Identifying the Influential Inputs for Network Output Variance Using Sparse Polynomial Chaos Expansion

Zhanlin Liu¹, Ashis G. Banerjee², and Youngjun Choe¹

Abstract—Sensitivity analysis (SA) is an important aspect of process automation. It often aims to identify the process inputs that influence the output of the variance significantly. Existing SA approaches typically consider the input-output relationship as a black-box and conduct extensive random sampling from the actual process or its high-fidelity simulation model to identify the influential inputs. In this paper, an alternate, novel approach is proposed using a sparse polynomial chaos expansion-based model for a class of input-output relationships represented as directed acyclic networks. The model exploits the relationship structure by recursively relating a network node to its direct predecessors to trace the output variance back to the inputs. It, thereby, estimates the Sobol indices, which measure the influence of each input on the output variance, accurately and efficiently. Theoretical analysis establishes the validity of the model as the prediction of the network output converges in probability to the true output under certain regularity conditions. Empirical evaluation on two manufacturing processes shows that the model estimates the Sobol indices accurately with far fewer observations than a state-of-the-art Monte Carlo sampling method.

Note to Practitioners—This paper is motivated by the problem of automated identification of the inputs that influence the variance of the output for networked processes without feedback control. Such processes arise in various natural and engineered systems, of which manufacturing operations are of particular interest to us, where the output variance represents the uncertainty in productivity and/or quality. Therefore, influential inputs identification allows us to quantify the effects of the various process parameters, such as operating conditions, material compositions and characteristic properties, in determining the uncertainties in the process outputs. We show that our identification method is guaranteed to quantify the effects accurately, and is expected to do so more efficiently (with fewer experimental observations) than a widely used stochastic sampling technique. In the future, we will like to evaluate the usefulness of the developed method on large-scale manufacturing and supply chain networks in actual production facilities.

Index Terms—directed acyclic graph, sensitivity analysis, Sobol index, uncertainty quantification

I. INTRODUCTION

Uncertainty quantification plays a critical role in controlling the uncertainties in process automation. Automated processes that neglect important uncertainties are, at minimum, unstable, and, in the worst case, have catastrophic process outcomes in terms of both quality and productivity. To quantify how such uncertainties propagate through the process, sensitivity analysis is widely used in process automation. The sensitivity analysis of this study focuses on characterizing how the process output’s variance is propagated from the inputs. This type of analysis is ubiquitous in different areas of automation science and engineering, such as thermodynamics [3], electromagnetism [4], power systems [5], building systems [6], and manufacturing [7].

How sensitive a random variable (e.g., process output) is with respect to another random variable (e.g., process input) is measured using a sensitivity index. Arguably, the most widely used sensitivity indices are the Sobol indices [8], which quantify how the independent inputs apportion the variance of the output. In practice, simple random sampling (from the actual process) or Monte Carlo sampling (from the simulation model of the process) is most commonly used to estimate the Sobol indices, where many observations of the inputs and output are available. A more resource-efficient alternative is to construct a model (or, metamodel) of the actual process (or, its simulation model when the computational cost is expensive), and use the model (or, metamodel) to estimate the Sobol indices [9].

Among such models, polynomial chaos expansion (PCE) is particularly conducive to estimating the Sobol indices, as detailed in Sec. I. In essence, the PCE expands a random variable (e.g., process output) in terms of orthonormal polynomials in other random variables (e.g., process inputs), and the expansion’s coefficients directly yield convergent estimators of the Sobol indices thanks to the orthogonality of the polynomials in a Hilbert space.

However, such models, including PCE, typically consider the input-output relationship of a process as a black-box for sensitivity analysis. This approach, while generally applicable to many processes, misses the opportunity to leverage the scientific/engineering knowledge of how the process actually works. Opening the black-box and utilizing the knowledge of the inner working can enable more effective modeling of the process, leading to more accurate and efficient sensitivity analysis.

To this end, this study considers a broad class of processes whose input-output relationships are expressed as directed acyclic graphs (DAGs), also known as directed acyclic networks. Since network-structured processes are ubiquitous in practice, several real-world systems can potentially benefit from this study, such as biological...
networks [10], supply chain systems [11], manufacturing operations [12], and process industries, in general [13]. In particular, this study uses two manufacturing processes (welding and injection molding) for illustration purposes. We review the construction of orthonormal polynomials for the PCE, the Hoeffding approximation, and the Sobol indices. We also review how to estimate the Sobol indices using the PCE.

### II. Technical Background

In this section, we first formally define process inputs and output that bear uncertainties. Then, we present the PCE and sparse PCE. We review the construction of orthonormal polynomials for the PCE, the Hoeffding decomposition, and the Sobol indices. We also review how to estimate the Sobol indices using the PCE.

#### A. Input random vector and output random variable

In this paper, we generally use the same notations as [14], including \( \mathbb{N}_0 := \mathbb{N} \cup \{0\} \). \( \mathbb{A}^n \subseteq \mathbb{R}^n \), \( n \in \mathbb{N} \), denotes a bounded or unbounded subdomain of \( \mathbb{R}^n \). Let \( \Omega \) be a sample space, and \( \mathcal{F} \) be a \( \sigma \)-algebra on \( \Omega \). \( (\Omega, \mathcal{F}, \mathbb{P}) \) is a probability space with a probability measure \( \mathbb{P} : \mathcal{F} \rightarrow [0,1] \). The Borel \( \sigma \)-algebra on \( \mathbb{A}^n \subseteq \mathbb{R}^n \) is represented as \( \mathcal{B}^n := B(\mathbb{A}^n) \). An \( \mathbb{A}^n \)-valued input random vector \( \mathbf{x} := (x_1, \ldots, x_n) : (\Omega, \mathcal{F}) \rightarrow (\mathbb{A}^n, \mathcal{B}^n) \) describes the uncertainties of \( n \) process inputs of interest.

To model a process output \( y \) using the PCE in \( \mathbf{x} \), we assume that \( y \) is a function of \( \mathbf{x} \) and is a square-integrable random variable defined on the same probability space \( (\Omega, \mathcal{F}, \mathbb{P}) \), written \( y(\mathbf{x}) \in L^2(\Omega, \mathcal{F}, \mathbb{P}) \).

#### B. Polynomial chaos expansion (PCE)

PCE approximates \( y \) using a finite number of orthonormal polynomials in \( \mathbf{x} \) as follows:

\[
\hat{y} = f(\mathbf{x}) \approx \sum_{i=0}^{P} \theta_i \psi_i(\mathbf{x}),
\]

where \( \theta_i \) and \( \psi_i(\mathbf{x}) \), \( i = 0, 1, 2, \ldots, P \), denote the PCE coefficients and orthonormal polynomials in \( \mathbf{x} \), respectively. \( P + 1 \) is the number of the orthonormal polynomials and equals \( \binom{n+p}{n} \) for the pre-specified highest polynomial order \( p \) and the dimension of \( \mathbf{x} \), \( \dim(\mathbf{x}) = n \). Thus, \( P + 1 \) increases exponentially in \( n \) and \( p \). As \( P \) increases, the approximation error in eq. (1) tends to zero [15].

In this paper, we adopt a regression-based method to obtain the PCE coefficients by solving an overdetermined linear system of equations in the least-squares sense as follows [16]:

\[
\min_{\theta \in \mathbb{R}^{P+1}} \sum_{j=1}^{m} \left( Y_j - \sum_{i=0}^{P} \theta_i \psi_i(\mathbf{X}_j) \right)^2,
\]

where \( \theta \) denotes \( (\theta_0, \theta_1, \ldots, \theta_P) \). \( Y_j \) and \( \mathbf{X}_j \) represent the output and the input vector of the \( j \)th observation, \( j = 1, \ldots, m \), respectively.

Note that in contrast to typical regression models whose coefficients explain how the expectation of the output would conditionally change when the inputs are varied, the PCE coefficients are used to interpret how the variance of the output is apportioned to the inputs.

Thanks to the orthogonality of the orthonormal polynomials, the lower order moments of the output \( y \) are approximated using the PCE coefficients in eq. (1) as follows:

\[
\mathbb{E}(y) \approx \theta_0,
\]

\[
\text{Var}(y) \approx \sum_{i=1}^{P} \theta_i^2,
\]

where \( \mathbb{E} \) is the expectation operator with respect to the probability measure \( \mathbb{P} \). The approximation errors in eq. (3) tend to zero as \( P \) in the PCE in eq. (1) increases.

#### C. Sparse PCE

The sparse PCE is extensively studied in the recent literature [17–21]. In this paper, we use \( l_1 \) minimization, specifically the least absolute shrinkage and selection operator (LASSO), to obtain a more parsimonious model than the model from eq. (2), by solving the following problem:

\[
\min_{\theta \in \mathbb{R}^{P+1}} \sum_{i=0}^{P} |\theta_i|,
\]

\[
\text{such that } \frac{\sum_{j=1}^{m} \left( Y_j - \sum_{i=0}^{P} \theta_i \psi_i(\mathbf{X}_j) \right)^2}{\sum_{j=1}^{m} (Y_j - \bar{Y})^2} \leq \Gamma,
\]

where \( \bar{Y} = \frac{1}{m} \sum_{j=1}^{m} Y_j \). The parameter \( \Gamma \) constrains the goodness-of-fit for the sparse PCE (e.g., \( \Gamma = 0 \) requires a
perfectly fitting model and \( \Gamma = 1 \) allows the model to be as simple as a constant model. The two application examples in Sec. \( \text{V} \) use \( \Gamma \) of 0.001.

D. Construction of multivariate orthonormal polynomials

A variety of PCEs have been proposed to construct orthonormal polynomials considering different types of input distributions. The Wiener chaos expansion, known as the first PCE, uses Hermite polynomials for independent Gaussian-distributed inputs \[22\]. Later PCEs allow for different input distributions and include the generalized PCE (gPCE) \[23\], the multi-element gPCE (ME-gPCE) \[24\], the moment-based arbitrary PCE (aPCE) \[25\], and the Gram-Schmidt based PCE (GS-PCE) \[26\]. In particular, the GS-PCE, which accounts for dependent inputs following arbitrary distributions \[27\], provides the basis for constructing the proposed model in this paper.

In this work, process inputs are assumed to be mutually independent. However, the other variables in the process (represented as a network) are allowed to be dependent on others. When the variables in \( x \) are mutually independent, the orthonormal polynomials are directly constructed as the tensor products of the univariate orthonormal polynomials as follows:

\[
\psi_i(x) = \psi_{\alpha_i}(x) := \prod_{j=1}^{n} \psi_{\alpha_{ij}}(x_j),
\]

where \( \alpha_i := (\alpha_{i1}, \alpha_{i2}, \ldots, \alpha_{in}) \). \( \psi_{\alpha_{ij}}(x_j) \) represents the \( \alpha_{ij} \)-th order orthonormal polynomial in input \( x_j \), \( \alpha_i \) is the \( i \)-th arbitrary vector satisfying \( |\alpha_i| := \sum_{j=1}^{n} |\alpha_{ij}| \leq p \), where \( p \) is the highest order of the polynomials in the PCE. When variables are dependent on each other, we construct orthonormal polynomials using the modified Gram-Schmidt algorithm, as proposed in \[28\].

E. Hoeffding decomposition and Sobol indices

Suppose the inputs in the \( n \)-dimensional vector \( x \) are mutually independent and \( y = f(x) \in L^2(\Omega, \mathcal{F}, \mathcal{P}) \). Denote the probability density function of \( x \) as \( \mu(x) \). The Hoeffding decomposition of \( f(x) \) is then defined as follows \[8\] \[29\]:

\[
f(x) := \sum_{u \subseteq \{1,2,\ldots,n\}} f_u(x_u),
\]

where \( f_\emptyset := f_0 \) is a constant and \( x_u := (x_j)_{j \in u} \) for \( u \neq \emptyset \). Such decomposition is unique if and only if the summands in eq. \( \text{I} \) are orthogonal to each other as follows \[8\]:

\[
\int f_u(x)f_v(x)\mu(x)dx = 0, \forall u, v \subseteq \{1,2,\ldots,n\}, v \neq u.
\]

Due to the orthogonal property in eq. \( \text{II} \), the functional decomposition of \( \text{Var}(y) \) is expressed as follows \[30\]:

\[
\text{Var}(y) = \int f^2(x)\mu(x)dx - f^2_\emptyset = \sum_{u \subseteq \{1,2,\ldots,n\}} D_u(y),
\]

where

\[
D_u(y) := \int f^2_u(x_u)\mu(x_u)dx_u = \text{Var}(E(y|x_u)) - \sum_{v \subseteq u \neq \emptyset} D_v(y).
\]

Based on the decomposition, our sensitivity analysis considers the first-order Sobol index \( S_{x_j} \) and total Sobol index \( ST_{x_j} \) of \( y \) with respect to \( x_j \) defined as follows:

\[
S_{x_j} := \frac{D_{\{j\}}(y)}{\text{Var}(y)},
\]

\[
ST_{x_j} := \sum_{u \ni x_j} S_u,
\]

where \( S_u := D_u(y)/\text{Var}(y) \). The first-order Sobol index \( S_{x_j} \) measures the main effect of input \( x_j \) on the output variance \( \text{Var}(y) \). The total Sobol index \( ST_{x_j} \) measures the total contribution of \( x_j \) to \( \text{Var}(y) \) including its main effect and interactions with other inputs \[31\].

F. PCE-based Sobol indices

The Sobol indices can be estimated directly using the PCE coefficients in eq. \( \text{I} \), making PCE particularly useful for the sensitivity analysis \[32\]. The first-order Sobol index is estimated as follows:

\[
S_{x_j} \approx \frac{\sum_{\alpha_i \in \mathcal{A}(j)} \theta^2_{\alpha_i}}{\sum_{i=1}^{p} \theta^2_i},
\]

where \( \theta_{\alpha_i} \) is the PCE coefficient with respect to \( \psi_{\alpha_i}(x) \) in eq. \( \text{I} \) and

\[
\mathcal{A}(j) := \{ \alpha_i \in \mathbb{N}^n : \alpha_{ij} \neq 0 \leftrightarrow j \in u, |\alpha_i| \leq p \}.
\]

The total Sobol index is estimated as follows:

\[
ST_{x_j} \approx \sum_{\mathcal{A}(j)} S_{\mathcal{A}^{\emptyset}},
\]

where

\[
S_{\mathcal{A}^{\emptyset}} \approx \frac{\sum_{\alpha_i \in \mathcal{A}^{\emptyset}} \theta^2_{\alpha_i}}{\sum_{i=1}^{p} \theta^2_i}.
\]

III. Methodology

In this section, we first define notations on the directed acyclic graph (DAG), which represents the network-structured process of interest. Then, we present three models to estimate the Sobol indices for the process output with respect to the process inputs. The first model called the naive PCE is a baseline model and directly approximates the process output as a function of the process inputs, viewing the process as a black-box. The second model called the network PCE uses the network structure of the process to effectively approximate the process output in terms of the process inputs. The third model called the sparse network PCE (SN-PCE) imposes sparsity on the second model to use even fewer observations for the sensitivity analysis than the other models.
A. Directed acyclic graph

Let $G = \text{DAG}(V,E)$ be the directed acyclic graph that represents the network-structured process of interest. $V = \{v_1, v_2, \ldots, v_{|V|}\}$ is the collection of all the nodes in $G$, where $|V|$ denotes the number of the nodes. Let $x_v$ denote the random variable represented by the node $v \in V$ and, for $v \subseteq V$, $x_v := (x_v)_{v \in V}$. $E \subseteq V \times V$ is the collection of all the directed edges in $G$, encoding all dependencies between the nodes. For example, $(v_i, v_j) \in E$ implies that there is an edge from node $v_i$ to node $v_j$, and hence $x_{v_j}$ depends on $x_{v_i}$. The adjacency matrix $A$ is defined as follows:

$$A_{ij} := \begin{cases} 1 & (v_i, v_j) \in E \\ 0 & (v_i, v_j) \notin E. \end{cases}$$

If $A_{ij} = 1$, then $v_i$ is called a direct predecessor of $v_j$. If $\sum_{j=1}^{|V|} A_{ji} = 0$, $v_i$ is termed a sink node. Let $S(G)$ denote all the source nodes in $G$. We call the variables in $x_{S(G)}$, network inputs and the variables represented by the sink nodes network outputs. The node corresponding to the network output $y$ is denoted by $v_y$.

We say that there exists a path from $v_i$ to $v_j$ if and only if either $A_{ij} = 1$ or there exists a sequence of nodes $(v_{k_1}, \ldots, v_{k_t})$ for $1 \leq t \leq |V| - 2$ such that $A_{i,k_1} \prod_{l=1}^{t-1} A_{k_l,k_{l+1}} A_{k_t,j} = 1$.

If there is such a path, we define $E(v_i, v_j) = 1$; otherwise, $E(v_i, v_j) = 0$. This function is useful for the naïve PCE, which uses the network inputs that influence $y$, denoted as $\xi := x_{S(G) \cap V_y}$ for

$$V_y := \{v_i \in V : E(v_i, v_y) = 1\}.$$

We assume the variables in $\xi$ are mutually independent hereafter to well-define the Sobol indices of $y$ with respect to $\xi$.

For the network PCE, which relates each node to its direct predecessors, we define

$$\mathcal{P}(x_v) := x_{\{v_i \in V : v_j \in v, A_{ij} = 1\} \cup (v \cap S(G))},$$

where $\{v_i \in V : v_j \in v, A_{ij} = 1\}$ represents the direct predecessors, if any, of the nodes in $v$. To well-define $\mathcal{P}(x_v)$, $v \cap S(G)$ represents the source nodes in $v$, which do not have any direct predecessors. For $l \in \mathbb{N}$, $\mathcal{P}^l(x_v)$ denotes applying the operator $\mathcal{P}(\cdot)$ on $x_v$ $l$ times.

The network PCE can be applied to any DAG, which contains any of the four possible 3-node motifs. Fig. 1 shows an example DAG, which contains all the four motifs (e.g., $\{v_1, v_2, v_7\}, \{v_2, v_7, v_8\}, \{v_4, v_5, v_9\}, \{v_6, v_{10}, v_{12}\}$). Note the network inputs $\xi = (x_{v_1}, x_{v_2}, x_{v_5}, x_{v_6})$ are mutually independent. The node $v_{13}$ is the sink node corresponding to the network output $y$. This example DAG will be used in the following subsections to illustrate the naïve PCE and the network PCE.

---

B. Naïve PCE

The naïve PCE is the standard PCE in eq. (1) that approximates $y$ directly as a function of the network inputs that influence $y$, $\xi = x_{S(G) \cap V_y}$, as follows:

$$\hat{y} = \sum_{i=0}^{P} \theta_i \psi_i(\xi).$$

This PCE directly yields the estimated Sobol indices of $y$ with respect to $\xi$ based on eqs. (5) and (6). The naïve PCE algorithm is summarized in Algorithm 1.

---

**Algorithm 1 Naïve PCE Algorithm**

**Input:** $G = \text{DAG}(V,E)$; at least $P+1$ observations of the network output $y$ and inputs $\xi = x_{S(G) \cap V_y}$.

**Output:** Sobol indices of $y$ with respect to each input in $\xi$.

1: Construct univariate orthonormal polynomials for each input in $\xi$.
2: Construct multivariate orthonormal polynomials for $\xi$ as the tensor products of the univariate orthonormal polynomials using eq. (5).
3: Estimate $\theta$ in eq. (10) by solving an equivalent problem to eq. (2).
4: Estimate the Sobol indices based on the estimated $\theta$ using eqs. (5) and (6).

---

As discussed in Sec. II-B, the number of orthonormal polynomials, $P$, increases exponentially in $\dim(\xi)$. Thus, this naïve approach of taking the network as a blackbox requires an exponentially increasing number of observations to solve an equivalent problem to eq. (2) as $\dim(\xi)$ increases. In other words, a sensitivity analysis with respect to a large number of network inputs requires a large number of observations for the naïve PCE. This issue is mitigated by the network PCE that explicitly considers the network structure.
C. Network PCE

The network PCE is proposed to leverage the known network structure of the process of interest to improve the efficiency and accuracy of sensitivity analysis. Intuitively speaking, this model recursively relates a network node to its direct predecessors to trace the output variance back to the network inputs. How uncertainties propagate through the network is effectively captured by the PCE coefficients in the model. The coefficients directly yield estimated Sobol indices of the output with respect to each input in the network.

The recursive modeling process for the network PCE starts from the sink node $v_y$ (e.g., $v_{13}$ in Fig. 1) and traces it back to the source nodes (e.g., $v_1, v_3, v_4, v_5, v_6$ in Fig. 1). The network output $y$ is first modeled as the PCE in $\mathcal{P}(y)$ (e.g., $(x_{v_{11}}, x_{v_{12}})$ in Fig. 1), which includes the variables corresponding to the direct predecessors of $v_y$. Then, their direct predecessors are recursively found until $y$ is modeled as the PCE in $\xi$, or equivalently, $\mathcal{P}^L(y)$, where $L := \inf \{l \in \mathbb{N} : \mathcal{P}(y) = \mathcal{P}^{l+1}(y) \}$ denotes the total number of iterations.

In the $l^{th}$ iteration of this recursive process for $l = 1, \ldots, L$, we need to find mutually independent vectors to use in a PCE (recall eq. 3). Thus, we define the \textit{mutually independent decomposition} of $\mathcal{P}^l(y)$ as follows:

$$ x_{v_i}^{(l)} := \left( x_{v_{i1}}^{(l)}, x_{v_{i2}}^{(l)}, \ldots, x_{v_{in_i}}^{(l)} \right), \quad (11) $$

which has an arbitrary order of the elements and satisfies the following two conditions:

1. $x_{v_i}^{(l)} \bot x_{v_j}^{(l)}, \forall i \neq j$;
2. $x_{v_i} \not\perp x_k$ for $v_i, v_j \in v_i^{(l)}, \forall i$.

Note $n_i^{(l)} := \dim (x_{v_i}^{(l)})$ is the number of elements of the tuple in eq. (11). For example, in Fig. 1 the mutually independent decompositions of $\mathcal{P}(y)$ and $\mathcal{P}^2(y)$ are $(x_{v_{11}}, x_{v_{12}})$ and $(x_{v_{7}}, x_{v_{8}}, x_{v_{9}}, x_{v_{10}})$, respectively. Hence, $n_1^{(1)} = 2$ and $n_1^{(2)} = 3$, not 4.

In the $l^{th}$ iteration, the network PCE approximates $y$ using the PCE as follows:

$$ \hat{y}^{(l)} := \sum_{i=0}^{P_i^{(l)}} \theta_i^{(l)} \psi_i^{(l)}(\mathcal{P}^l(y)), \quad (12) $$

where each orthonormal polynomial $\psi_i^{(l)}(\mathcal{P}^l(y))$ can be obtained using the mutually independent decomposition of $\mathcal{P}^l(y)$ in eq. (11) as follows:

$$ \psi_i^{(l)}(\mathcal{P}^l(y)) = \psi_i^{(l)}(\mathcal{P}^l(y)) := \prod_{j=1}^{n_l^{(l)}} \psi_{ij}^{(l)} \left( x_{v_j}^{(l)} \right), \quad (13) $$

Here $\alpha_i^{(l)} = \left( \alpha_{i1}, \ldots, \alpha_{in_i} \right)$ is the $i$-th arbitrary tuple satisfying $\sum_{j=1}^{n_l^{(l)}} |\alpha_{ij}^{(l)}| \leq P^{(l)}$ for the pre-specified highest polynomial order $P^{(l)}$. $\alpha_{ij}^{(l)}$ is the vector composed of the polynomial orders with respect to the variables in $x_{v_j}^{(l)}$ for $j = 1, 2, \ldots, n_l^{(l)}$. $\psi_{ij}^{(l)} \left( x_{v_j}^{(l)} \right)$ is an $|\alpha_{ij}^{(l)}|$-th order orthonormal polynomial in $x_{v_j}^{(l)}$ obtained using the modified Gram-Schmidt algorithm [28].

In the first iteration ($l = 1$), the PCE coefficients, $\theta_i^{(l)}, i = 0, 1, \ldots, P^{(l)}$, in eq. (12) are estimated by solving an equivalent problem to eq. (2) where only the notations are different. For the subsequent iterations ($l \geq 2$), the coefficients are calculated in a different way using the previous iteration’s coefficients, as detailed next.

To model $y$ as a function of $\mathcal{P}^{l+1}(y)$, or equivalently, $$ \left( \mathcal{P} \left( x_{v_1}^{(l)} \right), \mathcal{P} \left( x_{v_2}^{(l)} \right), \ldots, \mathcal{P} \left( x_{v_{n_l^{(l)}}}^{(l)} \right) \right), $$

the network PCE substitutes $\psi_i^{(l)} \left( x_{v_j}^{(l)} \right) \in$ eq. (13) with

$$ \hat{y}_i^{(l)} \left( \mathcal{P}^{l}(y) \right) := \sum_{k=0}^{P_i^{(l)}} \hat{\theta}_i^{(l)} \psi_i^{(l)} \left( \mathcal{P}^{l}(x_{v_j}^{(l)}) \right) \quad (14) $$

to obtain the approximation of eq. (13) as follows:

$$ \hat{y}_i^{(l)} \left( \mathcal{P}^{l}(y) \right) := \prod_{j=1}^{n_l^{(l)}} \hat{\psi}_{ij}^{(l)} \left( x_{v_j}^{(l)} \right). \quad (15) $$

Without loss of generality, we let the highest polynomial order $P^{(l)}$ of orthonormal polynomials in eq. (14) to be the constant $P^{(l+1)}$. Substituting $\hat{\psi}_i^{(l)} \left( \mathcal{P}^{l+1}(y) \right)$ in eq. (15) for $\hat{\psi}_i^{(l)} \left( \mathcal{P}^{l}(y) \right)$ in eq. (12) yields the approximation of $y$ for the $(l+1)^{th}$ iteration as follows:

$$ \hat{y}^{(l+1)} := \sum_{i=0}^{P^{(l)}} \theta_i^{(l)} \psi_i^{(l)}(\mathcal{P}^l(y)) \quad (16) $$

$$ := \sum_{i=0}^{P^{(l+1)}} \theta_i^{(l+1)} \psi_i^{(l+1)} \left( \mathcal{P}^{l+1}(y) \right), \quad (17) $$

where the PCE coefficient $\theta_i^{(l+1)}$ in eq. (17) is calculated after estimating the coefficients in eq. (14) (by solving an equivalent problem to eq. (2)) and rearranging the terms in eq. (16), which involve the previous iteration’s coefficients. This recursive approach of calculating the PCE coefficient helps reduce the minimally required number of observations compared to the naïve PCE, as explained later.

The above iteration ends when $y$ is approximated as the PCE in $\mathcal{P}^L(y)$, or equivalently, $\xi$ as follows:

$$ \hat{y}(L) := \sum_{i=0}^{P^{(L)}} \theta_i^{(L)} \psi_i(\xi), \quad (18) $$

where $P^{(L)}$ depends on the highest polynomial orders, $p^{(1)}, \ldots, p^{(L)}$. This recursive approximation process is valid as shown in Theorem 3 in Sec. IV, which proves the convergence of $\hat{y}(L)$ in eq. (18) to $y$ in probability. The PCE coefficients, $\theta_i^{(L)}, i = 1, \ldots, P^{(L)}$, in eq. (18) directly yield the estimated Sobol indices of $y$ with respect to each input in $\xi$, as described in Sec. IV. The network PCE algorithm is summarized in Algorithm 2.
Here, below eq. (1). That for the network PCE (see Input naïve PCE increases exponentially in dim(\( \varepsilon \)). The network PCE uses many orthonormal polynomials to capture all main effects and major interaction effects of the variables in the network on the output variance. Therefore, we propose the SN-PCE, which imposes \( l_1 \)-sparsity on the PCE coefficients to capture only significant pathways of uncertainty propagation in the network. Specifically, the SN-PCE solves an equivalent problem of eq. (4) (with the difference lying only in the notations) instead of eq. (2) in Steps 3 and 4 of Algorithm 2. The resulting parsimonious model can use even fewer observations than the network PCE (which can already save substantially over the naïve PCE) to estimate the PCE coefficients and, in turn, the Sobol indices. Also, because only significant effects appear in the model (with non-zero PCE coefficients), the model is easier to interpret than the other models.

### IV. Theoretical Result

In this section, we show that predicted outputs from the naïve PCE and the network PCE converge to the true network output in probability under certain regularity conditions. This validates the use of the PCEs for estimating Sobol indices to conduct a sensitivity analysis. Because the SN-PCE is a sparsity-imposed version of the network PCE, its validity follows from the validity of the network PCE and the sparse PCE.

Because the naïve PCE is the direct application of the standard PCE in eq. (1), the corresponding theoretical result (Theorem 1) directly follows from [14] by appropriately invoking Assumption 1 below. The result is still presented here mainly for comparison with the theoretical result on the network PCE (Theorem 3).

#### Assumption 1 (adapted from [14]). The random vector \( \mathbf{x} := (x_1, \ldots, x_n)^T : (\Omega, \mathcal{F}) \rightarrow (\mathbb{A}^n, \mathcal{B}^n) \)

1) has a continuous joint probability density function \( \mu(\mathbf{x}) \) with a bounded or unbounded support \( \mathbb{A}^n \subseteq \mathbb{R}^n \);
2) possesses absolute finite moments of all orders, that is, \( \forall j := (j_1, j_2, \ldots, j_n) \in \mathbb{N}^n_0 \),

\[
\mathbb{E} \left( \left| \mathbf{x}^j \right|^p \right) := \int_{\Omega} \left| \mathbf{x}^j(w) \right| d\mathcal{P}(w) < \infty,
\]
Proof. This is a direct result of Theorem 11 in [14].

Theorem 1. Suppose that for the network output $y(\xi) \in L^2(\Omega, F, P)$, $\xi = x_{S(G) \cap V_y}$ fulfills Assumption 1. Then, $\bar{y}$ in eq. (10) converges to $y$ in probability as $P \to \infty$.

Proof. Under the stated assumptions, $\psi^{(l)}_{\alpha_{ij}}(x_{v_{ij}})$ in eq. (13) is a square-integrable function of $\Omega$. Building on Lemma 2, Theorem 3 proves the convergence of the network PCE output in eq. (18).

Lemma 2. Suppose that $x_{v_{ij}}^{(l)}$ is a function of $\mathcal{P}(x_{v_{ij}})$ for $l = 1, \ldots, L - 1$ and $j = 1, \ldots, n(i)$, and that for the network output $y$, $x_{v_{ij}}$ fulfills Assumption 1. Then,

1) $\psi^{(l)}_{\alpha_{ij}}(x_{v_{ij}})$ in eq. (14) converges to $\psi^{(l)}_{\alpha_{ij}}(x_{v_{ij}})$ in eq. (13) in probability as $P_{ij}^{(l)} \to \infty$; and

2) $\psi^{(l)}_{\alpha_{ij}}(\mathcal{P}(y)) = \prod_{j=1}^{n(i)} \psi^{(l)}_{\alpha_{ij}}(x_{v_{ij}})$ in eq. (15) converges to $\psi^{(l)}_{\alpha_{ij}}(\mathcal{P}(y))$ in eq. (13) in probability as $P_{ij}^{(l)} \to \infty$.

for all $l = 1, \ldots, L - 1$ and all $\alpha_{ij}^{(l)} = (\alpha_{i1}^{(l)}, \ldots, \alpha_{in(i)}^{(l)})$ satisfying $\sum_{j=1}^{n(i)} |\alpha_{ij}^{(l)}| \leq p^{(l)}$.

Proof. Under the stated assumptions, $\psi^{(l)}_{\alpha_{ij}}(x_{v_{ij}})$ in eq. (13) is a square-integrable function of $\mathcal{P}(x_{v_{ij}})$. The PCE's advantage over the naive PCE. Lemma 2 validates the recursive modeling of a network node using its direct predecessors (described in Steps 1–5 in Algorithm 2).
The first statement follows from Theorem 11 in [13]. The second statement follows from the first statement by the continuous mapping theorem.

**Theorem 3.** Suppose that the assumptions in Lemma 2 hold for the network output \( y(\mathbf{x}_\nu(1)) \in \mathbb{L}^2(\Omega, \mathcal{F}, \mathcal{P}) \). Then, there exists an increasing function \( \gamma^{(l)}: \mathbb{N} \rightarrow \mathbb{N} \) such that if \( p^{(l+1)} = \gamma^{(l)}(p^{(l)}) \) for \( l = 1, \ldots, L - 1 \), \( \hat{y}^{(L)} \) in eq. (18) converges to \( y \) in probability as \( p^{(l)} \rightarrow \infty \), or equivalently, \( P^{(l)} \rightarrow \infty \).

**Proof.** The proof is based on mathematical induction.

**Base case** (iteration \( l = 1 \)). Let \( \gamma^{(0)} \) be an identify function and \( P^{(0)} := P^{(1)} \) so that \( p^{(1)} = \gamma^{(0)}(P^{(0)}) \). Based on Theorem 11 in [14],

\[
\hat{y}^{(1)} = \sum_{i=0}^{l} \theta_i^{(1)} \psi_i^{(1)}(\mathcal{P}(y))
\]

in eq. (12) with \( l = 1 \) converges to \( y(\mathbf{x}_\nu(1)) \in \mathbb{L}^2(\Omega, \mathcal{F}, \mathcal{P}) \) in probability as \( p^{(1)} \rightarrow \infty \), or equivalently, \( P^{(1)} \rightarrow \infty \).

**Inductive hypothesis.** For \( l \in \mathbb{N} \), suppose there exists an increasing function \( \gamma^{(l-1)}: \mathbb{N} \rightarrow \mathbb{N} \) such that if \( p^{(l)} = \gamma^{(l-1)}(P^{(l-1)}) \), \( \hat{y}^{(l)} \) in eq. (12) converges to \( y \) in probability as \( P^{(l)} \rightarrow \infty \).

**Inductive step.** We want to show that there exists an increasing function \( \gamma^{(l)}: \mathbb{N} \rightarrow \mathbb{N} \) such that if \( p^{(l+1)} = \gamma^{(l)}(P^{(l)}) \), \( \hat{y}^{(l+1)} \) in eq. (16) converges to \( y \) in probability as \( P^{(l)} \rightarrow \infty \).

To prove \( \hat{y}^{(l+1)} \rightarrow y \) under the aforementioned conditions, we show that for any \( \epsilon > 0 \) and any \( \delta > 0 \), there exists \( P_0^{(l)} \) such that \( \forall P^{(l)} \geq P_0^{(l)} \),

\[
\mathcal{P} \left( \left| \hat{y}^{(l+1)} - y \right| > \epsilon \right) = \mathcal{P} \left( \left| \sum_{i=0}^{l} \theta_i^{(1)} \psi_i^{(1)}(\mathcal{P}(y)) - y \right| > \epsilon \right) < \delta.
\]

Note that \( P^{(l)} \) is an increasing function of \( p^{(l)} \), \( l = 1, \ldots, l \). The right-hand side of eq. (23) can be rewritten as

\[
\mathcal{P} \left( \left| \sum_{i=0}^{l} \theta_i^{(1)} \psi_i^{(1)}(\mathcal{P}(y)) - y \right| > \epsilon \right) = \mathcal{P} \left( \left| \sum_{i=0}^{l} \theta_i^{(1)} \psi_i^{(1)}(\mathcal{P}(y)) - \sum_{i=0}^{l} \theta_i^{(1)} \psi_i^{(1)}(\mathcal{P}(y)) \right| > \epsilon \right) + \mathcal{P} \left( \left| \sum_{i=0}^{l} \theta_i^{(1)} \psi_i^{(1)}(\mathcal{P}(y)) - y \right| > \frac{\epsilon}{2} \right)
\]

by the triangular inequality. By the inductive hypothesis, there exists \( P_1^{(l)} \) such that \( \forall P^{(l)} \geq P_1^{(l)} \), the second term in eq. (24) satisfies

\[
\mathcal{P} \left( \left| \sum_{i=0}^{l} \theta_i^{(1)} \psi_i^{(1)}(\mathcal{P}(y)) - \sum_{i=0}^{l} \theta_i^{(1)} \psi_i^{(1)}(\mathcal{P}(y)) \right| > \frac{\epsilon}{2} \right) < \delta/2.
\]

The first term in eq. (24) can be upper-bounded using the triangular inequality as follows:

\[
\mathcal{P} \left( \left| \sum_{i=0}^{l} \theta_i^{(1)} \psi_i^{(1)}(\mathcal{P}(y)) - \sum_{i=0}^{l} \theta_i^{(1)} \psi_i^{(1)}(\mathcal{P}(y)) \right| > \frac{\epsilon}{2} \right) \leq \sum_{i=0}^{l} \mathcal{P} \left( \left| \psi_i^{(1)}(\mathcal{P}(y)) - \psi_i^{(1)}(\mathcal{P}(y)) \right| > \frac{\epsilon}{2} \right).
\]

Note that \( P_i^{(l)} \) in eq. (14) is an increasing function of the highest polynomial order \( p_{ij}^{(l)} \), which is assumed to be the constant \( p^{(l+1)} \) in Sec. III-C. By Lemma 2 there exists an increasing function \( \gamma^{(l)}: \mathbb{N} \rightarrow \mathbb{N} \) such that \( \forall p^{(l+1)} \geq \gamma^{(l)}(P^{(l)}) \), the summand in eq. (26) satisfies

\[
\mathcal{P} \left( \left| \psi_i^{(1)}(\mathcal{P}(y)) - \psi_i^{(1)}(\mathcal{P}(y)) \right| > \frac{\epsilon}{2} \right) < \frac{\delta}{2(P^{(l+1)} + 1)}
\]

for \( i = 0, 1, \ldots, P^{(l)} \), and for any \( P^{(l)} \in \mathbb{N} \). Therefore, eq. (26) is upper-bounded by \( \delta/2 \), \( \forall p^{(l+1)} \geq \gamma^{(l)}(P^{(l)}) \).

Putting this together with eq. (25) proves the existence of \( P_0^{(l)} := P^{(l)} \) such that \( \forall P^{(l)} \geq P_0^{(l)} \), eq. (23) is upper-bounded by \( \delta \), completing the proof of \( \hat{y}^{(l+1)} \rightarrow y \) as \( P^{(l)} \rightarrow \infty \) if \( p^{(l+1)} = \gamma^{(l)}(P^{(l)}) \). By mathematical induction, the conclusion of the theorem follows.

The increasing function \( \gamma^{(l)} \) in Theorem 3 prescribes how fast the highest polynomial order \( p^{(l+1)} = \gamma^{(l)}(P^{(l)}) \) should grow in relation to the number of orthonormal polynomials, \( P^{(l)} \), for \( l = 1, \ldots, L - 1 \) so that \( \hat{y}^{(L)} \) in eq. (18) converges to \( y \) in probability. Furthermore, to make the relation between \( p^{(l+1)} \) and \( P^{(l)} \) more explicit, using eqs. (20) and (21), let \( d^{(l)} := |D_0| \) and \( d^{(l)} := \bigcup_{1 \leq j \leq n^{(l)}} D_j^{(l-1)} \), \( l = 2, \ldots, L \), denote the number of nodes represented by \( \mathcal{P}(y) \) and \( \mathcal{P}(y) \) in eq. (12), respectively. Because

\[
P^{(l)} + 1 = \left( d^{(l)} + p^{(l)} \right),
\]

for \( l = 1, \ldots, L \), Stirling’s approximation yields

\[
p^{(l+1)} = \gamma^{(l)} \left( \mathcal{O} \left( \left( P^{(l)} d^{(l)} \right) \right) \right)
\]

using the big O notation.

For example, if \( \gamma^{(l)} \) is linear (or superlinear), then \( p^{(l+1)} \) should grow as fast as (or faster than) \( d^{(l)-th} \) power of \( p^{(l)} \), or equivalently, \( \prod_{l=1}^{L} d^{(l)-th} \) power of \( p^{(1)} \) for \( l = 1, \ldots, L - 1 \). Intuitively speaking, we should control the
approximation errors for the upstream nodes in the network more tightly to ensure that the approximation errors for the downstream nodes (especially the output node) are arbitrarily small. We note that it is beyond the scope of this paper to establish more detailed characteristics of $\gamma^{(l)}$.

The SN-PCE, which tends to use much smaller $P^{(l)}, l = 1, \ldots, L$, than the network PCE, mitigates the need for rapidly increasing $\rho^{(l)}, l = 1, \ldots, L$, while maintaining a similar approximation accuracy.

V. APPLICATIONS

For empirical evaluation of the proposed methodology, we conduct sensitivity analysis of two manufacturing processes, namely, the welding process and the injection molding process. Each process has multiple variables whose relationships are modeled as a network in [34]. We use the same modeling equations and notations therein (hence, some notation conflicts arise although their meanings are clear from the context).

We compare three methods, a state-of-the-art Monte Carlo method [35], the naïve PCE, and the SN-PCE, for estimating the first-order and total Sobol indices. The estimation is based on randomly generated observations of the process variables using the models in [34]. The estimation is replicated 200 times to calculate the sample mean and standard error of the estimated Sobol indices for each method.

As discussed in Sec. I-E, the Sobol indices measure the influence of each network input on the variance of the network output. Hereafter, we call some network inputs influential inputs if their first-order Sobol indices are $10^{-1}$ or larger; in other words, influential inputs explain 10% or more of the output variance without considering their interactions with other inputs.

The Monte Carlo method in [35] is used as a benchmark method because it is known to be more accurate than other Monte Carlo methods for estimating small Sobol indices. We use a large sample for the Monte Carlo method, namely, 10,000 observations and treat its sample indices. We use a large sample for the Monte Carlo method because it is known to be more accurate than other Monte Carlo methods for estimating small Sobol indices.

These observations are still sufficient because we use the highest polynomial order of 3 for both the naïve PCE and the SN-PCE, namely, 500 and 100, respectively. These samples sizes are still sufficient because we use the highest polynomial order of 3 for both the naïve PCE and the SN-PCE; the naïve PCE requires at least $364 = \binom{11+3}{3}$ observations for $\dim(\xi) = 11$ and the network PCE (i.e., SN-PCE without sparsity) requires at least $84 = \binom{6+4}{3}$ observations because eq. (19) equals 6. The SN-PCE could use even fewer observations because it identifies only 14 orthonormal polynomials (4% of those used in the naïve PCE) as necessary to approximate the network output of this particular process across all 200 replications.

In turn, the weld volume $V$ depends on six welding parameters (weld zone dimensions: $e$, $g$, $h$, $l$, and $t$; weld length $L$), and the total energy $E$ depends on $V$ and additional parameters, $\rho$, $C_p$, $T_i$, $T_f$, and $H$.

In turn, the weld volume $V$ depends on six welding parameters (weld zone dimensions: $e$, $g$, $h$, $l$, and $t$; weld length $L$) as follows:

$$V = L (0.75lh + gt + 0.5(l-9)(t-e)) .$$

The process inputs’ distributions are presented in Table I.

Compared to the Monte Carlo method that uses 10,000 observations, we use much fewer observations for the naïve PCE and the SN-PCE, namely, 500 and 100, respectively. These samples sizes are still sufficient because we use the highest polynomial order of 3 for both the naïve PCE and the SN-PCE; the naïve PCE requires at least $364 = \binom{11+3}{3}$ observations for $\dim(\xi) = 11$ and the network PCE (i.e., SN-PCE without sparsity) requires at least $84 = \binom{6+4}{3}$ observations because eq. (19) equals 6. The SN-PCE could use even fewer observations because it identifies only 14 orthonormal polynomials (4% of those used in the naïve PCE) as necessary to approximate the network output of this particular process across all 200 replications.

Table I shows the sample means and standard errors of the estimated Sobol indiceses for the three methods. Despite the vastly different sample sizes used for each method, the sample means are nearly identical across the methods (except for the non-influential inputs, which have total Sobol indices smaller than $10^{-1}$). This indicates the estimation bias is nearly zero for these methods. The standard errors are also very similar across the methods for the influential inputs, indicating that the SN-PCE achieves a similar accuracy as the other methods with a much smaller sample size.

Fig. 4 presents a Pareto chart of the first-order Sobol indices estimated from the SN-PCE. Along with Table I, the chart confirms that the weld zone dimensions ($h, g, t, e, l$) are the most influential inputs for the variance of the process output $E$. Also, the cumulative sum of the first-order Sobol indices approaches 100% in the chart, implying that the interactions between the inputs do not have significant effects on the variance of $E$. It echoes the finding from Table I that the first-order Sobol indices are approximately equal to the total Sobol indices across all the influential inputs.

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{dag.png}
\caption{This DAG represents the relationships among the variables in the welding process [34]; the weld volume $V$ depends on six welding parameters (weld zone dimensions: $e$, $g$, $h$, $l$, and $t$; weld length $L$), and the total energy $E$ depends on $V$ and additional parameters, $\rho$, $C_p$, $T_i$, $T_f$, and $H$.}
\end{figure}
TABLE I
Sample means and standard errors (rounded to two decimal places) of the estimated first-order and total Sobol indices based on 200 replications for the welding process. The inputs in the first column are sorted in descending order of the first-order Sobol indices estimated from the Monte Carlo method. For each replication, †Monte Carlo method, ‡Naïve PCE, and §SN-PCE use 10,000, 500, and 100 observations, respectively. For the influential inputs, SN-PCE attains similar standard errors as the other methods despite using the smallest sample size.

| Input | Distribution | Monte Carlo† | Naïve PCE‡ | SN-PCE§ |
|-------|--------------|--------------|------------|---------|
| h     | N(2.6,0.5)   | 2.78 ± 10^{-4} | 2.81 ± 10^{-4} | 2.80 ± 10^{-4} |
|       |              | ±0.00 ± 10^{-1} | ±0.01 ± 10^{-1} | ±0.01 ± 10^{-1} |
| g     | N(2,0.1)     | 2.32 ± 10^{-4} | 2.31 ± 10^{-4} | 2.34 ± 10^{-4} |
|       |              | ±0.00 ± 10^{-1} | ±0.01 ± 10^{-1} | ±0.02 ± 10^{-1} |
| t     | N(15,0.6)    | 2.28 ± 10^{-4} | 2.28 ± 10^{-4} | 2.25 ± 10^{-4} |
|       |              | ±0.00 ± 10^{-1} | ±0.01 ± 10^{-1} | ±0.02 ± 10^{-1} |
| e     | N(11,1)      | 1.46 ± 10^{-4} | 1.45 ± 10^{-4} | 1.46 ± 10^{-4} |
|       |              | ±0.00 ± 10^{-1} | ±0.01 ± 10^{-1} | ±0.01 ± 10^{-1} |
| l     | N(8.5,0.5)   | 1.07 ± 10^{-4} | 1.10 ± 10^{-4} | 1.12 ± 10^{-4} |
|       |              | ±0.00 ± 10^{-1} | ±0.01 ± 10^{-1} | ±0.01 ± 10^{-1} |
| L     | N(500,10)    | 1.95 ± 10^{-4} | 1.76 ± 10^{-4} | 2.00 ± 10^{-4} |
|       |              | ±0.00 ± 10^{-1} | ±0.01 ± 10^{-1} | ±0.01 ± 10^{-1} |
| $C_p$ | N(500,5)     | 9.72 ± 10^{-4} | 13.9 ± 10^{-4} | 9.79 ± 10^{-4} |
|       |              | ±0.02 ± 10^{-1} | ±0.05 ± 10^{-1} | ±0.05 ± 10^{-1} |
| $T_f$ | N(1628,10)   | 2.76 ± 10^{-4} | 1.57 ± 10^{-4} | 2.81 ± 10^{-4} |
|       |              | ±0.00 ± 10^{-1} | ±0.01 ± 10^{-1} | ±0.01 ± 10^{-1} |
| $T_i$ | N(303,0.3)   | 8.28 ± 10^{-4} | 1.93 ± 10^{-4} | 8.45 ± 10^{-4} |
|       |              | ±0.00 ± 10^{-1} | ±0.03 ± 10^{-1} | ±0.04 ± 10^{-1} |
| $\rho$| N(8238,10)   | 7.20 ± 10^{-4} | 1.93 ± 10^{-4} | 7.30 ± 10^{-4} |
|       |              | ±0.00 ± 10^{-1} | ±0.03 ± 10^{-1} | ±0.03 ± 10^{-1} |
| $H$   | N(2270,3)    | 3.32 ± 10^{-4} | 1.84 ± 10^{-4} | 3.41 ± 10^{-4} |
|       |              | ±0.00 ± 10^{-1} | ±0.02 ± 10^{-1} | ±0.02 ± 10^{-1} |

Fig. 4. Pareto chart of the first-order Sobol indices estimated using the SN-PCE for the welding process. The higher bar indicates that the input has a more influence (excluding interactions with other inputs) on the variance of the process output $E$.

B. Injection molding process

The injection molding process has more intricate relationships between process variables than the welding process, as depicted in Fig. [3]. The process output of interest is the energy consumed in resetting the process, $E_{\text{reset}}$. This energy depends on the melting energy $E_{\text{melt}}$, the injection energy $E_{\text{inj}}$, and the cooling energy $E_{\text{cool}}$ as follows: $E_{\text{reset}} = 0.25 (E_{\text{melt}} + E_{\text{inj}} + E_{\text{cool}})$. Here, $E_{\text{melt}} = P_{\text{melt}} \times V_{\text{shot}} / Q$, where

$$P_{\text{melt}} = \frac{1}{2} \left( \rho \times Q \times C_p \times (T_{\text{inj}} - T_{\text{pol}}) + \rho \times Q \times H_f \right),$$

$$V_{\text{shot}} = V_{\text{part}} \times \left( 1 + \frac{e}{100} + \frac{\Delta}{100} \right).$$

Here, $\rho$ (specific gravity), $C_p$ (heat capacity), $T_{\text{pol}}$ (initial polymer temperature), $e$ (shrinkage parameter), and $T_{\text{inj}}$ (injection temperature) are the network inputs. $Q$ (flow rate), $H_f$ (polymer heat of fusion), $V_{\text{part}}$ (volume of mold), and $\Delta$ (buffer) are constant parameters. On the other hand, $E_{\text{inj}} = P_{\text{inj}} \times V_{\text{part}}$ and

$$E_{\text{cool}} = \rho \times V_{\text{part}} \times (C_p \times (T_{\text{inj}} - T_{ej})), \frac{COP}{COP}$$

where $P_{\text{inj}}$ (injection pressure), $T_{ej}$ (ejection temperature), and $T_{\text{inj}}$ (injection temperature) are the network inputs. $COP$ (coefficient of performance of the cooling equipment) is a constant parameter. The network inputs’ distributions are presented in Table I.

To adequately model the more intricate network structure of the injection molding process, we use the highest polynomial order of 4 for both the naïve PCE and the SN-PCE, compared to 3 used for the welding process; the naïve PCE requires at least 330 = $\binom{7+4}{4}$ observations for $\text{dim}(\xi) = 7$ and the network PCE (i.e., SN-PCE without sparsity) requires at least 126 = $\binom{9+4}{4}$ observations because eq. [19] equals 5. Thus, we use 500 and 200 observations for the naïve PCE and the SN-PCE, respectively,
Fig. 5. This DAG represents the relationships among the variables in the injection molding process [34]; the yellow shaded nodes $E_{\text{melt}}$, $E_{\text{cool}}$, and $E_{\text{inj}}$ are the energies consumed in three subprocesses that depend on different blue shaded network inputs. The network output $E_{\text{reset}}$ depends on $E_{\text{melt}}$, $E_{\text{cool}}$, and $E_{\text{inj}}$.

compared to 500 and 100 used for the welding process. Yet, again, the SN-PCE could use even fewer observations because it identifies only 9 orthonormal polynomials (3% of those used in the naïve PCE) as necessary to approximate the network output of this particular process across all 200 replications.

**TABLE II**

Sample means and standard errors (rounded to two decimal places) of the estimated first-order Sobol indices based on 200 replications for the injection molding process. For each replication, §SN-PCE uses 200 observations. All the other setups are the same as in Table I.

| Input | Distribution | Monte Carlo | Naïve PCE | SN-PCE |
|-------|--------------|-------------|-----------|--------|
| $T_{\text{inj}}$ | $N(210, 3)$ | $4.77 \times 10^{-1}$ | $4.77 \times 10^{-1}$ | $4.78 \times 10^{-1}$ |
| $T_{\text{ej}}$ | $N(35, 3)$ | $2.62 \times 10^{-1}$ | $2.62 \times 10^{-1}$ | $2.61 \times 10^{-1}$ |
| $\rho$ | $U(950, 990)$ | $2.26 \times 10^{-1}$ | $2.26 \times 10^{-1}$ | $2.26 \times 10^{-1}$ |
| $T_{\text{pol}}$ | $N(40, 3)$ | $3.21 \times 10^{-2}$ | $3.21 \times 10^{-2}$ | $3.20 \times 10^{-2}$ |
| $C_{\rho}$ | $U(2250, 2260)$ | $2.61 \times 10^{-3}$ | $2.61 \times 10^{-3}$ | $2.60 \times 10^{-3}$ |
| $\epsilon$ | $U(0.018, 0.021)$ | $7.72 \times 10^{-9}$ | $7.76 \times 10^{-9}$ | $0$ |
| $P_{\text{inj}}$ | $N(90, 4)$ | $4.77 \times 10^{-14}$ | $4.77 \times 10^{-14}$ | $0$ |

Like the welding process, the injection molding process turns out to have the first-order Sobol indices approximately equal to the total Sobol indices for the influential inputs. Thus, we only report the first-order Sobol indices in Table I. Again, the SN-PCE attains similar standard errors as the other methods for the influential inputs despite using fewer observations. Fig. 6 shows that $T_{\text{inj}}$ determines nearly 50% of the variance of network output $E_{\text{reset}}$. $T_{\text{ej}}$ and $\rho$ have comparable effects (26% and 23%, respectively), while other inputs, $T_{\text{pol}}$, $C_{\rho}$, $\epsilon$, and $P_{\text{inj}}$, barely influence the variance of $E_{\text{reset}}$.

**VI. Conclusion**

This paper proposes the SN-PCE to model uncertainty propagation in a broad class of processes represented as DAGs. A DAG encodes the dependencies between the variables in a process, including the process output (sink node in the DAG) and inputs (source nodes in the DAG). The SN-PCE effectively captures how the inputs influence the output variance. Theoretically, it is shown that the network PCE (equivalent to the SN-PCE without sparsity) is valid in the sense that its prediction of the output converges in probability to the true output under reasonable assumptions. Empirically, the SN-PCE is shown to accurately estimate the Sobol indices of the output with respect to the inputs for two manufacturing processes. The SN-PCE uses substantially fewer observations than the black-box approaches (a state-of-the-art Monte Carlo method and the naïve PCE) to accurately identify the influential inputs, showing promise for efficient sensitivity analysis in process automation.

Future research may investigate extension of the proposed model to even more general networks. One direction could be to relax the assumption of mutual independence of the network inputs. While their dependencies would complicate the estimation and interpretation of the sensitivity indices, the indices proposed in [28] might help decode how the dependent network inputs influence the output. Another research direction would be to allow cycles (or, feedback loops) in the network, thereby, extending this work beyond directed acyclic networks.

**Acknowledgment**

This work was partially supported by the National Science Foundation (NSF grant CMMI-1824681).
References

[1] D. Djurdjanovic and J. Ni, “Stream-of-variation (SoV)-based measurement scheme analysis in multi-station machining systems,” IEEE Transactions on Automation Science and Engineering, vol. 3, no. 4, pp. 407–422, 2006.

[2] J. A. Marvel, “Performance metrics of speed and separation monitoring in shared workspaces,” IEEE Transactions on Automation Science and Engineering, vol. 10, no. 2, pp. 405–414, 2013.

[3] A. L. Costa and E. M. Queiroz, “Design optimization of shell-and-tube heat exchangers,” Applied Thermal Engineering, vol. 28, no. 14-15, pp. 1798–1805, 2008.

[4] P. C. Chen, V. Malbasa, Y. Dong, and M. Kezunovic, “Sensitivity analysis of voltage sag based fault location with distributed generation,” IEEE Transactions on Smart Grid, vol. 6, no. 4, pp. 2098–2106, 2015.

[5] F. Ni, M. Nijhuis, P. H. Nguyen, and J. F. Cobben, “Variance-based global sensitivity analysis for power systems,” IEEE Transactions on Power Systems, vol. 33, no. 2, pp. 1670–1682, 2018.

[6] S. Li, K. Deng, and M. Zhou, “Sensitivity analysis for building energy simulation model calibration via algorithmic differentiation,” IEEE Transactions on Automation Science and Engineering, vol. 14, no. 2, pp. 905–914, 2017.

[7] W. Huang and Z. Kong, “Process capability sensitivity analysis for design evaluation of multistage assembly processes,” IEEE Transactions on Automation Science and Engineering, vol. 7, no. 4, pp. 736–745, 2010.

[8] I. M. Sobol, “Sensitivity estimates for nonlinear mathematical models,” Mathematical Modelling and Computational Experiments, vol. 1, no. 4, pp. 407–414, 1993.

[9] B. Sudret, “Meta-models for structural reliability and uncertainty quantification,” arXiv preprint arXiv:1203.2062, 2012.

[10] R. J. Prill, P. A. Iglesias, and A. Levchenko, “Dynamic properties of network motifs contribute to biological network organization,” PLoS Biology, vol. 3, no. 11, pp. 1881–1892, 2005.

[11] D. Mogale, S. K. Kumar, and M. K. Tiwari, “Two stage Indian food grain supply chain network transportation-allocation model,” IFAC-PapersOnLine, vol. 49, no. 12, pp. 1767–1772, 2016.

[12] K. He, M. Jia, and Q. Xu, “Optimal sensor deployment for manufacturing process monitoring based on quantitative cause-effect graph,” IEEE Transactions on Automation Science and Engineering, vol. 13, no. 2, pp. 963–975, 2016.

[13] P. Agrawal and S. Rao, “Energy-aware scheduling of distributed systems,” IEEE Transactions on Automation Science and Engineering, vol. 11, no. 4, pp. 1163–1175, 2014.

[14] S. Rahman, “A polynomial chaos expansion in dependent random variables,” Journal of Mathematical Analysis and Applications, vol. 464, no. 1, pp. 749–775, 2018.

[15] R. H. Cameron and W. T. Martin, “The orthogonal development of non-linear functionals in series of Fourier-Hermite functionals,” Annals of Mathematics, vol. 48, no. 2, pp. 385–392, 1947.

[16] M. P. Pettersson, G. Iaccarino, and J. Nordström, Polynomial chaos methods for hyperbolic partial differential equations. Springer, 2015.

[17] G. Blatman and B. Sudret, “Sparse polynomial chaos expansions and adaptive stochastic finite elements using a regression approach,” Comptes Rendus Mécanique, vol. 336, no. 6, pp. 518–523, 2008.

[18] ——, “Efficient computation of global sensitivity indices using sparse polynomial chaos expansions,” Reliability Engineering & System Safety, vol. 95, no. 11, pp. 1216–1229, 2010.

[19] ——, “Adaptive sparse polynomial chaos expansion based on least angle regression,” Journal of Computational Physics, vol. 230, no. 6, pp. 2345–2367, 2011.

[20] J. D. Jakeman, M. S. Eldred, and K. Sargsyan, “Enhancing ℓ1-minimization estimates of polynomial chaos expansions using basis selection,” Journal of Computational Physics, vol. 289, pp. 18–34, 2015.

[21] J. Peng, J. Hampton, and A. Doostan, “On polynomial chaos expansion via gradient-enhanced ℓ1-minimization,” Journal of Computational Physics, vol. 310, pp. 440–458, 2016.

[22] N. Wiener, “The homogeneous chaos,” American Journal of Mathematics, vol. 60, no. 4, pp. 897–936, 1938.

[23] D. Xiu and G. E. Karniadakis, “The Wiener–Askey polynomial chaos for stochastic differential equations,” SIAM Journal on Scientific Computing, vol. 24, no. 2, pp. 619–644, 2002.

[24] X. Wan and G. E. Karniadakis, “Multi-element generalized polynomial chaos for arbitrary probability measures,” SIAM Journal on Scientific Computing, vol. 28, no. 3, pp. 901–928, 2006.

[25] S. Oladyshkin and W. Nowak, “Data-driven uncertainty quantification using the arbitrary polynomial chaos expansion,” Reliability Engineering & System Safety, vol. 106, pp. 179–190, 2012.

[26] J. A. Witteveen, S. Sarkar, and H. Bijl, “Modeling physical uncertainties in dynamic stall induced fluid–structure interaction of turbine blades using arbitrary polynomial chaos,” Computers & Structures, vol. 85, no. 11, pp. 866–878, 2007.

[27] M. Navarro, J. Witteveen, and J. Blom, “Polynomial chaos expansion for general multivariate distributions with correlated variables,” arXiv preprint arXiv:1406.5483, 2014.

[28] Z. Liu and Y. Choe, “Data-driven sensitivity indices for models with dependent inputs using the polynomial chaos expansion,” arXiv preprint arXiv:1803.10978, 2018.

[29] G. Chastaing, F. Gamboa, and C. Prieur, “Gener-
alized Hoeffding-Sobol decomposition for dependent variables-application to sensitivity analysis,” *Electronic Journal of Statistics*, vol. 6, pp. 2420–2448, 2012.

[30] T. Crestaux, O. Le Maître, and J. M. Martinez, “Polynomial chaos expansion for sensitivity analysis,” *Reliability Engineering & System Safety*, vol. 94, no. 7, pp. 1161–1172, 2009.

[31] T. Homma and A. Saltelli, “Importance measures in global sensitivity analysis of nonlinear models,” *Reliability Engineering & System Safety*, vol. 52, no. 1, pp. 1–17, 1996.

[32] B. Sudret, “Global sensitivity analysis using polynomial chaos expansions,” *Reliability Engineering & System Safety*, vol. 93, no. 7, pp. 964–979, 2008.

[33] C. Carstens, “Motifs in directed acyclic networks,” in 2013 *International Conference on Signal-Image Technology & Internet-Based Systems*, 2013, pp. 605–611.

[34] S. Nannapaneni and S. Mahadevan, “Uncertainty quantification in performance evaluation of manufacturing processes,” in 2014 *IEEE International Conference on Big Data*, 2014, pp. 996–1005.

[35] A. B. Owen, “Better estimation of small Sobol’ sensitivity indices,” *ACM Transactions on Modeling and Computer Simulation*, vol. 23, no. 2, pp. 11–17, 2013.

[36] E. Myshetskaya, “Monte Carlo estimators for small sensitivity indices,” *Monte Carlo Methods and Applications mcma*, vol. 13, no. 5-6, pp. 455–465, 2008.

Zhanlin Liu received the B.S. degree in Statistics from University of Iowa, Iowa City, IA, USA, in 2014, and the M.S. degree in Statistics from the University of Washington, Seattle, WA, USA, in 2016. He is currently working toward the Ph.D. degree in Industrial & Systems Engineering at the University of Washington, Seattle, WA, USA. His current research interests include uncertainty quantification, reliability analysis, and statistical modeling.

Ashis G. Banerjee (S’08-M’09) received the B.Tech. degree in Manufacturing Science and Engineering from the Indian Institute of Technology Kharagpur, Kharagpur, India, in 2004, the M.S. degree in Mechanical Engineering from the University of Maryland (UMD), College Park, MD, USA, in 2006, and the Ph.D. degree in Mechanical Engineering from UMD in 2009. He is currently an Assistant Professor of Industrial & Systems Engineering and Mechanical Engineering at the University of Washington, Seattle, WA, USA. Prior to this appointment, he was a Research Scientist at GE Global Research, Niskayuna, NY, USA. Previously, he was a Research Scientist and Postdoctoral Associate in the Computer Science and Artificial Intelligence Laboratory at Massachusetts Institute of Technology, Cambridge, MA, USA. His research interests include digital manufacturing, predictive and prescriptive analytics, and autonomous robotics.

Youngjun Choe received the B.Sc. degrees in Physics and Management Science from KAIST, Korea in 2010, and both the M.A. degree in Statistics and the Ph.D. degree in Industrial & Operations Engineering from the University of Michigan, Ann Arbor, MI, USA in 2016. He is currently an Assistant Professor of Industrial & Systems Engineering at the University of Washington, Seattle, WA, USA. His research centers around developing statistical methods to infer on extreme events using empirical and simulated data.