terms of which

$$(4.6) \qquad\qquad [\mathsf{S_m}]_{l\times l'} = [\mathsf{R_{mm}}]_{l\times l'}\sqrt{[\mathsf{S_m}]_{l\times l}\,[\mathsf{S_m}]_{l'\times l'}} \qquad \forall l, l' \in \mathbf{L}$$

All one can rely on – for any $l \in \mathbf{L}$ and any realization $[\mathsf{u}]_M = [u]_M$ – is

$$(4.7a) \qquad\qquad [\mathsf{S_0}]_{\mathbf{L}\times\mathbf{L}} = \left[\mathsf{S_0}^T\right]_{\mathbf{L}\times\mathbf{L}} = [\mathsf{0}]_{\mathbf{L}\times\mathbf{L}}$$

$$(4.7b) \qquad\qquad [\mathsf{S_M}]_{\mathbf{L}\times\mathbf{L}} = \left[\mathsf{S_M}^T\right]_{\mathbf{L}\times\mathbf{L}} = [\mathsf{R_{MM}}]_{\mathbf{L}\times\mathbf{L}}$$

$$(4.7c) \qquad [\mathsf{0}]_{l\times l} \leq \left|[\mathsf{S_m}]_{l\times l'}\right| \leq \sqrt{[\mathsf{S_m}]_{l\times l}\,[\mathsf{S_m}]_{l'\times l'}} \leq 1 \qquad \forall l, l' \in \mathbf{L}$$

So the void model $[\mathsf{y_0}]_{\mathbf{L}}$ still explains nothing, the full model $[\mathsf{y_0}]_{\mathbf{L}}$ still explains everything explicable, and every other mQU lies somewhere in between.

Let us pursue an informative toy example to illustrate this. Take some even M and define

$$w\colon [0,1]^{M/2} \to \mathbb{R} \quad \text{such that} \quad \mathbb{E}_{\mathbf{M/2}}[w] = 0 \quad \text{and} \quad \mathbb{V}_{\mathbf{M/2}}[w] = 1$$

to construct the $(L = 2)$ MQU

$$y([\mathsf{u}]_{\mathbf{M+1}}) = \begin{bmatrix} w([\mathsf{u}]_{\mathbf{M/2}}) + w([\mathsf{u}]_{\mathbf{M-M/2}}) \\ w([\mathsf{u}]_{\mathbf{M/2}}) - w([\mathsf{u}]_{\mathbf{M-M/2}}) \end{bmatrix}$$

The Sobol' matrix of the full model is easily calculated

$$\mathsf{S_M} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Two important reduced models have the Sobol' matrices

$$\mathsf{S_{M/2}} = \mathsf{S}_{\mathbf{M/2}}^T = \begin{bmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{bmatrix} \quad ; \quad \mathsf{S_{M-M/2}} = \mathsf{S}_{\mathbf{M-M/2}}^T = \begin{bmatrix} 1/2 & -1/2 \\ -1/2 & 1/2 \end{bmatrix}$$

The Sobol' matrices reveal that input axes $\mathbf{M/2}$ influence both outputs in the same sense, while input axes $\mathbf{M - M/2}$ influence the two outputs in opposite senses. In real-world examples, this information is often valuable. If the two components of y are the yield and the purity of a pharamaceutical product one would initially focus on inputs $\mathbf{M/2}$ when trying to maximise both outputs simultaneously. Alternatively, if the two components of y are the efficacy and the cost of an industrial process, one would initally vary inputs $\mathbf{M - M/2}$ in an effort to improve the tradeoff between the two outputs. Such prescriptions are particularly simple in this case because the total Sobol' matrices are equal to the closed Sobol' matrices, revealing that inputs $\mathbf{M/2}$ do not cooperate with inputs $\mathbf{M - M/2}$.

The direct tensorization of Sobol' index definition (3.4) would define the matrix

$$\left[\hat{\mathsf{S}}_{\mathbf{m}}\right]_{\mathbf{L \times L}} := \frac{[\mathsf{S_m}]_{\mathbf{L \times L}}}{[\mathsf{S_M}]_{\mathbf{L \times L}}} \quad \text{which is undefined whenever} \quad [\mathsf{S_M}]_{l \times l'} = 0 \text{ for some } l, l' \in \mathbf{L}$$

In our toy example, the most interesting information – the off-diagonal indices for two important reduced models – is undefined and completely lost by this definition.

We close this section by considering how a Sobol' matrix may be summarized in a single number. This is often desired to present "the" sensitivity of multi-output to a reduced set of inputs $\mathbf{m}$. The simple answer is to define a seminorm (like a norm, only positive semi-definite instead of definite) on the Sobol' matrix [38, pp.314]. The seminorm should be chosen according to one's interest in the multi-output. For example, one could use the determinant $|[\mathsf{S_m}]_{\mathbf{l \times l}}|$ (modulus in case $\mathbf{l}$ is singleton) of a chosen submatrix $\mathbf{l} \subseteq \mathbf{L}$. The Sobol' matrix provides a platform for investigating a variety of such measures. However, all matrices and measures remain RVs at this point, and the next two sections are devoted to extracting statistics – i.e. determined quantities – from these.

5. Sobol matrix statistics. At this stage, Sobol' matrices have been robustly defined as tensor RVs – i.e. functions of the undetermined input $[\mathsf{u}]_M$. This section extracts two determined matrix statistics from each RV: its expected value and its standard deviation or error.

Expected values are written as the italic version of the underlying RV, starting with

(5.1a)   marginal variance $[V_{\mathbf{m}}]_{\mathbf{L \times L}} := \mathbb{E}_M \, \mathbb{V}_{\mathbf{m}}[\mathsf{y_m}]_{\mathbf{L \times L}}$

(5.1b)   marginal deviation $[D_{\mathbf{m}}]_{\mathbf{L}} := \mathbb{E}_M \, \mathbb{D}_{\mathbf{m}}[\mathsf{y_m}]_{\mathbf{L}} \quad \Longrightarrow \quad [D_{\mathbf{m}}]_l = \sqrt{[V_{\mathbf{m}}]_{l \times l}} \quad \forall l \in \mathbf{L}$

The GSA statistics used to assess input relevance are the expected Sobol' matrices

(5.2a)   closed Sobol' matrix $[S_{\mathbf{m}}]_{\mathbf{L}^2} := \mathbb{E}_M \, [\mathsf{S_m}]_{\mathbf{L}^2} = \dfrac{[V_{\mathbf{m}}]_{\mathbf{L}^2}}{[D_{\mathbf{m}}]_{\mathbf{L}} \otimes [D_{\mathbf{m}}]_{\mathbf{L}}}$

(5.2b)   total Sobol' matrix $\left[S_{\mathbf{M-m}}^T\right]_{\mathbf{L}^2} := \mathbb{E}_M \left[\mathsf{S}_{\mathbf{M-m}}^T\right]_{\mathbf{L}^2} = [S_{\mathbf{M}}]_{\mathbf{L}^2} - [S_{\mathbf{m}}]_{\mathbf{L}^2}$

309   In order to express standard errors – due to undetermined input $[\mathsf{u}]_M$ – the notation
310 introduced in (3.3) is extended to define the matrix standard deviation $\mathbb{D}_M[\bullet]_{\mathbf{L}\times\mathbf{L}}$ of a matrix
311 RV $[\bullet]_{\mathbf{L}\times\mathbf{L}}$

312   (5.3) $$\mathbb{D}_M[\bullet]_{l\times l'} := \sqrt{\mathbb{V}_M\big[[\bullet]_{l\times l'}\big]} \qquad \forall l, l' \in \mathbf{L}$$

313 The GSA statistics used to assess the standard error of Sobol' matrices are

314   (5.4a)   closed Sobol' matrix error $[T_{\mathbf{m}}]_{\mathbf{L}^2} := \mathbb{D}_M[\mathsf{S}_{\mathbf{m}}]_{\mathbf{L}^2}$

315   (5.4b)   total Sobol' matrix error $\big[T^T_{\mathbf{M}-\mathbf{m}}\big]_{\mathbf{L}^2} := [T_{\mathbf{M}}]_{\mathbf{L}^2} + [T_{\mathbf{m}}]_{\mathbf{L}^2} \geq \mathbb{D}_M\big[\mathsf{S}^T_{\mathbf{M}-\mathbf{m}}\big]_{\mathbf{L}^2}$

316 The total Sobol' matrix error is a conservative statistic which achieves equality on the diagonal,
317 and is robust and sufficiently precise for most practical purposes off the diagonal. Attempts
318 at greater precision are apt to yield nonsense when implemented on a computer. This is
319 because the total Sobol' matrix (4.3) is the difference between two terms which are often
320 highly correlated with each other. Tiny differences between correlated terms are swamped by
321 numerical error in implementation, so the resulting computation is wildly unreliable.
322   To calculate the closed Sobol' matrix error $[T_{\mathbf{m}}]_{\mathbf{L}\times\mathbf{L}}$ we use the Taylor series method [23,
323 pp.353], which is valid provided $\mathbb{V}_{\mathbf{M}}[\mathsf{y}_{\mathbf{M}}]_{l\times l}$ is well approximated by its mean

324                          $$[V_{\mathbf{M}}]_{l\times l} \gg \big|\mathbb{V}_{\mathbf{M}}[\mathsf{y}_{\mathbf{M}}]_{l\times l} - [V_{\mathbf{M}}]_{l\times l}\big|$$

325 This is essentially the positive variance clause in the definition (2.2) of an MQU, designed to
326 prohibit constant or pure noise outputs which do not depend on any of the determined input
327 axes $\mathbf{M}$.
328   The covariance between two marginal covariance matrix RVs is the determined 4-tensor

329   (5.5) $$[W_{\mathbf{m}\mathbf{m}'}]_{\mathbf{L}^4} := \mathbb{V}_M\big[\mathbb{V}_{\mathbf{m}}[\mathsf{y}_{\mathbf{m}}]_{\mathbf{L}\times\mathbf{L}}, \mathbb{V}_{\mathbf{m}'}[\mathsf{y}_{\mathbf{m}'}]_{\mathbf{L}\times\mathbf{L}}\big] \qquad \forall \mathbf{m}, \mathbf{m}' \in \mathbf{M}$$

330 used to define the determined matrix $[Q_{\mathbf{m}}]_{\mathbf{L}\times\mathbf{L}}$ elementwise

331   (5.6)

$$\begin{aligned}
[Q_{\mathbf{m}}]_{l\times l'} := {}& [W_{\mathbf{m}\mathbf{m}}]_{(l\times l')^2} \\
&- [V_{\mathbf{m}}]_{l\times l'} \sum_{l^{\ddagger}\in\{l,l'\}} \frac{[W_{\mathbf{m}\mathbf{M}}]_{l^{\ddagger}\times l^{\ddagger}\times l\times l'}}{[D_{\mathbf{M}}]^2_{l^{\ddagger}}} \\
&+ \frac{[V_{\mathbf{m}}]^2_{l\times l'}}{4} \sum_{l^{\ddagger}\in\{l,l'\}} \frac{[W_{\mathbf{M}\mathbf{M}}]_{l^{\ddagger}\times l^{\ddagger}\times l\times l}}{[D_{\mathbf{M}}]^2_{l^{\ddagger}}[D_{\mathbf{M}}]^2_{l}} + \frac{[W_{\mathbf{M}\mathbf{M}}]_{l^{\ddagger}\times l^{\ddagger}\times l'\times l'}}{[D_{\mathbf{M}}]^2_{l^{\ddagger}}\otimes[D_{\mathbf{M}}]^2_{l'}}
\end{aligned}$$

332 The Taylor series estimate of the closed Sobol matrix error (5.4a) is finally calculated elemen-
333 twise as

334   (5.7) $$[T_{\mathbf{m}}]_{l\times l'} := \mathbb{D}_M[\mathsf{S}_{\mathbf{m}}]_{l\times l'} = \frac{\sqrt{[Q_{\mathbf{m}}]_{l\times l'}}}{[D_{\mathbf{M}}]_l[D_{\mathbf{M}}]_{l'}}$$

335 It is satisfying to note that these equations enforce

336                          $$[T_{\mathbf{M}}]_{l\times l} = 0 \quad \text{on the diagonal} \quad [\mathsf{S}_{\mathbf{M}}]_{l\times l} = 1$$

6. Sobol' matrix statistics from MQU moments. The central problem in calculating errors on Sobol' matrices is that they involve ineluctable covariances over undetermined noise between differently marginalized SPs. But marginalization and covariance determination are both a matter of taking expectations. Using Fubini's theorem [47, pp.77] the ineluctable can be avoided by reversing the order of expectations – taking moments over ungoverned noise, then marginalizing.

Section 2 invoked the Kolmogorov extension theorem [34, pp.124] to guarantee the existence of a tensor-valued SP called a finite-dimensional distribution

$$\left[y([\mathsf{u}]_{\mathbf{M+1}\times\mathbf{N}})\right]_{\mathbf{L}\times\mathbf{N}} \quad \text{for any} \quad N \in \mathbb{Z}^+$$

This used to construct MQU moments as follows. The first moment is the determined statistic

(6.1) $$\left[\mu_{\mathbf{M}}\right]_{\mathbf{L}} := \mathbb{E}_M\left[y([\mathsf{u}]_{\mathbf{M+1}})\right]_{\mathbf{L}}$$

engendering the centralized MQU

(6.2) $$\left[\mathsf{e}_{\mathbf{M}}\right]_{\mathbf{L}} := \left[y([\mathsf{u}]_{\mathbf{M+1}})\right]_{\mathbf{L}} - \left[\mu_{\mathbf{M}}\right]_{\mathbf{L}}$$

The Nth MQU moment is the determined statistic

(6.3) $$\left[\mu_{\mathbf{M}...\mathbf{M}^{n\prime}...\mathbf{M}^{(N-1)\prime}}\right]_{\mathbf{L}^N} := \mathbb{E}_M[[\mathsf{e}_{\mathbf{M}}]_{\mathbf{L}} \otimes \cdots \otimes [\mathsf{e}_{\mathbf{M}^{n\prime}}]_{\mathbf{L}^{n\prime}} \otimes \cdots \otimes [\mathsf{e}_{\mathbf{M}^{(N-1)\prime}}]_{\mathbf{L}^{(N-1)\prime}}]$$

where, to be clear

$$n \in \mathbf{N}$$
$$\mathbf{m}^{n\prime} \subseteq \mathbf{M}^{n\prime} := \mathbf{M} \supseteq \mathbf{m}$$
$$\mathbf{l}^{n\prime} \subseteq \mathbf{L}^{n\prime} := \mathbf{L} \supseteq \mathbf{l}$$

Throughout this work, primes on uppercase constants are for bookkeeping only, they do not affect the value. Primes on lowercase variables do affect the value, so it may or may not be the case that $\mathbf{m}^{n\prime} = \mathbf{m}$ for example. An Nth mQU moment is a determined statistic obtained by marginalizing an Nth MQU moment

(6.4) $$\begin{aligned}\left[\mu_{\mathbf{m}...\mathbf{m}^{(N-1)\prime}}\right]_{\mathbf{L}^N} &:= \mathbb{E}_{\mathbf{m}}\ldots\mathbb{E}_{\mathbf{m}^{(N-1)\prime}}\mathbb{E}_M[[\mathsf{e}_{\mathbf{M}}]_{\mathbf{L}} \otimes \cdots \otimes [\mathsf{e}_{\mathbf{M}^{(N-1)\prime}}]_{\mathbf{L}^{(N-1)\prime}}] \\ &= \mathbb{E}_M[[\mathsf{e}_{\mathbf{m}}]_{\mathbf{L}} \otimes \cdots \otimes [\mathsf{e}_{\mathbf{m}^{(N-1)\prime}}]_{\mathbf{L}^{(N-1)\prime}}]\end{aligned}$$

The last line relies on Fubini's theorem. The law of iterated expectations further entails

(6.5) $$\left[\mu_{\mathbf{0}...\mathbf{0}\mathbf{m}^{n\prime}...\mathbf{m}^{(N-1)\prime}}\right]_{\mathbf{L}^N} = \mathbb{E}_{\mathbf{m}}\left[\mu_{\mathbf{m}...\mathbf{m}\mathbf{m}^{n\prime}...\mathbf{m}^{(N-1)\prime}}\right]_{\mathbf{L}^N} = \mathbb{E}_{\mathbf{M}}\left[\mu_{\mathbf{M}...\mathbf{M}\mathbf{m}^{n\prime}...\mathbf{m}^{(N-1)\prime}}\right]_{\mathbf{L}^N}$$

This reduction will be used repeatedly in the remainder of this section. Definitions (2.2), (3.2), and (5.1) conveniently zero the fully marginalized quantities

(6.6) $$\mathbb{V}_{\mathbf{0}}[\mathsf{y}_{\mathbf{0}}]_{\mathbf{L}^2} = [V_{\mathbf{0}}]_{\mathbf{L}^2} = [\mu_{\mathbf{0}}]_{\mathbf{L}}^2 = [0]_{\mathbf{L}^2}$$

although $[\mu_{\mathbf{00}}]_{\mathbf{L}^2} \geq 0$ in general.

The expected conditional variance in (5.1) amounts to

$$
\begin{aligned}
[V_{\mathbf{m}}]_{\mathbf{L}^2} &:= \mathbb{E}_M \mathbb{V}_{\mathbf{m}}[\mathbf{y}_{\mathbf{m}}]_{\mathbf{L}^2} = \mathbb{E}_M \mathbb{E}_{\mathbf{m}}\left[[\mathbf{y}_{\mathbf{m}}]_{\mathbf{L}}^2 - [\mathbf{y}_{\mathbf{0}}]_{\mathbf{L}}^2\right] \\
&= \mathbb{E}_{\mathbf{m}} \mathbb{E}_M\left[[\mathbf{e}_{\mathbf{m}} + \mu_{\mathbf{m}}]_{\mathbf{L}}^2\right] - \mathbb{E}_M\left[[\mathbf{e}_{\mathbf{0}} + \mu_{\mathbf{0}}]_{\mathbf{L}}^2\right] \\
&= \mathbb{E}_{\mathbf{m}}\left[[\mu_{\mathbf{mm}}]_{\mathbf{L}^2} + [\mu_{\mathbf{m}}]_{\mathbf{L}}^2\right] - [\mu_{\mathbf{00}}]_{\mathbf{L}^2} - [\mu_{\mathbf{0}}]_{\mathbf{L}}^2 \\
&= \mathbb{E}_{\mathbf{m}}\left[[\mu_{\mathbf{m}}]_{\mathbf{L}}^2\right]
\end{aligned}
\tag{6.7}
$$

Substituting this formula in (5.1a) and (5.2) determines the closed and total Sobol' matrices in terms of mQU moments.

The covariance between conditional variances in (5.5) is

$$
\begin{aligned}
[W_{\mathbf{mm}'}]_{\mathbf{L}^2 \times \mathbf{L}'^2} &:= \mathbb{V}_M[\mathbb{V}_{\mathbf{m}}[\mathbf{y}_{\mathbf{m}}]_{\mathbf{L}^2}, \mathbb{V}_{\mathbf{m}'}[\mathbf{y}_{\mathbf{m}'}]_{\mathbf{L}'^2}] \\
&= \mathbb{V}_M\left[\mathbb{E}_{\mathbf{m}}\left[[\mathbf{y}_{\mathbf{m}}]_{\mathbf{L}}^2 - [\mathbf{y}_{\mathbf{0}}]_{\mathbf{L}}^2\right], \mathbb{E}_{\mathbf{m}'}\left[[\mathbf{y}_{\mathbf{m}'}]_{\mathbf{L}'}^2 - [\mathbf{y}_{\mathbf{0}}]_{\mathbf{L}'}^2\right]\right] \\
&= \mathbb{E}_M\left[\mathbb{E}_{\mathbf{m}}\left[[\mathbf{y}_{\mathbf{m}}]_{\mathbf{L}}^2 - [\mathbf{y}_{\mathbf{0}}]_{\mathbf{L}}^2\right] \otimes \mathbb{E}_{\mathbf{m}'}\left[[\mathbf{y}_{\mathbf{m}'}]_{\mathbf{L}'}^2 - [\mathbf{y}_{\mathbf{0}}]_{\mathbf{L}'}^2\right]\right] - [V_{\mathbf{m}}]_{\mathbf{L}^2} \otimes [V_{\mathbf{m}'}]_{\mathbf{L}'^2} \\
&= [A_{\mathbf{mm}'} - A_{\mathbf{0m}'} - A_{\mathbf{m0}} + A_{\mathbf{00}}]_{\mathbf{L}^2 \times \mathbf{L}'^2}
\end{aligned}
$$

where

$$
\begin{aligned}
[A_{\mathbf{mm}'}]_{\mathbf{L}^2 \times \mathbf{L}'^2} &:= \mathbb{E}_M \mathbb{E}_{\mathbf{m}'} \mathbb{E}_{\mathbf{m}}\left[[\mathbf{y}_{\mathbf{m}}]_{\mathbf{L}}^2 \otimes [\mathbf{y}_{\mathbf{m}'}]_{\mathbf{L}'}^2\right] - [V_{\mathbf{m}}]_{\mathbf{L}^2} \otimes [V_{\mathbf{m}'}]_{\mathbf{L}'^2} \\
&= \mathbb{E}_{\mathbf{m}} \mathbb{E}_{\mathbf{m}'} \mathbb{E}_M\left[[\mathbf{e}_{\mathbf{m}} + \mu_{\mathbf{m}}]_{\mathbf{L}}^2 \otimes [\mathbf{e}_{\mathbf{m}'} + \mu_{\mathbf{m}'}]_{\mathbf{L}'}^2 - [\mu_{\mathbf{m}}]_{\mathbf{L}}^2 \otimes [\mu_{\mathbf{m}'}]_{\mathbf{L}'}^2\right]
\end{aligned}
$$

exploiting the fact that $V_{\mathbf{0}} = [0]_{\mathbf{L}^2}$. Equation (6.5) cancels all terms beginning with $[\mathbf{e}_{\mathbf{m}}]_{\mathbf{L}}^2$, across $A_{\mathbf{mm}'} - A_{\mathbf{0m}'} - A_{\mathbf{m0}} + A_{\mathbf{00}}$. All remaining terms ending in $[\mu_{\mathbf{m}'}]_{\mathbf{L}'}^2$ are eliminated by centralization $\mathbb{E}_M[\mathbf{e}_{\mathbf{m}}] = 0$. Similar arguments eliminate $[\mathbf{e}_{\mathbf{m}'}]_{\mathbf{L}'}^2$ and $[\mu_{\mathbf{m}}]_{\mathbf{L}}^2$. Effectively then

$$
[A_{\mathbf{mm}'}]_{\mathbf{L}^4} = \sum_{\pi(\mathbf{L}^2)} \sum_{\pi(\mathbf{L}'^2)} \mathbb{E}_{\mathbf{m}} \mathbb{E}_{\mathbf{m}'} [\mu_{\mathbf{m}} \otimes \mu_{\mathbf{mm}'} \otimes \mu_{\mathbf{m}'}]_{\mathbf{L}^2 \times \mathbf{L}'^2}
$$

so (6.6) entails

$$
[W_{\mathbf{mm}'}]_{\mathbf{L}^4} = \sum_{\pi(\mathbf{L}^2)} \sum_{\pi(\mathbf{L}'^2)} \mathbb{E}_{\mathbf{m}} \mathbb{E}_{\mathbf{m}'} [\mu_{\mathbf{m}} \otimes \mu_{\mathbf{mm}'} \otimes \mu_{\mathbf{m}'}]_{\mathbf{L}^2 \times \mathbf{L}'^2}
\tag{6.8}
$$

where each summation is over permutations of tensor axes

$$
\pi(\mathbf{L}^2) := \left\{(\mathbf{L} \times \mathbf{L}''), (\mathbf{L}'' \times \mathbf{L})\right\} \quad ; \quad \pi(\mathbf{L}'^2) := \left\{(\mathbf{L}' \times \mathbf{L}'''), (\mathbf{L}''' \times \mathbf{L}')\right\}
$$

Substituting (6.8) in (5.4) and (5.6) determines the closed and total Sobol' matrix errors in terms of marginalized MQU moments.

Equation (6.8) has an important property. Any constant term E added to the MQU variance $\mu_{\mathbf{mm'}} \mapsto \mu_{\mathbf{mm'}} + E$ adds nothing to $W_{\mathbf{mm'}}$ by reduction (6.5). Perhaps, surprisingly, adding homoskedastic noise to an MQU directly affects neither $S_{\mathbf{m}}$ nor $T_{\mathbf{m}}$.

So Sobol' matrices may be calculated from the first MQU moment alone. Their standard errors may be calculated from the first two MQU moments alone. The first MQU moment $[\mu_{\mathbf{M}}]_{\mathbf{L}}$ is simply the mean prediction of the MQU, a function of $[u]_{\mathbf{M}}$. The second MQU moment $[\mu_{\mathbf{MM}}]_{\mathbf{L}^2}$ is known as the covariance function or kernel of an SP

$$(6.9) \qquad [\mu_{\mathbf{MM'}}]_{\mathbf{L}\times\mathbf{L'}} = \left[k([u]_{\mathbf{M}}, [u']_{\mathbf{M'}})\right]_{\mathbf{L}\times\mathbf{L'}} := \mathbb{V}_M\left[\left[y([\mathsf{u}]_{\mathbf{M}+1})\right]_{\mathbf{L}}, \left[y\left([\mathsf{u'}]_{\mathbf{M'}+1}\right)\right]_{\mathbf{L'}}\right]$$

It expresses the linkage between MQU predictions at two determined inputs, and is central to the theory and implementation of GPs [32].

Analytic expressions for Sobol' matrices and their standard errors are given in [30] for GPs with a Radial Basis Function (RBF) kernel [32]. These have been implemented in Python as the rom-comma package [2], which is used in the next two sections to benchmark the calculation of Sobol' matrices and their standard errors from MQU moments.

7. Test functions. The SALib package [5] implements a number of scalar test functions for benchmarking sensitivity analysis. This study uses 3 of these

$$(7.1a) \qquad \text{Ishigami } [22]: \quad \text{ish}([u]_{\mathbf{3}}; A, B) := \left(1 + B[u]_2^4\right)\sin([u]_0) + A\sin([u]_1)^2$$

$$(7.1b) \qquad \text{Sobol' G } [37]: \quad \text{sob}([u]_{\mathbf{5}}; [A]_{\mathbf{5}}, [B]_{\mathbf{5}}) := \prod_{m=0}^{4} \frac{(1 + [B]_m)\,|2[u]_m - 1|^{[B]_m} + [A]_m}{1 + [A]_m}$$

$$(7.1c) \qquad \text{Oakley 2004 } [31]: \quad \text{oak}([u]_{\mathbf{5}}; [A]_{\mathbf{5}}, [B]_{\mathbf{5}\times\mathbf{5}}) := [u]_{\mathbf{5}}[A]_{\mathbf{5}} + [u]_{\mathbf{5}}[B]_{\mathbf{5}\times\mathbf{5'}}[u]_{\mathbf{5'}}$$

The last of these uses the Einstein summation convention for tensor contraction. It is just a quadratic form in $[u]_{\mathbf{5}}$ parametrized by the matrix $[B]_{\mathbf{5}\times\mathbf{5}}$ plus a linear term parametrized by the vector $[A]_{\mathbf{5}}$. To parametrize the (modified) Sobol' G function and (restricted) Oakley 2004 function we define the vectors

$$(7.2) \qquad [A_g]_{\mathbf{5}} := \begin{bmatrix} 3 \\ 6 \\ 9 \\ 18 \\ 27 \end{bmatrix} \quad ; \quad [A_G]_{\mathbf{5}} := \begin{bmatrix} 1/2 \\ 1 \\ 2 \\ 4 \\ 8 \end{bmatrix} \quad ; \quad [A_O]_{\mathbf{5}} := \begin{bmatrix} 5 \\ 35/8 \\ 15/4 \\ 25/8 \\ 5/2 \end{bmatrix}$$

and the matrices

$$(7.3) \qquad [B_+]_{\mathbf{5}\times\mathbf{5}} := \begin{bmatrix} 5 & 29/6 & 14/3 & 9/2 & 13/3 \\ 25/6 & 4 & 23/6 & 11/3 & 7/2 \\ 10/3 & 19/6 & 3 & 17/6 & 8/3 \\ 5/2 & 7/3 & 13/6 & 2 & 11/6 \\ 5/3 & 3/2 & 4/3 & 7/6 & 1 \end{bmatrix} \quad ; \quad [B_-]_{m\times m'} := [B_+]_{4-m\times 4-m'}$$

410   The $L = 9$ MNU used for benchmarking is

411   (7.4)
$$f([u]_\mathbf{M}) := \begin{bmatrix} \mathrm{ish}(2\pi[u]_\mathbf{3} - \pi[1]_\mathbf{3}; 7, 1/10) \\ \mathrm{ish}(2\pi[u]_\mathbf{3} - \pi[1]_\mathbf{3}; 20, 1) \\ \mathrm{ish}(2\pi[u]_\mathbf{3} - \pi[1]_\mathbf{3}; 0, 0) \\ \mathrm{sob}([u]_\mathbf{5}; [A_g]_\mathbf{5}, [2]_\mathbf{5}) \\ \mathrm{sob}([u]_\mathbf{5}; [A_G]_\mathbf{5}, [2]_\mathbf{5}) \\ \mathrm{sob}([u]_\mathbf{5}; [A_G]_\mathbf{5}, [4]_\mathbf{5}) \\ \mathrm{oak}(2[u]_\mathbf{5} - [1]_\mathbf{5}; [A_O]_\mathbf{5}, [0]_{\mathbf{5}\times\mathbf{5}}) \\ \mathrm{oak}(2[u]_\mathbf{5} - [1]_\mathbf{5}; [A_O]_\mathbf{5}, [B_+]_{\mathbf{5}\times\mathbf{5}}) \\ \mathrm{oak}(2[u]_\mathbf{5} - [1]_\mathbf{5}; -[A_O]_\mathbf{5}, [B_-]_{\mathbf{5}\times\mathbf{5}}) \end{bmatrix}$$

412   The correlation matrix of this MNU is

413   $S_\mathbf{5} = \begin{bmatrix} 1.000 & 0.896 & 0.560 & -0.073 & -0.078 & -0.131 & 0.254 & 0.125 & -0.159 \\ 0.896 & 1.000 & 0.593 & -0.032 & -0.034 & -0.057 & 0.268 & 0.146 & -0.161 \\ 0.560 & 0.593 & 1.000 & 0.000 & 0.000 & 0.000 & 0.453 & 0.264 & -0.264 \\ -0.073 & -0.032 & 0.000 & 1.000 & 0.944 & 0.825 & 0.000 & 0.251 & 0.136 \\ -0.078 & -0.034 & 0.000 & 0.944 & 1.000 & 0.926 & 0.000 & 0.232 & 0.137 \\ -0.131 & -0.057 & 0.000 & 0.825 & 0.926 & 1.000 & 0.000 & 0.197 & 0.116 \\ 0.254 & 0.268 & 0.453 & 0.000 & 0.000 & 0.000 & 1.000 & 0.582 & -0.582 \\ 0.125 & 0.146 & 0.264 & 0.251 & 0.232 & 0.197 & 0.582 & 1.000 & 0.206 \\ -0.159 & -0.161 & -0.264 & 0.136 & 0.137 & 0.116 & -0.582 & 0.206 & 1.000 \end{bmatrix}$

414   The Sobol' G functions $[f]_3, [f]_4, [f]_5$ are invariant under the transformation $[u]_m \mapsto [1 - u]_m$ –
415   they possess the reflection symmetries of an even function. The sine function $[f]_2$ and the linear
416   function $[f]_6$ preserve magnitude and change sign under the transformation $[u]_m \mapsto [1 - u]_m$
417   – they possess rotational symmetries of an odd function. As a result, the correlation matrix
418   contains a central rectangle of three Sobol' G functions bordered by zero correlations.
419   The remaining closed Sobol' matrices of the test MNU are as follows

420   $S_\mathbf{4} = \begin{bmatrix} 1.000 & 0.896 & 0.560 & -0.073 & -0.078 & -0.131 & 0.254 & 0.125 & -0.159 \\ 0.896 & 1.000 & 0.593 & -0.032 & -0.034 & -0.057 & 0.268 & 0.146 & -0.161 \\ 0.560 & 0.593 & 1.000 & 0.000 & 0.000 & 0.000 & 0.453 & 0.264 & -0.264 \\ -0.073 & -0.032 & 0.000 & 0.986 & 0.929 & 0.811 & 0.000 & 0.247 & 0.116 \\ -0.078 & -0.034 & 0.000 & 0.929 & 0.979 & 0.904 & 0.000 & 0.229 & 0.118 \\ -0.131 & -0.057 & 0.000 & 0.811 & 0.904 & 0.970 & 0.000 & 0.194 & 0.100 \\ 0.254 & 0.268 & 0.453 & 0.000 & 0.000 & 0.000 & 0.916 & 0.533 & -0.533 \\ 0.125 & 0.146 & 0.264 & 0.247 & 0.229 & 0.194 & 0.533 & 0.839 & 0.031 \\ -0.159 & -0.161 & -0.264 & 0.116 & 0.118 & 0.100 & -0.533 & 0.031 & 0.591 \end{bmatrix}$

421

$$S_3 = \begin{bmatrix} 1.000 & 0.896 & 0.560 & -0.073 & -0.078 & -0.131 & 0.254 & 0.125 & -0.159 \\ 0.896 & 1.000 & 0.593 & -0.032 & -0.034 & -0.057 & 0.268 & 0.146 & -0.161 \\ 0.560 & 0.593 & 1.000 & 0.000 & 0.000 & 0.000 & 0.453 & 0.264 & -0.264 \\ -0.073 & -0.032 & 0.000 & 0.956 & 0.889 & 0.774 & 0.000 & 0.235 & 0.093 \\ -0.078 & -0.034 & 0.000 & 0.889 & 0.912 & 0.833 & 0.000 & 0.215 & 0.091 \\ -0.131 & -0.057 & 0.000 & 0.774 & 0.833 & 0.877 & 0.000 & 0.183 & 0.077 \\ 0.254 & 0.268 & 0.453 & 0.000 & 0.000 & 0.000 & 0.784 & 0.457 & -0.457 \\ 0.125 & 0.146 & 0.264 & 0.235 & 0.215 & 0.183 & 0.457 & 0.622 & -0.096 \\ -0.159 & -0.161 & -0.264 & 0.093 & 0.091 & 0.077 & -0.457 & -0.096 & 0.359 \end{bmatrix}$$

422

423

$$S_2 = \begin{bmatrix} 0.756 & 0.525 & 0.560 & -0.073 & -0.078 & -0.131 & 0.254 & 0.125 & -0.159 \\ 0.525 & 0.435 & 0.593 & -0.032 & -0.034 & -0.057 & 0.268 & 0.146 & -0.161 \\ 0.560 & 0.593 & 1.000 & 0.000 & 0.000 & 0.000 & 0.453 & 0.264 & -0.264 \\ -0.073 & -0.032 & 0.000 & 0.848 & 0.765 & 0.661 & 0.000 & 0.202 & 0.059 \\ -0.078 & -0.034 & 0.000 & 0.765 & 0.741 & 0.660 & 0.000 & 0.181 & 0.057 \\ -0.131 & -0.057 & 0.000 & 0.661 & 0.660 & 0.664 & 0.000 & 0.154 & 0.048 \\ 0.254 & 0.268 & 0.453 & 0.000 & 0.000 & 0.000 & 0.595 & 0.346 & -0.346 \\ 0.125 & 0.146 & 0.264 & 0.202 & 0.181 & 0.154 & 0.346 & 0.375 & -0.145 \\ -0.159 & -0.161 & -0.264 & 0.059 & 0.057 & 0.048 & -0.346 & -0.145 & 0.221 \end{bmatrix}$$

424

425

$$S_1 = \begin{bmatrix} 0.314 & 0.332 & 0.560 & 0.000 & 0.000 & 0.000 & 0.254 & 0.148 & -0.148 \\ 0.332 & 0.351 & 0.593 & 0.000 & 0.000 & 0.000 & 0.268 & 0.156 & -0.156 \\ 0.560 & 0.593 & 1.000 & 0.000 & 0.000 & 0.000 & 0.453 & 0.264 & -0.264 \\ 0.000 & 0.000 & 0.000 & 0.632 & 0.515 & 0.438 & 0.000 & 0.139 & 0.028 \\ 0.000 & 0.000 & 0.000 & 0.515 & 0.420 & 0.357 & 0.000 & 0.113 & 0.023 \\ 0.000 & 0.000 & 0.000 & 0.438 & 0.357 & 0.331 & 0.000 & 0.096 & 0.019 \\ 0.254 & 0.268 & 0.453 & 0.000 & 0.000 & 0.000 & 0.337 & 0.196 & -0.196 \\ 0.148 & 0.156 & 0.264 & 0.139 & 0.113 & 0.096 & 0.196 & 0.145 & -0.108 \\ -0.148 & -0.156 & -0.264 & 0.028 & 0.023 & 0.019 & -0.196 & -0.108 & 0.115 \end{bmatrix}$$

426

427 Additional input dimensions do not affect test MNU evaluation, so obviously

428
$$S_m = S_5 \quad \forall m \geq 5$$

429 Histograms of Sobol' index values across the test MNU are shown in Figure 1. The bench-
430 marking of first order indices will reveal superb agreement, but this could merely indicate the
431 benchmarking calculation is biased toward zero, because the first order indices almost all have
432 small magnitudes. The closed indices have a much more reasonable spread of values and are
433 therefore suitable for benchmarking.
434   Uncertainty is manufactured by adding iid (independent, identically distributed) Gaussian
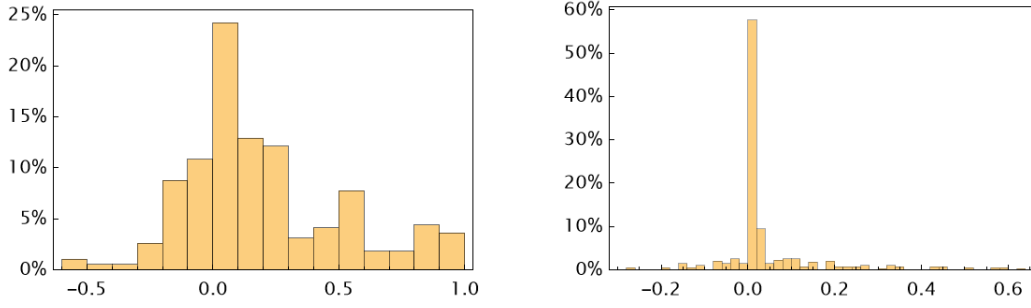
Figure 1. *Frequency of closed and first order Sobol' index values across 9 outputs and 5 inputs.*

noise of magnitude E to the normalized MNU using the identity matrix $\langle 1 \rangle$ to define

$$(7.5a) \qquad [y([u]_{\mathbf{M} \times \mathbf{N}})]_{l \times \mathbf{N}} := (1 + E^2)^{-1/2} \left(\left[\bar{f}([u]_{\mathbf{M} \times \mathbf{N}}) \right]_{l \times \mathbf{N}} + E \, [\mathsf{e}]_{(\mathbf{l+1})\mathbf{N} - \mathbf{lN}} \right)$$

$$(7.5b) \qquad \left[\bar{f}([u]_{\mathbf{M} \times \mathbf{N}}) \right]_{l \times \mathbf{N}} := \left([f([u]_{\mathbf{M} \times \mathbf{N}})]_{l \times \mathbf{N}} - \mathbb{E}_{\mathbf{N}} \left[f([u]_{\mathbf{M} \times \mathbf{N}})]_{l} \right) / \mathbb{D}_{\mathbf{N}}[f([u]_{\mathbf{M} \times \mathbf{N}})]_{l}$$

$$(7.5c) \qquad\qquad [\mathsf{e}]_{\mathbf{LN}} \sim \mathcal{N} \big([0]_{\mathbf{LN}}, \langle 1 \rangle_{\mathbf{LN} \times \mathbf{LN}} \big)$$

Test MQUs are constructed by fitting a GP with an RBF kernel [32] to $[y([u]_{\mathbf{M} \times \mathbf{N}})]_{l \times \mathbf{N}}$. The suite of test MQUs exhaustively encompasses

$M \in \{5, 7\} \quad ; \quad L = 9$

$N \in \{30, 50, 70, 90, 110, 130, 150, 170, 190, 210, 230, 260, 290, 320, 360, 400, 440, 480, 525, 575,$

$\qquad 630, 690, 755, 825, 900, 980, 1065, 1105, 1200, 1300, 1410, 1530, 1660, 1800, 1950, 2110,$

$\qquad 2280, 2460, 2710, 2930, 3170, 3430, 3710, 4000, 4300, 4600, 4920\}$

$E \in \{0.0025, 0.005, 0.01, 0.025, 0.05, 0.075, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9,$

$\qquad 1.0, 1.2, 1.5, 2.0, 5.0\}$

There are 47 values for N, the number of regression (training) samples. A GP regressed over 5 or 7 inputs using less than 100 samples cannot be expected to perform well. There are 20 values for E, the noise to signal ratio of the test MQU. Where $E > 1$, Gaussian noise dominates the output and GP regression cannot be expected to perform well.

The quality of regression was monitored by 2-fold sampling, wherein a latin hypercube of $2N$ MQU samples is randomly split in half. One half is used for regression (training) and the other for validation (testing) in the first fold, the roles reversed in the second fold. This makes a total of nearly 17k MQU individual outputs, for just over 1.8m closed Sobol' indices over $M \in \{5, 7\}$. Although the results are somewhat similar, $M = 5$ gives a nice spread of Sobol' matrix element magnitudes, whereas $M = 7$ invites the curse of dimensionality [6, 8] by incorporating irrelevant input dimensions. The Sobol' matrices for these irrelevant dimensions is of particular interest, as it enables dimension reduction via GSA.

8. Benchmarking. The suite of test functions has been implemented as a Python script using the rom-comma package [2], to perform benchmarking of Sobol' matrix calculations and

their errors. This section describes the key results. A more detailed presentation, including GP calculation details, is given in [30].

The first task is to assess the reliability of the GP regression used to construct the test MQU, particularly given the extreme cases we have included. Figure 2 shows the standard deviation of prediction, Figure 3 the Root Mean Square Error from 2-fold validation. The former indicates how accurate the GP thinks its predictions are, the latter how good they actually are against independent test data. The two measures agree quite well, although the GP slightly overestimates its own accuracy.
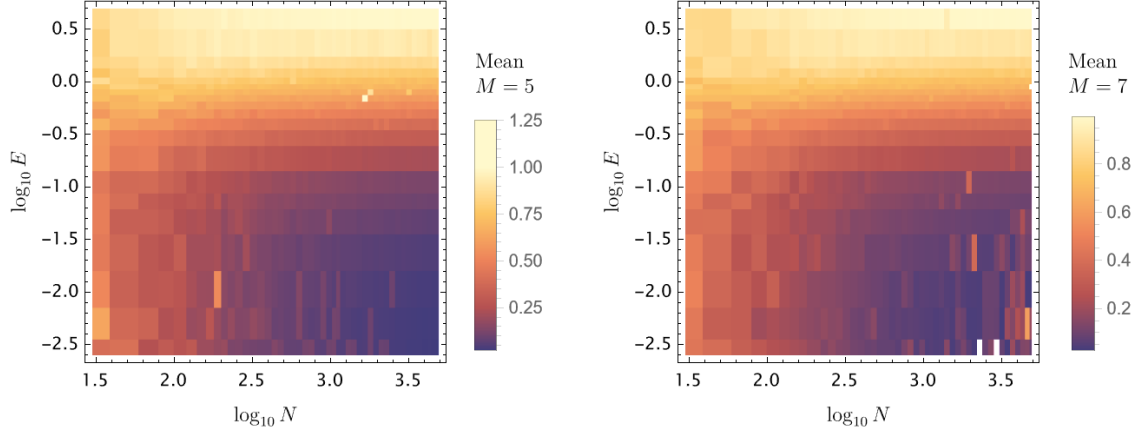
Figure 2. *The Standard Deviation (SD) of prediction for the benchmark GPs. Each plot point is the mean over 2 folds and 9 outputs.*
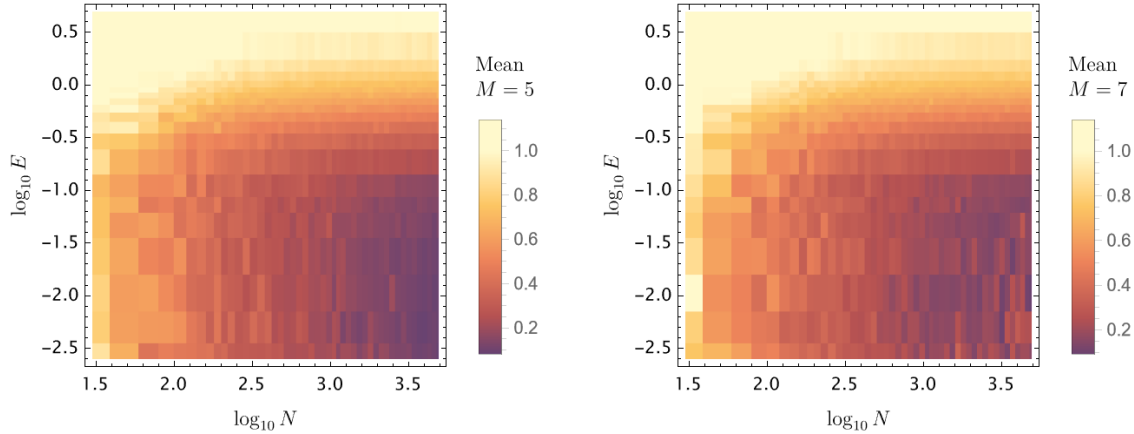

Figure 3. *The Mean Root Mean Square Error (RMSE) of prediction for the benchmark GPs, obtained from 2-fold validation. Each plot point is the mean over 2 folds and 9 outputs.*

Recall from (7.5) that each underlying MQU (GP) has been scaled to a total variation over training data of $\mathbb{D}_\mathbf{N}[y([u]_{\mathbf{M}\times\mathbf{N}})]_l = 1$. Therefore, predictions with an RMSE≥ 1 are uninformative, even overfit: the mean of the training data is a better predictor than the GP. The figures show this occurring for $E > 10^{0.5}$. There is very marked and consistent

473 deterioration in predictive GP performance with increasing E, decreasing N and increasing M.
474 The mean prediction error is 30% or more whenever $E > 20\%$ or $N < 100$. This description is
475 largely valid for each GP, even though the results are displayed as mean values so that extreme
476 outliers are visible. Severe outliers are numerically unstable GPs, appearing as blemishes in
477 Figure 2. Numerical instability results from overfitting, and is a well-understood pitfall of GP
478 regression, which is highly susceptible to the curse of dimensionality [6, 8], readily diagnosed
479 and sometimes remediable. Given k-fold validation, one would normally remove these GPs,
480 or try alternative optimizations to obtain a reliable GP regression.
481   In order to assess the performance of GSA, we have not removed numerically unsta-
482 ble, overfit GPs using k-fold validation as should be done in practice. Instead, the results
483 are cleaned similarly by filtering out numerically impossible GSA results. Any Sobol' index
484 $[S_{\mathbf{m}}]_{l \times l} \notin [-0.001, 1.001]$ or Sobol' matrix standard error $[T_{\mathbf{m}}]_{l \times l'} \notin [-0.001, 1.001]$ prompts
485 us to remove $[y]_l, [y]_{l'}$ entirely from that fold (k, M, N, E). If needed, such filtering should be
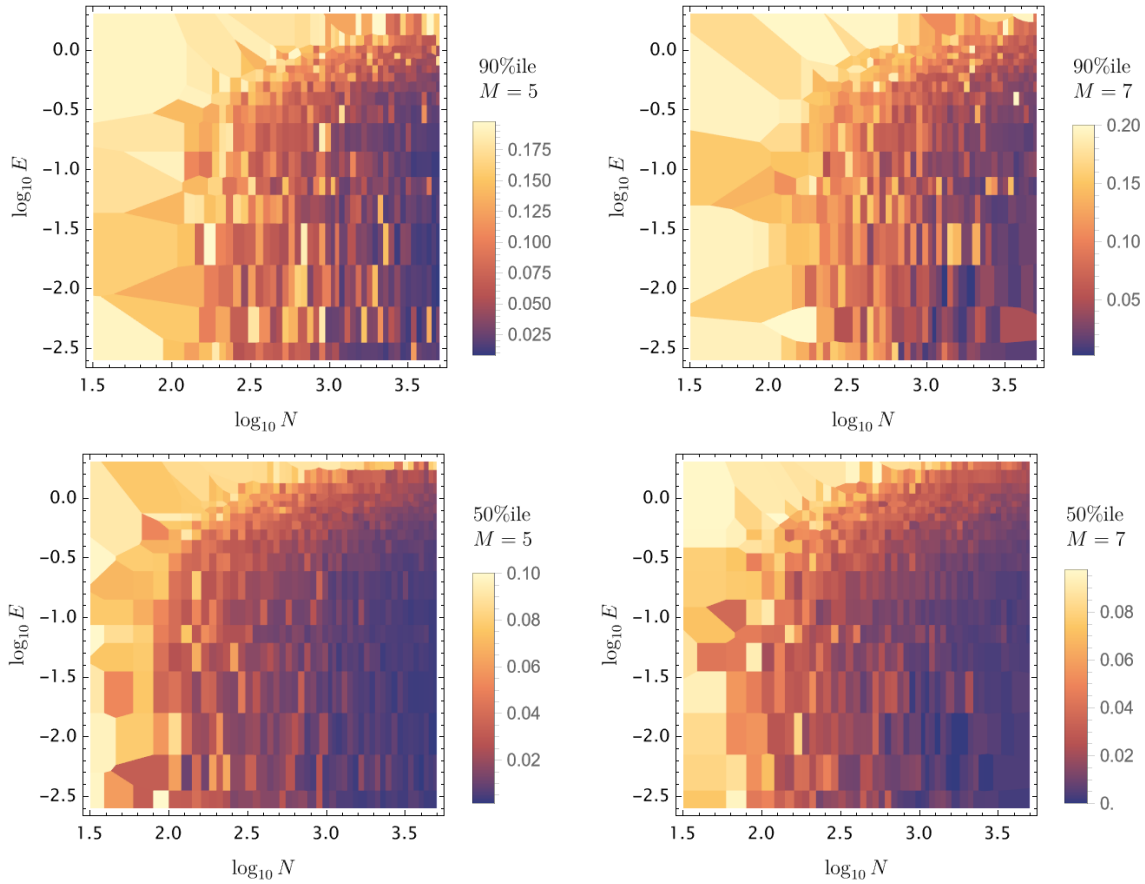486 applied in practice.

Figure 4. *The absolute error $[A_{\mathbf{m}}]_{l \times l'}$ of the closed Sobol' matrix element $[S_{\mathbf{m}}]_{l \times l'}$ calculated from MQU moments. Ground truth is the MNU closed Sobol' matrix reported in section 7. Each plot point is the 90% quantile (top row) or median (bottom row) A over 2 folds, $L^2 = 81$ matrix elements and $M \in \{5, 7\}$ closed matrices.*

Figure 4 shows the absolute error in Sobol' matrix elements calculated from MQU (i.e. GP) moments. The accuracy is far greater than predictive accuracy: GPs whose prediction accuracy is much worse than 30% generate median Sobol' matrices to an accuracy of 0.05-0.10. Provided $E \leq 50\%$ and $N \geq 100$, one can confidently expect 90% of Sobol' matrices to be accurate within 0.15, and most Sobol' matrices (the median) to be good to within 0.02-0.04. $N = 500$ samples nearly always provide Sobol' matrices to within 0.01 of the true value. In line with GP prediction accuracy, the estimates deteriorate with decreasing N and increasing M, as expected. However, deterioration with increasing E is much less apparent: increasing noise has little effect on GSA via MQU moments. This behaviour was predicted immediately following (6.8), and should apply widely.
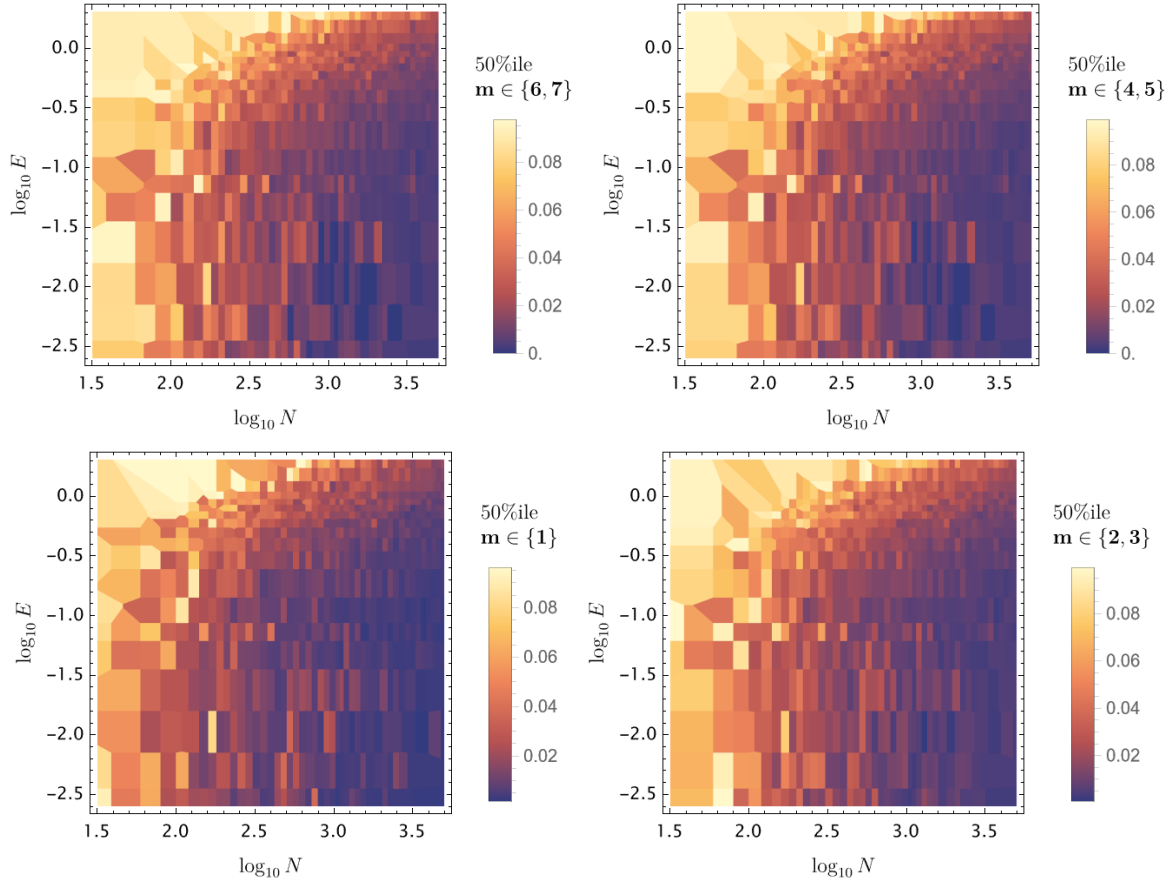

Figure 5. *The absolute error* $[A^T_{\mathbf{M-m}}]_{l \times l'}$ *of the total Sobol' matrix element* $[S^T_{\mathbf{M-m}}]_{l \times l'}$ *calculated from MQU moments. Ground truth is* $S_{\mathbf{M}} - S_{\mathbf{m}}$ *calculated from the MNU closed Sobol' matrix reported in* section 7. *Each plot point is the median* A^T *over 2 folds,* $L^2 = 81$ *matrix elements and one or two total matrices. Only MQUs with* $M = 7$ *have been used.*

One would like to know how the accuracy is affected by which Sobol' matrix is being measured. For the purposes of dimension reduction, inputs axes $\mathbf{m}$ whose complementary total Sobol' matrix $S^T_{\mathbf{M-m}}$ is small are irrelevant, and may be ignored. The test MNU has been arranged such that input relevance mostly decreases as m increases, and must be zero

for $m > 5$. Figure 5 shows the median absolute error in $S^T_{\mathbf{M-m}}$ as input axes are removed one or two at a time. There is remarkable stability and consistency: the accuracy of the total index shows little or no dependence on $\mathbf{m}$, even though its value $S^T_{\mathbf{M-m}}$ actually follows a strong trend.
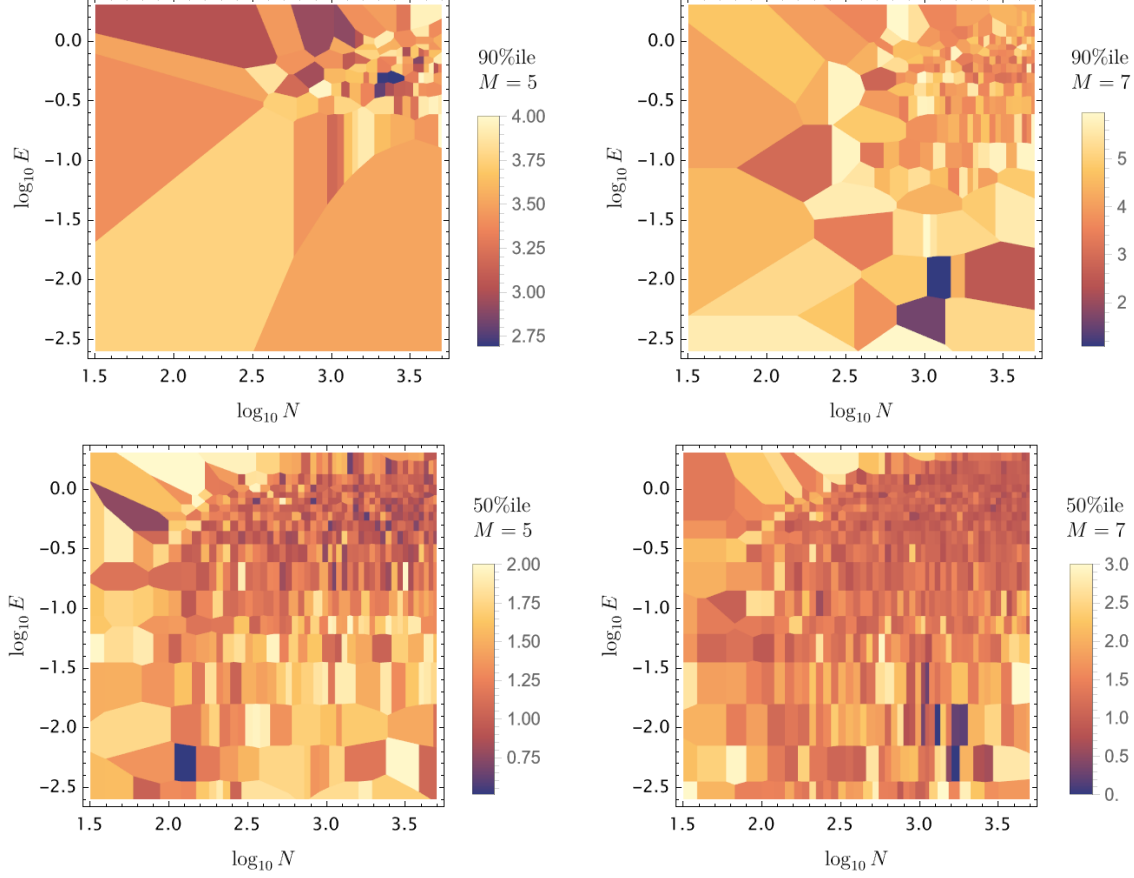

Figure 6. *The standardized score $[A_{\mathbf{m}}]_{l \times l'}/[T_{\mathbf{m}}]_{l \times l'}$ of the closed Sobol' matrix element $[S_{\mathbf{m}}]_{l \times l'}$ with standard error $[T_{\mathbf{m}}]_{l \times l'}$ calculated from MQU moments. Ground truth is the MNU Sobol' matrix reported in section 7. Each plot point is the 90% quantile (top row) or median (bottom row) A/T over 2 folds, $L^2 = 81$ matrix elements and $M \in \{5, 7\}$ closed matrices.*

MQU moments provide standard errors $[T_{\mathbf{m}}]_{l \times l'}$ on Sobol' matrix elements in section 5. Normalizing the results depicted in Figure 4 by these standard errors produces the standardized score for the closed Sobol' matrix element $[S_{\mathbf{m}}]_{l \times l'}$ shown in Figure 6. One does not expect $[S_{\mathbf{m}}]_{l \times l'}$ to be normally distributed, so standardized scores values are not expected to follow rules such as 95% of results score 2 or less. Rather, one is looking for stable and consistent scores over any choice of E, N, M. This means that the standard error $[T_{\mathbf{m}}]_{l \times l'}$ has a meaning which is largely independent of context, and provides a consistent guide to the accuracy of $[S_{\mathbf{m}}]_{l \times l'}$. Looking at Figure 6, one sees a median standardized score consistently less than 2. The 90% quantile shows less consistency as M increases, growing from ≈ 3.5 for $M = 5$ to ≈ 5.0 for $M = 7$. The reliability – but not necessarily the value – of standard errors on Sobol'

matrices computed from GP moments are very susceptible to the curse of dimensionality. We regard them as the natural extension of the Sobol' index definition to multi-output systems.

9. Conclusions. In this paper we have presented the theory and implementation of Sobol' indices extended to multi-outputs in the form of Sobol' matrices. These essentially ascribe the correlation between output components to the influence of various inputs. The diagonal elements of the Sobol' matrix are precisely the Sobol' indices of the output components, and the closed Sobol' matrix $\mathsf{S_M}$ considering all inputs is just the multi-output correlation matrix. This is deliberately intended to provide insights into the influence of inputs on the linkages (correlations) between output components. Every element of a Sobol matrix lies within $[0, 1]$.

The formal development assumes a multi-output model with quantified uncertainty (MQU) which is essentially a stochastic process (SP). The Sobol' matrix and its standard error have been expressed in terms of the first two moments of this SP. When benchmarked using GPs regressed to standard test functions with noise, the calculation is remarkably accurate up to $M = 7$ input dimensions. Sobol' matrices of 0.02 accuracy are usually obtained with just 300 samples, and even 90 samples will usually provide estimates accurate to within 0.08 of the true value. Sobol' matrices and their uncertainties are not directly affected by homoskedastic uncertainty or noise in an MQU. When the noise to signal ratio exceeds 1 accuracy is indirectly impaired by the woeful performance of the MQU as a predictor. The accuracy of total Sobol' matrices also appears hardly affected by the number of relevant inputs or irrelevant inputs included up $M = 7$. The standard error of Sobol' matrices indicate that most Sobol' matrices are accurate to within 2 standard errors. It should be ascertained whether these observations persist with more input dimensions $M > 7$. This would be very useful for reducing high dimensional systems to their relevant inputs.

Clearly the MQU moment method of GSA developed here looks very powerful when input dimensionality is moderate and data is scarce, or noisy, or both. It does not scale well with the number of outputs or samples: if data is abundant, other methods may be preferable. In any case, if one wishes to study the influence of various inputs on the correlations between outputs, Sobol' matrices provide a coherent framework for doing so.

REFERENCES

[1] *NumPy*, 2023-08-19, https://numpy.org.
[2] *NumPy*, 2023-08-19, https://numpy.org.
[3] *PyTorch*, 2023-08-19, https://pytorch.org.
[4] *TensorFlow*, 2023-08-19, https://tensorflow.org.
[5] *SALib*, 2023-09-25, https://salib.readthedocs.io/en/latest/.
[6] N. ALTMAN AND M. KRZYWINSKI, *The curse(s) of dimensionality*, Nature Methods, 15 (2018), pp. 399–400, https://doi.org/10.1038/s41592-018-0019-x.
[7] J. E. ANGUS, *The probability integral transform and related results*, SIAM Review, 36 (1994), pp. 652–654, https://doi.org/10.1137/1036146.
[8] M. BINOIS AND N. WYCOFF, *A survey on high-dimensional gaussian process modeling with application to bayesian optimization*, Nov. 2021, https://arxiv.org/abs/2111.05040.
[9] J. K. BLITZSTEIN AND J. HWANG, *Introduction to Probability, Second Edition*, Taylor & Francis Group, 2019.
[10] K. CAMPBELL, M. D. MCKAY, AND B. J. WILLIAMS, *Sensitivity analysis when model outputs are functions*, Reliability Engineering & System Safety, 91 (2006), pp. 1468–1472, https://doi.org/10.1016/j.

559   ress.2005.11.049.

[11] G. Chastaing, F. Gamboa, and C. Prieur, *Generalized hoeffding-sobol decomposition for dependent variables -application to sensitivity analysis*, (2011), https://doi.org/10.48550/ARXIV.1112.1788, https://arxiv.org/abs/1112.1788.

[12] W. Chen, R. Jin, and A. Sudjianto, *Analytical variance-based global sensitivity analysis in simulation-based design under uncertainty*, Journal of Mechanical Design, 127 (2005), p. 875, https://doi.org/10.1115/1.1904642.

[13] K. Cheng, Z. Lu, and K. Zhang, *Multivariate output global sensitivity analysis using multi-output support vector regression*, Structural and Multidisciplinary Optimization, 59 (2019), pp. 2177–2187, https://doi.org/10.1007/s00158-018-2184-z.

[14] M. Chevreuil, R. Lebrun, A. Nouy, and P. Rai, *A least-squares method for sparse low rank approximation of multivariate functions*, SIAM/ASA Journal on Uncertainty Quantification, 3 (2015), pp. 897–921, https://doi.org/10.1137/13091899X, https://arxiv.org/abs/http://arxiv.org/abs/1305.0030v2.

[15] D. Chicco, M. J. Warrens, and G. Jurman, *The coefficient of determination r-squared is more informative than SMAPE, MAE, MAPE, MSE and RMSE in regression analysis evaluation*, PeerJ Computer Science, 7 (2021-07), p. e623, https://doi.org/10.7717/peerj-cs.623.

[16] C. Cortes and V. Vapnik, *Support-vector networks*, Machine Learning, 20 (1995), pp. 273–297, https://doi.org/10.1007/bf00994018.

[17] F. Gamboa, A. Janon, T. Klein, and A. Lagnoux, *Sensitivity indices for multivariate outputs*, Comptes Rendus Mathematique, 351 (2013), pp. 307–310, https://doi.org/10.1016/j.crma.2013.04.016.

[18] O. Garcia-Cabrejo and A. Valocchi, *Global sensitivity analysis for multivariate output using polynomial chaos expansion*, Reliability Engineering & System Safety, 126 (2014), pp. 25–36, https://doi.org/10.1016/j.ress.2014.01.005.

[19] R. Ghanem, D. Higdon, H. Owhadi, et al., *Handbook of uncertainty quantification*, vol. 6, Springer, 2017.

[20] R. G. Ghanem and P. D. Spanos, *Spectral techniques for stochastic finite elements*, Archives of Computational Methods in Engineering, 4 (1997), pp. 63–100, https://doi.org/10.1007/BF02818931.

[21] T. Homma and A. Saltelli, *Importance measures in global sensitivity analysis of nonlinear models*, Reliability Engineering & System Safety, 52 (1996), pp. 1–17, https://doi.org/10.1016/0951-8320(96)00002-6.

[22] T. Ishigami and T. Homma, *An importance quantification technique in uncertainty analysis for computer models*, in [1990] Proceedings. First International Symposium on Uncertainty Modeling and Analysis, IEEE Comput. Soc. Press, https://doi.org/10.1109/isuma.1990.151285.

[23] M. G. Kendall, *Kendall's advanced theory of statistics*, John Wiley & Sons, 1994.

[24] D. Khoshnevisan, *Multiparameter Processes*, Springer Monographs in Mathematics Ser., Springer New York, New York, NY, 2002. Description based on publisher supplied metadata and other sources.

[25] K. Konakli and B. Sudret, *Global sensitivity analysis using low-rank tensor approximations*, Reliability Engineering & System Safety, 156 (2016), pp. 64–83, https://doi.org/10.1016/j.ress.2016.07.012.

[26] M. Lamboni, H. Monod, and D. Makowski, *Multivariate sensitivity analysis to measure global contribution of input factors in dynamic models*, Reliability Engineering & System Safety, 96 (2011), pp. 450–459, https://doi.org/10.1016/j.ress.2010.12.002.

[27] B. Lamoureux, N. Mechbal, and J. R. Massé, *A combined sensitivity analysis and kriging surrogate modeling for early validation of health indicators*, Reliability Engineering and System Safety, 130 (2014), pp. 12–26, https://doi.org/10.1016/j.ress.2014.03.007.

[28] Q. Liu, N. Tong, and X. Han, *A global sensitivity analysis method for multi-input multi-output system and its application in structural design*, International Journal of Computational Methods, 19 (2021), https://doi.org/10.1142/s021987622141005x.

[29] A. Marrel, B. Iooss, B. Laurent, and O. Roustant, *Calculations of sobol indices for the gaussian process metamodel*, Reliability Engineering & System Safety, 94 (2009), pp. 742–751, https://doi.org/10.1016/j.ress.2008.07.008.

[30] Y. A. S. Milton Robert A., Brown Solomon F., *In preparation*, 2024.

[31] J. E. Oakley and A. O'Hagan, *Probabilistic sensitivity analysis of complex models: a bayesian approach*,

Journal of the Royal Statistical Society: Series B (Statistical Methodology), 66 (2004), pp. 751–769, https://doi.org/10.1111/j.1467-9868.2004.05304.x.

[32] C. E. Rasmussen and C. K. I. Williams, *Gaussian Processes for Machine Learning (Adaptive Computation and Machine Learning series)*, The MIT Press, 2005.

[33] S. Razavi, A. Jakeman, A. Saltelli, C. Prieur, B. Iooss, E. Borgonovo, E. Plischke, S. L. Piano, T. Iwanaga, W. Becker, S. Tarantola, J. H. Guillaume, J. Jakeman, H. Gupta, N. Melillo, G. Rabitti, V. Chabridon, Q. Duan, X. Sun, S. Smith, R. Sheikholeslami, N. Hosseini, M. Asadzadeh, A. Puy, S. Kucherenko, and H. R. Maier, *The future of sensitivity analysis: An essential discipline for systems modeling and policy support*, Environmental Modelling & Software, 137 (2021-03), p. 104954, https://doi.org/10.1016/j.envsoft.2020.104954.

[34] L. C. G. Rogers and D. Williams, *Diffusions, Markov Processes, and Martingales*, Cambridge University Press, 2000.

[35] J. Sacks, W. J. Welch, T. J. Mitchell, and H. P. Wynn, *Design and analysis of computer experiments*, Statistical Science, 4 (1989), pp. 409–423.

[36] A. Saltelli, K. Aleksankina, W. Becker, P. Fennell, F. Ferretti, N. Holst, S. Li, and Q. Wu, *Why so many published sensitivity analyses are false: A systematic review of sensitivity analysis practices*, Environmental Modelling & Software, 114 (2019-04), pp. 29–39, https://doi.org/10.1016/j.envsoft.2019.01.012.

[37] A. Saltelli, P. Annoni, I. Azzini, F. Campolongo, M. Ratto, and S. Tarantola, *Variance based sensitivity analysis of model output. design and estimator for the total sensitivity index*, 181 (2010-02), pp. 259–270, https://doi.org/10.1016/j.cpc.2009.09.018.

[38] E. Schechter, *Handbook of analysis and its foundations*, Academic Press, San Diego, 1997.

[39] V. Skorokhod, *Basic Principles and Applications of Probability Theory*, Springer Berlin Heidelberg, 2005.

[40] I. Sobol, *Sensitivity estimates for nonlinear mathematical models*, Mathematical Modelling and Computational Experiments, 4 (1993), pp. 407–414.

[41] I. M. Sobol, *Global sensitivity indices for nonlinear mathematical models and their monte carlo estimates*, Mathematics and Computers in Simulation, 55 (2001), pp. 271–280.

[42] I. M. Sobol and S. S. Kucherenko, *Global sensitivity indices for nonlinear mathematical models. review*, Wilmott, 2005 (2005), pp. 56–61, https://doi.org/10.1002/wilm.42820050114.

[43] A. Srivastava, A. K. Subramaniyan, and L. Wang, *Analytical global sensitivity analysis with gaussian processes*, Artificial Intelligence for Engineering Design, Analysis and Manufacturing, 31 (2017), pp. 235–250, https://doi.org/10.1017/s0890060417000142.

[44] B. Sudret, *Global sensitivity analysis using polynomial chaos expansions*, Reliability Engineering & System Safety, 93 (2008), pp. 964–979, https://doi.org/10.1016/j.ress.2007.04.002.

[45] A. Villani, *Another note on the inclusion $L_p(\mu) \subset L_q(\mu)$*, The American Mathematical Monthly, 92 (1985), p. 485, https://doi.org/10.2307/2322503.

[46] P. Wiederkehr, *Global sensitivity analysis with dependent inputs*, master's thesis, 2018.

[47] D. Williams, *Probability with Martingales*, Cambridge University Press, 1991.

[48] Z. Wu, D. Wang, P. O. N, F. Hu, and W. Zhang, *Global sensitivity analysis using a gaussian radial basis function metamodel*, Reliability Engineering & System Safety, 154 (2016), pp. 171–179, https://doi.org/10.1016/j.ress.2016.06.006.

[49] S. Xiao, Z. Lu, and F. Qin, *Estimation of the generalized sobol's sensitivity index for multivariate output model using unscented transformation*, Journal of Structural Engineering, 143 (2017), https://doi.org/10.1061/(asce)st.1943-541x.0001721.

[50] D. Xiu, *Numerical Methods for Stochastic Computations: A Spectral Method Approach*, Princeton University Press, 2010.

[51] D. Xiu and G. E. Karniadakis, *The wiener–askey polynomial chaos for stochastic differential equations*, SIAM Journal on Scientific Computing, 24 (2002), pp. 619–644, https://doi.org/10.1137/s1064827501387826.

[52] C. Xu, P. Zhu, Z. Liu, and W. Tao, *Mapping-based hierarchical sensitivity analysis for multilevel systems with multidimensional correlations*, Journal of Mechanical Design, 143 (2020), https://doi.org/10.1115/1.4047689.

[53] K. Zhang, Z. Lu, K. Cheng, L. Wang, and Y. Guo, *Global sensitivity analysis for multivariate*

667   *output model and dynamic models*, Reliability Engineering & System Safety, 204 (2020), p. 107195,
668   https://doi.org/10.1016/j.ress.2020.107195.