Extreme learning machines for variance-based global sensitivity analysis\textsuperscript{*,**}  

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Abstract

Variance-based global sensitivity analysis (GSA) can provide a wealth of information when applied to complex models. A well-known Achilles’ heel of this approach is its computational cost which often renders it unfeasible in practice. An appealing alternative is to analyze instead the sensitivity of a surrogate model with the goal of lowering computational costs while maintaining sufficient accuracy. Should a surrogate be “simple” enough to be amenable to the analytical calculations of its Sobol’ indices, the cost of GSA is essentially reduced to the construction of the surrogate. We propose a new class of sparse weight Extreme Learning Machines (SW-ELMs) which, when considered as surrogates in the context of GSA, admit analytical formulas for their Sobol’ indices and, unlike the standard ELMs, yield accurate approximations of these indices. The effectiveness of this approach is illustrated through both traditional benchmarks in the field and on a chemical reaction network.

Keywords: Global sensitivity analysis, Sobol’ indices, neural networks, extreme learning machines, surrogate models, sparsification

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1. Introduction

A key insight into the behavior of a generic model of the form
\[ y = f(x), \quad x \in \mathbb{R}^d, y \in \mathbb{R}, \]  
(1)
is to understand the impact of the uncertainty in the entries of \( x = (x_1, \ldots, x_d) \) on the uncertainty in the model output \( y \); this can be addressed by performing global sensitivity analysis (GSA)\textsuperscript{[1, 2, 3]}. We focus on variance based GSA\textsuperscript{[4, 5, 6]} whereby one seeks to quantify the relative contributions of the entries of \( x \) to the variance of \( f \). Specifically, we rely on the Sobol’ indices\textsuperscript{[5]} and assume that the entries of \( x \) in (1) can be regarded as independent uniformly distributed random variables—which is common in applications.

Computing Sobol’ indices generally involves a costly sampling procedure and multiple applications of Monte Carlo integration. This is not feasible if the input dimension \( d \) is large, a common situation in engineering applications. Often, an initial parameter screening procedure can be applied to reduce the input dimension, before a more detailed variance-based GSA is conducted; see e.g.,\textsuperscript{[7]}. Also, specific problem structures may enable input dimension reduction in creative ways.

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An interesting example is the work [8], where the authors consider hierarchical models and devise a multi-level method for dimensionality reduction coupled with variable grouping to reduce the number of function evaluations. Nonetheless, when evaluating the model $f$ is prohibitively expensive, Monte Carlo methods for computing Sobol’ indices are not viable. In such cases, a widely used approach is to construct a surrogate model $\hat{f} \approx f$ whose Sobol’ indices can be computed efficiently [9, 10].

A number of surrogate models have been proposed for accelerating variance based GSA. These include polynomial chaos expansions (PCE) [11, 12], multivariate adaptive regression splines (MARS) [13, 14], Gaussian processes [15, 16, 17], Bayesian adaptive regression trees (BART) [18], random forests [19], support vector machines [20], artificial neural networks (ANN) [21], autoregressive models [22], and radial basis functions (RBF) [23]. See [9, 24] for an overview of surrogate-based methods for GSA.

In surrogate-based approaches, the user builds the surrogate model and estimates the surrogate’s Sobol’ indices by Monte Carlo integration. This process introduces two sources of error in the Sobol’ indices. The first one is due to the approximation error of the surrogate and the second one due to the error in estimating the surrogate’s Sobol’ indices. Sampling of the surrogate is often considerably cheaper than sampling the underlying model. However, this sampling can still be costly. In the best case, analytic formulas for the surrogate’s Sobol’ indices are known. Then, the issues caused by Monte Carlo sampling disappear altogether. Certain statistical surrogates such as Gaussian processes [16, 17] and BART [18], offer analytic Sobol’ indices along with accompanying uncertainty bounds. The statistical nature of these surrogates, however, means sampling is needed to compute Sobol’ indices. This could be potentially costly, especially compared to certain numerical surrogate models for which Sobol’ indices can be computed analytically for practically no additional cost [9]. Examples of such approaches include PCEs [11, 12] or RBFs [25, 26].

In the case of PCE surrogates, analytic formulas for Sobol’ indices derived from the PC coefficients with no additional sampling needed [11, 12]. Unsurprisingly, PCE has become a workhorse method for computing Sobol’ indices and uncertainty analysis in general. This has spawned a number of methods for computing and using PCEs for uncertainty analysis. Non-intrusive project-based approaches involve computing the PC coefficients using quadrature. For high-dimensional inputs, this is untenable and motivates regression-based approaches. A major challenge with PCE is that the PC basis can grow to gargantuan sizes as the degree of the expansion is increased. This necessitates sparse regression methods to reduce the size of basis [27]. A survey of these methods can be found in [28]. We also point to [29, 30, 31, 32, 33], for recent developments regarding PCE-based approaches for uncertainty quantification. Overall, PCEs provide an efficient computational tool for fast uncertainty analysis in problems with low to moderate parameter dimensions.

In this article, we present a new approach which uses extreme learning machine (ELM) surrogates—a class of neural networks—for which Sobol’ indices can be computed analytically. Our contribution expands the limited toolbox of fast surrogate models with analytic formulas for Sobol’ indices. Having ready access to such analytic formulas enables the users to compute these indices without any costly Monte Carlo sampling procedures. The existing surrogate modeling approaches that have this feature each have their strengths and weaknesses, making them suitable for specific applications of interest. When studying black box models, it is seldom obvious which surrogate is the best choice. In such applications where one does not know the true values of the sensitivity indices, it is beneficial to have access to different tools to compute the indices. This can be useful for confirming the reliability of one’s results. An example of this is [34], where comparing the Sobol’ indices of PCE and ANN surrogates provides verifiable GSA. Notably, however, the ANN surrogate requires much more time to produce GSA results.

ELMs are a class of single layer neural networks [35, 36, 37] where, unlike traditional neural networks, one draws weights and biases of the hidden layer randomly. Consequently, training an ELM amounts to solving a linear least squares problem to estimate the output layer weights; see Section 2 for more details. Though the idea of randomly sampling weights may appear far-fetched, ELMs are a theoretically sound approach. As a trade-off, ELMs may require more hidden layer neurons than traditional neural networks to achieve the same results. Generally, ELMs have proven
to be a powerful tool in a wide range of applications \[38, 39\].

Our motivation for considering ELMs for GSA is twofold:

- they are simple and inexpensive to train: only a linear least squares problem needs to be solved,
- through a judicious choice of the activation function, analytic formulas for the Sobol’ indices can be derived; see Section 3.

Also, ELMs provide a flexible surrogate modeling framework: they do not make strong demands on the distribution of the inputs or the regularity of the input-output map. Additionally, ELMs are well suited to tackle nonlinear and high-dimensional models. The use of neural networks for surrogate-based uncertainty quantification has been the object of recent research efforts. Among many others, \[40, 41, 42, 43, 44, 45\] have for instance used neural network surrogates for GSA. To our knowledge, however, the present work is the first of its kind to derive analytic formulas for Sobol’ indices of neural network surrogates.

To be used reliably for variance based GSA, the surrogate \( \hat{f} \) must capture some key structural properties of the exact model \( f \). To illustrate this point, consider (1) with \( x \in \mathbb{R}^3 \) and assume \( f \) has mean zero. The ANOVA decomposition of \( f \) is given by

\[
f(x_1, x_2, x_3) = \sum_{i=1}^{3} f_i(x_i) + f_{12}(x_1, x_2) + f_{13}(x_1, x_3) + f_{23}(x_2, x_3) + f_{123}(x_1, x_2, x_3),
\]

where \( f_i = \mathbb{E}(f|x_i) \), \( f_{ij} = \mathbb{E}(f|x_i, x_j) - f_i - f_j \), and \( f_{123} = f - \sum_{i=1}^{3} f_i - \sum_{i<j} f_{ij} \). A key observation is that the variance of \( f \) can be decomposed as the sum of the variances of the individual terms in the ANOVA. This makes it possible to quantify the contributions of the individual inputs (or a group of inputs) to the total variance of \( f \) and leads to definition of Sobol’ indices. To provide accurate estimates of Sobol’ indices, a surrogate \( \hat{f} \) must emulate the main effect terms \( \{ f_i \}_{i=1}^{d} \) as well as the higher order interaction terms in (2). As discussed in Section 4, standard ELMs may fail to correctly capture the impact of variable interactions on output variance, leading to inaccurate Sobol’ indices. We resolve this shortcoming by introducing sparsity to the hidden layer weights. The sparsification technique is most closely related to network pruning, a common method that improves training efficiency for neural networks \[46, 47\]. This unique feature of our method preserves the speed and simplicity of ELM while also allowing the surrogate to better incorporate model behavior. We demonstrate the efficiency of the proposed approach on standard benchmark problems, an application from biochemistry, and a high-dimensional problem; see Section 5.

2. Extreme learning machines

A single layer neural network (SLNN) with \( n \) hidden layer neurons and a scalar output has the form

\[
g(x) = \sum_{j=1}^{n} \beta_j \phi(w_j^\top x + b_j),
\]

where \( w_j \in \mathbb{R}^d \), \( b_j \in \mathbb{R} \), \( j = 1, \ldots, n \), are the weights and biases of the hidden layer, \( \beta_j, j = 1, \ldots, n \), are the weights of the output layer, and \( \phi \) is the hidden layer activation function. For a given number of neurons \( n \) and a given activation function \( \phi \), we set

\[
\mathcal{M}_n(\phi) = \left\{ \sum_{j=1}^{n} \beta_j \phi(w_j^\top x + b_j) : b_j, \beta_j \in \mathbb{R}, w_j \in \mathbb{R}^d \right\}.
\]

It is known that SLNNs are universal approximators since, when using non-polynomial continuous activation functions, they are dense in \( C(\mathbb{R}^d) \) \[18\]; more precisely, if \( \phi \in C(\mathbb{R}) \) is not polynomial and
where \( f \in \mathcal{C}(K) \) and \( K \) is a compact subset of \( \mathbb{R}^d \) then, for any \( \epsilon > 0 \), there exists \( n \) and \( g_n \in M_n(\phi) \) such that
\[
\max_{x \in K} |f(x) - g_n(x)| < \epsilon.
\]
(5)

In addition, SLNNs are universal approximators on \( L^p(\mathbb{R}^d) \), for \( p \in [1, \infty) \), when the activation function is not a polynomial (almost everywhere) \([49, 36]\).

The standard approach to train (3) is to determine all hidden layer weights and biases and output weights by solving a nonlinear least squares problem.

In an extreme learning machine (ELM) \([35]\), the weight vectors \( w_j \) and biases \( b_j \), \( j = 1, \ldots, n \), of the hidden layer are not determined as part of a regression process but rather are chosen randomly. Training an ELM then only involves determining the output layer weights \( \{\beta_j\}_{j=1}^n \) by solving a linear least squares problem. Remarkably, even though it bypasses training the hidden layer weights—and replaces a costly nonlinear least squares problem by a linear one—ELMs are (almost surely) universal approximators on \( L^2(\mathbb{R}^d) \).

2.1. Computing ELM surrogates

Let
\[
W = [w_1, w_2, \ldots, w_n]^T,
\]
\[
b = [b_1, b_2, \ldots, b_n]^T,
\]
\[
\beta = [\beta_1, \beta_2, \ldots, \beta_n]^T;
\]
the ELM (3) takes the form
\[
g(x) = \beta^T \phi(W x + b),
\]
(6)
where \( \phi \) is understood to act componentwise. The entries of the weight matrix \( W \) and bias vector \( b \) are sampled independently from a continuous probability distribution \( D \). It is important to note that this is done before the training, and a fixed realization of \( W \) and \( b \) is used in all subsequent computations.

To construct a surrogate, the model \( f \) is sampled at \( \{x_i\}_{i=1}^m \), yielding \( y_i = f(x_i), i = 1, \ldots, m \). We then find \( \beta \) by solving
\[
\min_{\beta \in \mathbb{R}^n} \|H \beta - y\|_2^2,
\]
(7)
where \( y = [y_1, \ldots, y_m]^T \) and \( H_{ij} = \phi(w_j^T x_i + b_j) \) for \( i, j \in \{1, \ldots, m\} \times \{1, \ldots, n\} \).

In our computations, we implement a regularized least squares problem to control the magnitude of the solution \( \beta \):
\[
\min_{\beta} \frac{1}{2} \|H \beta - y\|_2^2 + \frac{\alpha}{2} \|\beta\|_2^2,
\]
(8)
with \( \alpha > 0 \), the solution of which is
\[
\beta^* = (H^T H + \alpha I)^{-1} H^T y.
\]

The regularization parameter \( \alpha \) can be selected using the L-curve method or generalized cross validation (GCV) \([50]\). We construct the hidden layer weight matrix and bias vector by sampling individual values from the standard normal distribution and use Latin hypercube sampling (LHS) to sample points in the training set \( \{x_i\}_{i=1}^m \).
3. Global sensitivity analysis using ELMs

For each entry $x_k$, $k = 1, \ldots, d$, the first-order Sobol’ index $S_k$ and total Sobol’ index $S_k^{\text{tot}}$ of a surrogate $y = \hat{f}(x)$ are defined as

$$S_k = \frac{\text{var}(\hat{f}_k)}{\text{var}(\hat{f})}, \quad S_k^{\text{tot}} = 1 - \frac{\text{var}(\mathbb{E}(\hat{f}|x_l, l \neq k))}{\text{var}(\hat{f})},$$

where $\hat{f}_k(x_k) = \mathbb{E}(\hat{f}|x_k) - \mathbb{E}(\hat{f})$; see e.g., [6]. Henceforth, we assume that the entries of the input vector $x$ are independent and uniformly distributed on the interval $[0, 1]$ and, therefore, the input domain is $[0, 1]^d$. It is straightforward to extend the proposed approach to the case where entries of $x$ are independent uniformly distributed random variables on arbitrary closed and bounded intervals.

To obtain analytic formulas for the Sobol’ indices while avoiding Monte Carlo approximations, we must be able to easily compute the mean, variance, and partial variances of the surrogate. By carefully choosing the activation function, we can design $\hat{f}$ as an ELM which (i) suits the above requirement and (ii) preserves the universal approximation property. Activation functions traditionally used in machine learning are not suited for our purpose as the corresponding calculations in (9) become impractical or impossible. Instead, we choose an exponential activation function $\phi(t) = e^t$,

which results in

$$\hat{f}(x) = \sum_{j=1}^n \beta_j e^{w_j^T x + b_j} = \sum_{j=1}^n \left( \beta_j e^{b_j} \prod_{l=1}^d e^{w_{j,l} x_l} \right).$$

Since $\phi$ is a continuous non-polynomial function, the results cited in Section 2 apply and ELMs constructed this way still have the universal approximation property.

We now compute the first and second moments of (10).

**Lemma 3.1.** The mean and variance of the ELM (10) are

$$\mathbb{E}(\hat{f}) = \sum_{j=1}^n \left( \beta_j e^{b_j} \prod_{l=1}^d \epsilon(w_{j,l}) \right)$$

and

$$\text{var}(\hat{f}) = \sum_{j=1}^n \beta_j \beta_i e^{b_j + b_i} \left( \prod_{l=1}^d \epsilon(w_{j,l} + w_{i,l}) - \prod_{r=1}^d \epsilon(w_{j,r}) \epsilon(w_{i,r}) \right),$$

where $\epsilon(t) = \begin{cases} \frac{e^t - 1}{t}, & t \neq 0 \\ 1, & t = 0 \end{cases}$

**Proof.** See Appendix A

Using Lemma 3.1 we obtain analytic expressions for the Sobol’ indices of (10).

**Proposition 3.2.** The first-order and total Sobol’ indices of the ELM (10) are given by

$$S_k = \frac{1}{\text{var}(\hat{f})} \sum_{j=1}^n \beta_j \beta_i e^{b_j + b_i} \left( \epsilon(w_{j,k} + w_{i,k}) - \epsilon(w_{j,k}) \epsilon(w_{i,k}) \right) \prod_{l \neq k} \epsilon(w_{j,l}) \epsilon(w_{i,l})$$

and

$$S_k^{\text{tot}} = 1 - \frac{1}{\text{var}(\hat{f})} \sum_{j=1}^n \beta_j \beta_i e^{b_j + b_i} \epsilon(w_{i,k}) \left( \prod_{r \neq k} \epsilon(w_{j,r} + w_{i,r}) - \prod_{l \neq k} \epsilon(w_{j,r}) \epsilon(w_{i,l}) \right),$$

respectively, for $k = 1, \ldots, d$.

**Proof.** See Appendix A
4. Sparse weight ELMs

ELM surrogates are constructed by randomly sampling the hidden layer weight matrix \( W \) and bias vector \( b \) from the standard normal distribution. As pointed out in Section 2, an ELM surrogate \( \hat{f} \) can be found to satisfy

\[
\hat{f} \approx f
\]

as accurately as desired. Our goal is however not so much to construct \( \hat{f} \) satisfying (13) within a given tolerance but rather to construct \( \hat{f} \) such that

\[
S(\hat{f}) \approx S(f),
\]

where \( S \) stands here for any of the Sobol’ indices from Proposition 3.2 and \( S(f) \) can be computed at low cost. To ensure that the Sobol’ indices computed from \( f \) yield a reliable description of the variable interactions, we thus have to construct a surrogate \( \hat{f} \) that not only satisfies (13) but also

\[
\hat{f}_u \approx f_u, \quad \text{for any } u \subset \{1, \ldots, d\},
\]

where \( f_u \) and \( \hat{f}_u \) are the terms corresponding to the subset \( u \) in the ANOVA decomposition of \( f \) and \( \hat{f} \) respectively.

4.1. ELMs and variable interactions

Simple examples show that the amount of variable interactions in \( f \) plays a key role in either achieving or failing to achieve (14). As an illustration, consider the following parametrized function

\[
f_\delta(x) = \sum_{i=1}^{d} x_i + \delta \prod_{j=1}^{d} (1 + x_j), \quad x \in [0,1]^d,
\]

where \( \delta \) controls the amount of variable interactions. When \( \delta = 0 \), \( f_\delta \) is fully additive: there are no variable interactions and thus the first-order and corresponding total Sobol indices are equal. For \( \delta > 0 \), there are interactions between the variables that increase in importance as \( \delta \) increases. By construction, we also observe that the individual entries \( x_i, i = 1, \ldots, d \), all share the same Sobol’ indices; this feature is not present when considering the ELM surrogate \( \hat{f} \) instead of \( f \) because of approximation errors. The first-order and total Sobol’ indices of (16) can be found analytically and are given in Appendix B. Therefore, by varying \( \delta \), we can explore how variable interactions affect accuracy in both (13) and (14).

To approximate the Sobol’ indices of (16) with \( d = 15 \), we construct ELMs of the form (10) as follows:

1: collect \( m = 900 \) training points sampled by LHS
2: construct ELMs with \( n = 300 \) neurons
3: compute the surrogate relative error

\[
E_{\text{surr}} = \frac{1}{\sqrt{\sum_{j=1}^{s} y_j^2}} \sqrt{\sum_{j=1}^{s} (\hat{f}(x_j) - y_j)^2}, \quad y_j = f(x_j) \quad j = 1, \ldots, s,
\]

using \( s = 1000 \) validation points sampled by LHS
4: select a regularization parameter \( \alpha = 10^{-3} \) by the L-curve method
5: compute Sobol’ indices of the ELM surrogate using (11) and (12)
Figure 1: Example with $d = 15$. Top left: Surrogate relative error; bottom left: first-order Sobol’ indices $S_i(f)$ and $S_i(\hat{f})$ of $x_i$, $i = 1, \ldots, 15$ and corresponding mean; bottom right: total Sobol’ indices $S_{i}^{\text{tot}}(f)$ and $S_{i}^{\text{tot}}(\hat{f})$ of $x_i$, $i = 1, \ldots, 15$, and corresponding mean; top right: interaction indices $I_i := S_{i}^{\text{tot}} - S_{i}$, $i = 1, \ldots, 15$, for both $f$ and $\hat{f}$.

Fig. 1 (top left) illustrates that, unsurprisingly, the surrogate relative error—which measures the discrepancy in (13)—increases as the amount of interactions increases with $\delta$. Interestingly, the situation is reversed when looking at the accuracy of the Sobol’ indices through (14). Indeed, Fig. 1 (bottom left) shows that while $S_i(\hat{f})$ is a close approximation of $S_i(f)$, for any $i = 1, \ldots, d$, at the larger values of $\delta$, the relative accuracy of the corresponding approximations decreases for smaller levels of interaction (i.e., smaller values of $\delta$). The variance of the $S_i(f)$’s, which again should ideally all have the value $S_1(f) = \cdots = S_d(f)$, also increases with smaller values of $\delta$. The total Sobol’ indices and their approximations largely behave in similar fashion, see Fig. 1 (bottom right). This example shows that ELM based surrogates have a tendency to overestimate variable interactions, a point made clear in Fig. 1 (top right) where the interaction indices $I_i := S_{i}^{\text{tot}} - S_{i}$, $i = 1, \ldots, d$ are considered.

These results demonstrate that, for variance based GSA, standard ELM may fail to effectively adapt when applied to models featuring different degrees of contribution from interaction terms to the output variance.

4.2. Hidden layer weight sparsification

We propose sparsifying the hidden layer weight matrix $W$ before training the output weights as a means of controlling the influence of variable interactions. Specifically, we replace $W$ by a sparse weight matrix $\bar{W}$ defined as

$$\bar{W} = B \circ W,$$

(18)
where $B$ is a $n \times d$-matrix with independent Bernoulli entries, i.e.,

$$B_{ij} = \begin{cases} 0 & \text{with probability } p, \\ 1 & \text{with probability } 1 - p \end{cases},$$

and where $\circ$ stands for elementwise matrix multiplication. The sparsification parameter $p \in [0, 1)$ determines how sparse the hidden layer weight matrix is. If $p = 0$, then $\tilde{W} = W$ and the method reverts to standard ELM; when $p$ is selected to be near 1, the weight matrix $\tilde{W}$ is sparse. This technique strays from the ELM theory which assumes sampling weights from a continuous probability distribution to guarantee universal approximation.

We implement the sparse weight ELM (SW-ELM) approach, i.e., ELM with $\tilde{W}$ instead of $W$ as a hidden layer weight matrix, on example (16). Figure 2 illustrates the results for a range of values of the sparsification parameter $p$ and for three values of $\delta$ corresponding to low variable interactions ($\delta = 10^{-8}$), limited variable interactions ($\delta = 10^{-3}$), and strong variable interactions ($\delta = 10^{8}$). In the case of low variable interactions ($\delta = 10^{-8}$), Figure 2 shows that using a sparse weight matrix can dramatically increase the accuracy of both the ELM surrogate and of the Sobol’ indices computed using that surrogate. Sparsifying the weight matrix may thus lead to significant improvements in GSA results when dealing with models with few interaction terms. On the other hand, in cases where interaction terms are prominent in the model, sparsifying the hidden layer weight matrix may offer no improvement or may even result in loss of accuracy.

### 4.3. Selection of sparsification parameter

Figure 2 suggests a framework for how to implement SW-ELM for a given model; indeed, for fixed values of $\delta$ and varying values of $p$, we observe similar trends in the surrogate error and in the total Sobol’ index approximation error. This indicates that we may use the surrogate error as a guideline when searching for the best sparsification parameter.

We propose creating a validation set alongside the training set when using SW-ELM surrogates for GSA. Subsequently, we select $r$ values of the sparsification parameter $p$ and construct corresponding sparse weight matrices. Then, ELMs are trained using each weight matrix and the validation set is used to compute the surrogate error for each ELM. This serves as a diagnostic tool to aid in deciding whether sparsification may improve Sobol’ index approximation. If sparsification yields an improved surrogate error, then we use the SW-ELM with the lowest surrogate error to approximate...
Sobol’ indices. If, on the other hand, sparsification does not yield a notable improvement then we may default to using standard ELM. We summarize the method in Algorithm 1.

**Algorithm 1** GSA with sparse weight ELM

**Input:** (i) Model $f$; (ii) training set $\{x_i, y_i\}_{i=1}^m$; (iii) validation set $\{x'_j, y'_j\}_{j=1}^s$; (iv) number of neurons $n$; (v) candidate sparsification values $\{p_l\}_{l=1}^r$ (with $p_1 = 0$)

**Output:** (i) First order Sobol’ indices $\{S_k\}_{k=1}^n$ and (ii) total Sobol’ indices $\{S^\text{tot}_k\}_{k=1}^n$

1. Generate weight matrix $W_0$ and bias vector $b$ using a standard normal distribution
2. for $l = 1, \ldots, r$ do
   3. Construct $W_l = B \circ W_0$ with $B$ from (19) with $p = p_l$
   4. Determine regularization parameter $\alpha_l$ by the L-curve method
   5. Find output weights $\beta_l$ by training ELM using $W_l, b, \alpha_l$ (see (8))
   6. Compute relative surrogate error $E_l = E_\text{surr}$ (see (17))
3. end for
4. Select hidden layer weight matrix $W$ and output weights $\beta$ corresponding to sparsification parameter that gives smallest relative surrogate error
5. With $W, \beta$, and $b$, compute first order Sobol’ indices $\{S_k\}_{k=1}^n$ and total Sobol’ indices $\{S^\text{tot}_k\}_{k=1}^n$ using (11) and (12), respectively

We illustrate the power of this method by repeating the experiment in Fig. 1 for (16) using SW-ELM instead of ELM. Fig. 3 displays the total Sobol’ indices for both surrogates as well as the exact indices. SW-ELM displays increased accuracy and reduced variance across all tested ranges of interaction strength.

In the context of GSA, SW-ELM displays better accuracy and flexibility than standard ELM. The proposed implementation is only marginally more costly than standard ELM as there is no need to re-sample training or validation points for each ELM.

![Figure 3: Example (16) true analytic total Sobol’ indices compared to those approximated by standard ELM and sparse weight ELM (SW-ELM). All approximated indices are plotted along with means for each $\delta$.](image-url)
5. Computational results

5.1. Analytic example: Sobol’ g-function

The Sobol’ g-function \[ \text{[4]} \]

\[
 f(x) = \prod_{i=1}^{d} g_i(x_i) \quad x \in [0,1]^d, \quad g_i(x_i) = \frac{|4x_i - 2| + a_i}{1 + a_i}, \quad i = 1, \ldots, d, \tag{20}
\]

is commonly used as a benchmark to test new methods; its nonlinearity and lack of smoothness make approximating its Sobol’ indices a significant challenge. Moreover, we can compare to the true Sobol’ indices. Formulas for these can be found in the appendix to [51]. The constants \( a_i \), chosen from the interval \((-1, \infty)\), can be tuned to determine which input variables are important. The closer \( a_i \) is to \(-1\), the more “important” \( x_i \) becomes. On the other hand, the relative importance of \( x_i \) diminishes with larger values of \( a_i \). For our test, we take the input dimension \( d = 8 \) and let \( a = [1, 2, 5, 10, 20, 50, 100, 500] \) as in [11].

We train our SW-ELM surrogates with 160 hidden layer neurons using 400 training points and 100 validation points, all sampled by Latin hypercube sampling (LHS). The regularization parameter \( \alpha = 10^{-3} \) is selected by the L-curve method. The sparsification parameter \( p \) is determined through Algorithm 1. While Fig. 4 does not show drastic improvements in error, we nevertheless conclude from this test that sparsifying may improve our approximations when performing GSA; we select the sparsification parameter \( p = 0.85 \). Sobol’ indices estimated by SW-ELM are compared to their true analytic values.

![Figure 4: Sparsification test for 8-dimensional g-function (20) with \( a = [1, 2, 5, 10, 20, 50, 100, 500] \). Relative surrogate error is estimated using validation set with 100 points.](image)

As can seen from Fig. 5, SW-ELM correctly ranks the Sobol’ indices and successfully identifies the most influential input variables. For important input variables, each approximated first-order Sobol’ index is within 5% relative error of the respective true first-order Sobol’ index while each approximated total Sobol’ index is within 7% relative error of the respective true total Sobol’ index.

We use this benchmark example to study how numerical accuracy of SW-ELM affects the accuracy of GSA. In the experiment, we train SW-ELMs to a certain accuracy level by adding neurons and training points until the surrogate reaches the accuracy level. Each surrogate uses two training points for every neuron. We decrease the surrogate relative error from 15% to 5% and record the relative error of the first-order and total Sobol’ index estimates for the inputs \( x_1, x_2, x_3 \). The relations between numerical error and GSA error are shown in Fig. 6. The experiment shows that SW-ELM can provide accurate GSA estimates, especially for the more influential inputs, despite 11% numerical error. Still, reducing the numerical error has a demonstrative effect on GSA. As we decrease the error to 5%, the Sobol’ indices become much more accurate.
Figure 5: 8-dimensional g-function (20) with \(a = [1, 2, 5, 10, 20, 50, 100, 500]\). First-order (left) and total (right) Sobol’ indices approximated via SW-ELM and computed analytically.

Figure 6: 8-dimensional g-function (20) with \(a = [1, 2, 5, 10, 20, 50, 100, 500]\). Effect of reducing numerical error on the relative error of first-order (left) and total (right) Sobol’ indices estimated by SW-ELM.

5.2. Genetic oscillator

We examine the performance of the proposed approach on a challenging application problem from biochemistry, specifically, the genetic oscillator system which describes the time evolution of molecular species involved in the regulation of circadian rhythm [52]. The reaction network consists of sixteen reactions and involves nine species. The reactions, the corresponding propensity functions, and the nominal values of the rate parameters are given in Section 5.2. We consider the reaction rate equations (RREs), described by a nonlinear system of ordinary differential equations (ODEs), for this reaction network; see e.g., [52], [53], or [54], which we follow in the specific problem formulation used in the present study. We focus on the uncertainty in the reaction rate parameters. A uniform distribution is attached to each rate parameter on an interval given by a ±5% perturbation from the corresponding nominal value. We use a random vector \(x \in \mathbb{R}^{16}\), whose entries are uniformly distributed on \([0, 1]\), to parameterize the uncertainty in the reaction rates. The vector of reaction rates is obtained by applying a linear transformation to \(x\) that maps the entries of \(x\) to the respective physical ranges. In the present study, we consider the quantity of interest (QoI) given by

\[
 f(x) = \frac{1}{T} \int_0^T R(t; x) \, dt, \tag{21}
\]

where \(R(t; x)\) is the concentration of the species \(R\) present in the system at time \(t\), and \(T\) is the final simulation time. Notice that computing \(R(t; x)\), for \(t \in [0, T]\), requires solving the system of RREs with the reaction rates set according to \(x\). This system, for the present application, is given by a stiff system of nonlinear ODEs. Thus, evaluations of the QoI in (21) are computationally expensive.
| Reaction                              | Propensity Function | Parameter | Value |
|--------------------------------------|--------------------|-----------|-------|
| $P_a \rightarrow P_a + mRNA_a$      | $\alpha_A P_a$     | $\alpha_A$ | 50.0  |
| $P_r \rightarrow P_r + mRNA_r$      | $\alpha_R P_r$     | $\alpha_R$ | 0.01  |
| $mRNA_a \rightarrow mRNA_a + A$     | $\beta_A mRNA_a$   | $\beta_A$ | 50.0  |
| $mRNA_r \rightarrow mRNA_r + R$     | $\beta_R mRNA_r$   | $\beta_R$ | 5.0   |
| $A + R \rightarrow C$               | $\gamma_C AR$      | $\gamma_C$ | 20.0  |
| $P_a + A \rightarrow P_a - A$       | $\gamma_A P_a A$   | $\gamma_A$ | 1.0   |
| $P_a - A \rightarrow P_a + A$       | $\theta_A P_a - A$ | $\theta_A$ | 50.0  |
| $P_r + A \rightarrow P_r - A$       | $\gamma_R P_r A$   | $\gamma_R$ | 1.0   |
| $P_r - A \rightarrow P_r + A$       | $\theta_R P_r - A$ | $\theta_R$ | 1.0   |
| $A \rightarrow \emptyset$           | $\delta_A A$       | $\delta_A$ | 1.0   |
| $R \rightarrow \emptyset$           | $\delta_R R$       | $\delta_R$ | 0.2   |
| $mRNA_a \rightarrow \emptyset$      | $\delta_M mRNA_a$  | $\delta_M A$ | 10.0  |
| $mRNA_r \rightarrow \emptyset$      | $\delta_M mRNA_r$  | $\delta_M R$ | 0.5   |
| $C \rightarrow R$                   | $\delta_C C$       | $\delta_C$ | 1.0   |
| $P_a - A \rightarrow P_a - A + mRNA_a$ | $\alpha_a \alpha_A P_a - A$ | $\alpha_a$ | 10.0  |
| $P_r - A \rightarrow P_r - A + mRNA_r$ | $\alpha_r \alpha_R P_r - A$ | $\alpha_r$ | 5000  |

Table 1: Genetic oscillator reactions, propensity functions, parameters and nominal values of the parameters [53, 54].

Fig. 7 (top row) presents approximations for first-order and total Sobol’ indices when using standard ELM. The experiment uses 3000 training points and 1000 neurons. The regularization parameter $\alpha = 10^{-4}$ is selected by the L-curve method. We observe that approximation using standard ELM leads to overestimates, particularly for unimportant input variables, of the total Sobol’ indices and underestimates of the first-order Sobol’ indices; this is a clear case of standard ELM overestimating contributions to the output variance by higher order interactions.

Let us instead tackle this problem using SW-ELM; we train our surrogates with again 3000 training points, using 1000 hidden layer neurons, and 100 validation points, all sampled by LHS. Regarding sparsification, we follow Algorithm 1. The results of these tests are displayed in Fig. 8 (left), and show that as the hidden layer weight matrix become more sparse, the error in the surrogate improves dramatically; we select the sparsification parameter $p = 0.8$. Fig. 7 (middle row), displays the resulting approximated Sobol’ indices and compares with the Sobol’ indices approximated by Monte Carlo methods with $10^6$ sample points. Given that the Sobol’ indices computed via Monte Carlo methods are a close representation of the true Sobol’ indices, SW-ELM provides an accurate approximation of the indices.

We can further challenge the performance of SW-ELM. We train surrogates with with only 150 training points, using 50 hidden layer neurons, and 100 validation points. The results of sparsification tests are displayed in Fig. 8 (right). We select the sparsification parameter $p = 0.9$. Fig. 7 (bottom row) displays the resulting approximated Sobol’ indices. SW-ELM with 150 training points or 3000 training points gives very similar results. This indicates that SW-ELM is extremely efficient for this problem—a modest number of training samples are sufficient for obtaining accurate sensitivity analysis results.

As shown in Fig. 7, the first-order Sobol’ indices and the total Sobol’ indices are very close to each other for this application. This suggests that there are few, if any, higher order variable interactions present in the QoI function (21). The fact that the sparsity of the weight matrix had a significant influence over the quality of the ELM surrogate, as seen in Fig. 8, further supports
5.3. High-dimensional example

In this section, we use our proposed approach to perform GSA in a model governed by a system of ordinary differential equations (ODEs) with 50 uncertain inputs. Specifically, we consider a linear homogeneous ODE system,

\[ \dot{x} = -Ax, \quad x(0) = x_0, \]

where \( x(t) = [x_1(t), \ldots, x_{50}(t)]^\top \) and \( A \in \mathbb{R}^{50 \times 50} \). Note that the solution of this system is given by \( x(t) = e^{-tA}x_0 \).
In the present example, we assume $A$ is symmetric. Thus, $A$ has spectral decomposition $A = Q\Lambda Q^\top$, where $Q$ is orthogonal and $\Lambda$ is diagonal with the eigenvalues $\lambda_1, \ldots, \lambda_{50}$ of $A$ as its diagonal entries. This allows us to express the solution as

$$x(t) = Qe^{-t\Lambda}Q^\top x_0,$$

where $e^{-t\Lambda}$ is the diagonal matrix taking $e^{-t\lambda_1}, \ldots, e^{-t\lambda_{50}}$ as its diagonal entries. In this example, we consider a symmetric matrix $A$ with a known orthogonal matrix $Q$ of eigenvectors and uncertain eigenvalues. That is, the diagonal entries of $\Lambda$ in Equation (23) are uncertain. We assume these eigenvalues take nominal values $\lambda_k = \frac{1}{k}$, $k = 1, \ldots, 50$. Each eigenvalue is assumed to follow a uniform distribution on an interval given by a $\pm 5\%$ perturbation from the respective nominal value. We consider the quantity of interest, $f(\theta) = x_{50}(10)$, which is the last entry in the solution vector $x(t) = Qe^{-t\Lambda}Q^\top x_0$ at time $t = 10$. For further details on the setup of the problem, see Appendix C.

In Fig. 10, we see the results of the sparsification test. The experiment uses 700 training points, 350 neurons, and 100 validation points to compute surrogate error. As shown in Fig. 9, the surrogate error reaches a minimum when $p = 0.95$, indicating that a very sparse weight matrix should be used. Fig. 10 demonstrates the accuracy of the total Sobol’ indices estimated using SW-ELM. These are compared to total Sobol’ indices estimated using Monte Carlo integration which we treat as the ground truth. The Sobol’ indices reveal the absence of variable interactions, justifying the use of a very sparse weight matrix.

6. Conclusion

The use of SW-ELM as a surrogate in the context of variance based GSA allows the user to completely eschew Monte Carlo integration which is a perennial bottleneck in this field. The numerical results we present above make a strong case for further study of the approach. In particular, there is in general very little known theoretically regarding the link from (13) (accurate surrogate) to (14) (accurate GSA). In our particular case, we note further that SW-ELM is not strictly covered by the existing theory [35] as the distribution we use for $W$ is not continuous.

A key point in our approach is the ability to analytically compute the Sobol’ indices of $\hat{f}$. This is where the assumption of independent uniformly distributed parameters is crucial. Further work will
Figure 9: Sparsification test for (24) on a 100 point validation set. ELMs trained with 700 training points and 350 neurons. Surrogate relative error reaches a minimum of $2.73 \times 10^{-4}$ on the validation set at $p = 0.95$.

reveal to what extent this assumption might be weakened. A deeper understanding of the proposed sparsification process might also result in further improvement of the proposed approach.

References

[1] A. Saltelli, M. Ratto, T. Andres, F. Campolongo, J. Cariboni, D. Gatelli, M. Saisana, S. Tarantola, Global sensitivity analysis: the primer, John Wiley & Sons, 2008.

[2] B. Iooss, P. Le Maître, A Review on Global Sensitivity Analysis Methods, Springer US, Boston, MA, 2015, pp. 101–122.
B. Iooss, A. Saltelli, Introduction to sensitivity analysis, in: R. Ghanem, D. Higdon, H. Owhadi (Eds.), Handbook of uncertainty quantification, Springer, 2017, pp. 1103–1122.

A. Saltelli, I. Sobol’, Sensitivity analysis for nonlinear mathematical models: numerical experience, Matematicheskoe Modelirovanie 7 (11) (1995) 16–28.

I. Sobol’, Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates, Mathematics and Computers in Simulation 55 (1–3) (2001) 271–280, the Second IMACS Seminar on Monte Carlo Methods.

C. Prieur, S. Tarantola, Variance-based sensitivity analysis: Theory and estimation algorithms, in: R. Ghanem, D. Higdon, H. Owhadi (Eds.), Handbook of Uncertainty Quantification, Springer, 2017, pp. 1217–1239.

J. Hart, P. Gremaud, T. David, Global sensitivity analysis of high-dimensional neuroscience models: An example of neurovascular coupling, Bulletin of mathematical biology 81 (6) (2019) 1805–1828.

A. Tabandeh, N. Sharma, P. Gardoni, Uncertainty propagation in risk and resilience analysis of hierarchical systems, Reliability Engineering & System Safety 219 (2022) 108208.

L. Le Gratiet, S. Marelli, B. Sudret, Metamodel-based sensitivity analysis: polynomial chaos expansions and Gaussian processes, in: R. Ghanem, D. Higdon, H. Owhadi (Eds.), Handbook of Uncertainty Quantification, Springer, 2017.

K. Sargsyan, Surrogate models for uncertainty propagation and sensitivity analysis, in: R. Ghanem, D. Higdon, H. Owhadi (Eds.), Handbook of uncertainty quantification, Springer, 2017.

B. Sudret, Global sensitivity analysis using polynomial chaos expansions, Journal = Reliability Engineering & System Safety 93 (7) (2008) 964–979, bayesian Networks in Dependability.

T. Crestaux, O. Le Maître, J.-M. Martinez, Polynomial chaos expansion for sensitivity analysis, Reliability Engineering & System Safety 94 (7) (2009) 1161–1172, special Issue on Sensitivity Analysis.

J. H. Friedman, Multivariate adaptive regression splines, The Annals of Statistics 19 (1) (1991) 1–141, with discussion and a rejoinder by the author.

J. Hart, A. Alexanderian, P. Gremaud, Efficient computation of Sobol’ indices for stochastic models, SIAM Journal on Scientific Computing. 39 (4) (2017) A1514–A1530.

A. Marrel, B. Iooss, B. Laurent, O. Roustant, Calculations of Sobol’ indices for the Gaussian process metamodel, Reliability Engineering & System Safety 94 (3) (2009) 742–751.

J. E. Oakley, A. O’Hagan, Probabilistic sensitivity analysis of complex models: a Bayesian approach, Journal of the Royal Statistical Society: Series B (Statistical Methodology) 66 (3) (2004) 751–769.

R. Jin, W. Chen, A. Sudjianto, Analytical metamodel-based global sensitivity analysis and uncertainty propagation for robust design, SAE transactions (2004) 121–128.

A. Horiguchi, M. T. Pratola, T. J. Santner, Assessing variable activity for Bayesian regression trees, Reliability Engineering & System Safety 207 (2021) 107391.

A. Antoniadis, S. Lambert-Lacroix, J.-M. Poggi, Random forests for global sensitivity analysis: A selective review, Reliability Engineering & System Safety 206 (2021) 107312.
[20] M. Steiner, J.-M. Bourinet, T. Lahmer, An adaptive sampling method for global sensitivity analysis based on least-squares support vector regression, Reliability Engineering & System Safety 183 (2019) 323–340.

[21] E. Fock, Global Sensitivity Analysis Approach for Input Selection and System Identification Purposes—A New Framework for Feedforward Neural Networks, IEEE Transactions on Neural Networks and Learning Systems 25 (8) (2014) 1484–1495.

[22] A. Datteo, G. Busca, G. Quattromani, A. Cigada, On the use of AR models for SHM: A global sensitivity and uncertainty analysis framework, Reliability Engineering & System Safety 170 (2018) 99–115.

[23] E. Todri, A. Amenaghawon, I. Del Val, D. Leak, C. Kontoravdi, S. Kucherenko, N. Shah, Global sensitivity analysis and meta-modeling of an ethanol production process, Chemical Engineering Science 114 (2014) 114–127.

[24] K. Cheng, L. Zhenzhou, C. Ling, S. Zhou, Surrogate-assisted global sensitivity analysis: an overview, Structural and Multidisciplinary Optimization 61 (2020).

[25] Z. Wu, D. Wang, P. N. Okolo, F. Hu, W. Zhang, Global sensitivity analysis using a Gaussian Radial Basis Function metamodel, Reliability Engineering & System Safety 154 (2016) 171–179.

[26] Z. Wu, W. Wang, D. Wang, K. Zhao, W. Zhang, Global sensitivity analysis using orthogonal augmented radial basis function, Reliability Engineering & System Safety 185 (2019) 291–302.

[27] G. Blatman, B. Sudret, Efficient computation of global sensitivity indices using sparse polynomial chaos expansions, Reliability Engineering & System Safety 95 (11) (2010) 1216–1229.

[28] N. Lüthen, S. Marelli, B. Sudret, Sparse Polynomial Chaos Expansions: Literature Survey and Benchmark, SIAM/ASA Journal on Uncertainty Quantification 9 (2) (2021) 593–649.

[29] A. Alexanderian, P. A. Gremaud, R. C. Smith, Variance-based sensitivity analysis for time-dependent processes, Reliability Engineering & System Safety 196 (2020) 106722.

[30] M. Ehre, I. Papaioannou, D. Straub, Global sensitivity analysis in high dimensions with PLS-PCE, Reliability Engineering & System Safety 198 (2020) 106861.

[31] Y. Zhou, Z. Lu, J. Hu, Y. Hu, Surrogate modeling of high-dimensional problems via data-driven polynomial chaos expansions and sparse partial least square, Computer Methods in Applied Mechanics and Engineering 364 (2020) 112906.

[32] N. Lüthen, S. Marelli, B. Sudret, Automatic selection of basis-adaptive sparse polynomial chaos expansions for engineering applications, International Journal for Uncertainty Quantification 12 (3) (2022) 49–74.

[33] S. M. Almohammadi, O. P. L. Maître, O. M. Knio, Computational Challenges in Sampling and Representation of Uncertain Reaction Kinetics in Large Dimensions, International Journal for Uncertainty Quantification 12 (1) (2022) 1–24.

[34] Q. Zhang, Y.-G. Zhao, K. Kolozvari, L. Xu, Reliability analysis of reinforced concrete structure against progressive collapse, Reliability Engineering & System Safety 228 (2022) 108831.

[35] G.-B. Huang, Q.-Y. Zhu, C.-K. Siew, Extreme learning machine: Theory and applications, Neurocomputing 70 (1) (2006) 489–501, neural Networks.

[36] G.-B. Huang, D. Wang, Y. Lan, Extreme learning machines: a survey, International Journal of Machine Learning and Cybernetics 2 (2) (2011) 107–122.
[37] P. Jorgensen, D. E. Stewart, Approximation Properties of Ridge Functions and Extreme Learning Machines, SIAM Journal on Mathematics of Data Science 3 (3) (2021) 815–832.

[38] G. Huang, G.-B. Huang, S. Song, K. You, Trends in extreme learning machines: A review, Neural Networks 61 (2015) 32–48.

[39] J. Wang, S. Lu, S.-H. Wang, Y.-D. Zhang, A review on extreme learning machine, Multimedia Tools and Applications 81 (29) (2022) 41611–41660.

[40] J. Nagawkar, L. Leifsson, Efficient Global Sensitivity Analysis of Model-Based Ultrasonic Non-destructive Testing Systems Using Machine Learning and Sobol’ Indices, Journal of Nondestructive Evaluation, Diagnostics and Prognostics of Engineering Systems 4 (4) (2021).

[41] J. Walzberg, A. Carpenter, G. A. Heath, Role of the social factors in success of solar photovoltaic reuse and recycle programmes, Nature Energy 6 (9) (2021) 913–924.

[42] S. Li, B. Yang, F. Qi, Accelerate global sensitivity analysis using artificial neural network algorithm: Case studies for combustion kinetic model, Combustion and Flame 168 (2016) 53–64.

[43] B. Kapusuzoglu, S. Mahadevan, Information fusion and machine learning for sensitivity analysis using physics knowledge and experimental data, Reliability Engineering & System Safety 214 (2021) 107734.

[44] D. Ye, A. Nikishova, L. Veen, P. Zun, A. G. Hoekstra, Non-intrusive and semi-intrusive uncertainty quantification of a multiscale in-stent restenosis model, Reliability Engineering & System Safety 214 (2021) 107734.

[45] Y. Zhao, X. Cheng, T. Zhang, L. Wang, W. Shao, J. Wiart, A global–local attention network for uncertainty analysis of ground penetrating radar modeling, Reliability Engineering & System Safety 234 (2023) 109176.

[46] A. Engelbrecht, A new pruning heuristic based on variance analysis of sensitivity information, Neural Networks, IEEE Transactions on 12 (2001) 1386 – 1399.

[47] D. Blalock, J. J. Gonzalez Ortiz, J. Frankle, J. Guttag, What is the state of neural network pruning?, Proceedings of machine learning and systems 2 (2020) 129–146.

[48] A. Pinkus, Approximation theory of the MLP model in neural networks, Acta Numerica 8 (1999) 143–195.

[49] M. Leskno, V. Y. Lin, A. Pinkus, S. Schocken, Multilayer feedforward networks with a non-polynomial activation function can approximate any function, Neural Networks 6 (6) (1993) 861–867.

[50] P. C. Hansen, Getting Serious: Choosing the Regularization Parameter, Society for Industrial and Applied Mathematics, 2010, Ch. 5, pp. 85–107.

[51] A. Saltelli, P. Annoni, I. Azzini, F. Campolongo, M. Ratto, S. Tarantola, Variance based sensitivity analysis of model output. Design and estimator for the total sensitivity index, Computer Physics Communications 181 (2) (2010) 259–270.

[52] J. M. Vilar, H. Y. Kueh, N. Barkai, S. Leibler, Mechanisms of noise-resistance in genetic oscillators, Proceedings of the National Academy of Sciences 99 (9) (2002) 5988–5992.
Appendix A. Derivation of analytic formulas for ELM surrogate

Appendix A.1. Proof of Lemma 3.1
Proof. For the surrogate presented in this paper, we will derive expressions for the mean and variance. Recall the expression for the ELM (10) and the definition of the function \( \epsilon(t) \), given in the statement of the lemma,

\[
\epsilon(t) := \int_0^1 e^{tx} \, dx = \begin{cases} 
\frac{e^t - 1}{t}, & t \neq 0, \\
1, & t = 0.
\end{cases}
\]

We first find the expression for the mean:

\[
\mathbb{E}(\hat{f}) = \int_{[0,1]^d} \left( \sum_{j=1}^n \beta_j e^{b_j} \prod_{l=1}^d e^{w_{j,l} x_l} \right) dx = \sum_{j=1}^n \left( \beta_j e^{b_j} \prod_{l=1}^d \int_0^1 e^{w_{j,l} x_l} \, dx_l \right).
\]

Therefore, the mean can be expressed as

\[
\mathbb{E}(\hat{f}) = \sum_{j=1}^n \left( \beta_j e^{b_j} \prod_{l=1}^d \epsilon(w_{j,l}) \right).
\]

Next, we find the expression for the variance:

\[
\text{var}(\hat{f}) = \mathbb{E}(\hat{f}^2) - \mathbb{E}(\hat{f})^2 = \int_{[0,1]^d} \left( \sum_{j=1}^n \beta_j e^{b_j} \prod_{l=1}^d e^{w_{j,l} x_l} \right)^2 dx - \mathbb{E}(\hat{f})^2
\]
\[
= \sum_{j,i=1}^n \left( \beta_j \beta_i e^{b_j+b_i} \prod_{l=1}^d \epsilon(w_{j,l}+w_{i,l}) \right) - \mathbb{E}(\hat{f})^2
\]
\[
= \sum_{j,i=1}^n \beta_j \beta_i e^{b_j+b_i} \prod_{l=1}^d \left( \epsilon(w_{j,l}+w_{i,l}) - \prod_{r=1}^d \epsilon(w_{j,r}) \epsilon(w_{i,r}) \right).
\]

\[\square\]

Appendix A.2. Proof of Proposition 3.2
Proof. For the surrogate presented in this paper, we will derive expressions for the general formulas for regular and total Sobol’ indices and offer simplified expressions for indices corresponding to single variables. Recall the expression for the ELM (10) and the function \( \epsilon(t) \), and let \( \mathbb{E}(\hat{f}) \) and \( \text{var}(\hat{f}) \) be as presented in Lemma 3.1.

Given subset of variables of \( \{x_1, \ldots, x_d\} \), we first derive the expressions for Sobol’ indices,

\[
S_u = \frac{\text{var}(\hat{f}_u)}{\text{var}(\hat{f})}, \quad \hat{f}_u := \sum_{v \subseteq u} (-1)^{|v|-|u|} \mathbb{E}(\hat{f}|x_l, \ l \in v),
\]

where \( \hat{f}_u \) is the surrogate built from the variables \( u \) , and \( S_u \) is the \( u \)-th Sobol’ index.
where \( u \subseteq \{1, \ldots, d\} \). Since terms in the ANOVA decomposition have the property that \( \text{var}(\hat{f}_u) = \mathbb{E}(\hat{f}_u^2) - \mathbb{E}^2(\hat{f}_u) \) we can we can express the Sobol’ index \( S_u \) for (10) as

\[
S_u = \frac{\text{var}(\hat{f}_u)}{\text{var}(f)} = \mathbb{E}(\hat{f}_u^2) - \mathbb{E}^2(\hat{f}_u)
\]

\[
= \frac{1}{\text{var}(f)} \int_{[0,1]^d} \left( \sum_{u \subseteq v} \sum_{j=1}^n (-1)^{|u|-|v|} \beta_j e^{b_j} \left( \prod_{l \in v} e^{w_{j,l}} \right) \left( \prod_{r \not\in v} e^{(w_{j,r} - \beta_l |v|)} \right) \right)^2 \text{d}x
\]

\[
= \frac{1}{\text{var}(f)} \sum_{u \subseteq v} \sum_{j=1}^n (-1)^{|u|-|v|} \int_{[0,1]^d} \left( \beta_j e^{b_j} \left( \prod_{l \in v} e^{w_{j,l}} \right) \left( \prod_{r \not\in v} e^{(w_{j,r})} \right) \right)^2 \text{d}x
\]

When we only consider the single variable case or, in other words, when \( u = \{k\} \), then we arrive at equation (11) for the first-order Sobol’ indices:

\[
S_k = \frac{1}{\text{var}(f)} \sum_{j=1}^n \left( \beta_j e^{b_j} \cdot \left( \prod_{l \neq k} e^{w_{j,l}} \right) \left( \prod_{r \not\in \{k\}} e^{(w_{j,r})} \right) \right) - \mathbb{E}(\hat{f})^2
\]

\[
= \frac{1}{\text{var}(f)} \sum_{j=1}^n \beta_j e^{b_j} \left( \prod_{l \neq k} e^{w_{j,l}} \right) \left( \prod_{r \not\in \{k\}} e^{(w_{j,r})} \right) - \mathbb{E}(\hat{f})^2.
\]

Now we derive the expressions for the total Sobol’ indices for a given subset of variables of \( \{x_1, \ldots, x_d\} \),

\[
S^\text{tot}_u = 1 - \frac{\text{var}(\mathbb{E}(\hat{f}|x_r, r \not\in u))}{\text{var}(f)}
\]

where \( u \subseteq \{1, \ldots, d\} \). We find the expression for the total index \( S^\text{tot}_u \) for (11):

\[
S^\text{tot}_u = 1 - \frac{1}{\text{var}(f)} \left( \int_{[0,1]^d} \left( \sum_{j=1}^n \beta_j e^{b_j} \left( \prod_{l \in u} e^{w_{j,l}} \right) \left( \prod_{r \not\in u} e^{w_{j,r} - \beta_l |u|} \right) \right)^2 \text{d}x - \mathbb{E}(\hat{f})^2 \right)
\]

\[
= 1 - \frac{1}{\text{var}(f)} \left( \sum_{j=1}^n \beta_j e^{b_j} \left( \prod_{l \in u} e^{w_{j,l}} \right) \left( \prod_{r \not\in u} e^{(w_{j,r} + w_{i,r})} \right) - \mathbb{E}(\hat{f})^2 \right).
\]

When we consider the total Sobol’ index corresponding to a single variable \( x_k \), we have expression (12):

\[
S^\text{tot}_k = 1 - \frac{1}{\text{var}(f)} \left( \sum_{j=1}^n \beta_j e^{b_j} \left( \prod_{l \neq k} e^{w_{j,l} + w_{i,l}} \right) - \mathbb{E}(\hat{f})^2 \right)
\]

\[
= 1 - \frac{1}{\text{var}(f)} \sum_{j=1}^n \beta_j e^{b_j} \left( \prod_{l \neq k} e^{w_{j,l} + w_{i,l}} \right) - \mathbb{E}(\hat{f})^2.
\]

\[\square\]

Appendix  B. Sobol’ indices of analytic example (16)

Here we present formulas for the analytic first-order and total Sobol’ indices for (16), given an input dimension \( d \) and parameter \( \delta \). The first-order Sobol indices are the same for all \( k = 1, \ldots, d \).
The total Sobol’ indices are also the same for \( k = 1, \ldots, d \). The first-order and total Sobol’ indices are given by

\[
S_k = \frac{\text{var}(E(f_\delta | x_k))}{\text{var}(f_\delta)} \quad \text{and} \quad S_{k}^{\text{tot}} = 1 - \frac{\text{var}(E(f_\delta | x_l, l \neq k))}{\text{var}(f_\delta)},
\]

where

\[
\text{var}(f_\delta) = \frac{d\delta}{9} \left( \frac{3}{2} \right)^d + \delta^2 \left( \left( \frac{7}{3} \right)^d - \left( \frac{9}{7} \right)^d \right) + \frac{d}{12},
\]

\[
\text{var}(E(f_\delta | x_k)) = \frac{\delta^2}{27} \left( \frac{9}{4} \right)^d + \frac{\delta^2}{9} \left( \frac{3}{2} \right)^d + \frac{1}{12},
\]

\[
\text{var}(E(f_\delta | x_l, l \neq k)) = \frac{\delta(d-1)}{9} \left( \frac{3}{2} \right)^d + \delta^2 \left( \frac{27}{28} \left( \frac{7}{3} \right)^d - \left( \frac{9}{4} \right)^d \right) + \frac{d-1}{12}.
\]

Appendix C. Setup of the model in Section 5.3

Here we describe our choices for \( x_0 \) and \( Q \) in (23), as implemented in MATLAB. For the initial state, \( x_0 \), we take \( x_0 = [1 \ldots 1]^T \). We chose \( Q \) by generating a random orthogonal matrix as follows. First, we generated a matrix \( P \) whose entries are independent draws from standard normal distribution. This was done using MATLAB’s randn command. The random seed was fixed using \texttt{rand(1)}. Subsequently, the matrix \( Q \) was obtained by performing a QR factorization \( P = QR \), where \( Q \) is orthogonal and \( R \) is upper triangular, and retaining \( Q \). The QR factorization was computed using MATLAB’s \texttt{qr} command.