Explainable Neural Network for Sensitivity Analysis of Lithium-ion Battery Smart Production

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***Abstract*—Battery production is crucial for determining the quality of electrode, which in turn affects the manufactured battery performance. As battery production is complicated with strongly coupled intermediate and control parameters, an efficient solution that can perform a reliable sensitivity analysis of the production terms of interest and forecast key battery properties in the early production phase is urgently required. This paper performs detailed sensitivity analysis of key production terms on determining the properties of manufactured battery electrode via advanced data-driven modelling. To be specific, an explainable neural network named generalized additive model with structured interaction (GAM-SI) is designed to predict two key battery properties, including electrode mass loading and porosity, while the effects of four early production terms on manufactured batteries are explained and analysed. The experimental results reveal that the proposed method is able to accurately predict battery electrode properties in the mixing and coating stages. In addition, the importance ratio ranking, global interpretation and local interpretation of both the main effects and pairwise interactions can be effectively visualized by the designed neural network. Due to the merits of interpretability, the proposed GAM-SI can help engineers gain important insights for understanding complicated production behavior, further benefitting smart battery production.**

***Index Terms*—Battery management, battery manufacturing, data science, explainable artificial intelligence, sensitivity analysis.**

I. Introduction

DUE to the merits of high energy density and low self-discharging rate, lithium-ion (Li-ion) batteries have established themselves as important components of modern energy systems for renewable energy storage and transportation electrification sectors [1]. However, a key step in limiting the wider application of Li-ion batteries relies on the understanding and improvement of their production [2]. As a highly complex chain, the production parameters within each stage of battery manufacturing directly affect the properties of intermediate products such as electrodes, which in turn significantly affects the manufactured battery performance. In this context, conducting an efficient sensitivity analysis of the battery production parameters is of utmost importance with regard to smart monitoring/control of battery production [3].

A production line for Li-ion batteries usually comprises numerous mechanical, electrical and chemical processes with many closely interlinked production parameters [4]. Battery engineers usually rely on experimental tests, trial and error to perform the sensitivity analysis of these parameters in the respective battery production line [5]. These solutions lead to high time and labor costs, inaccurate quality management, and challenges in monitoring/capturing the properties of the manufactured battery products in early production phases. Against this background, efficient strategies for reliably analysing production parameters and providing satisfactory early predictions of battery properties are urgently needed.

With the rapid development of artificial intelligence (AI) and automation technology, data-driven methods have become powerful tools in the field of battery management [6]. To date, numerous data-driven strategies have been developed for battery state estimation [7]−[9], ageing prediction under both cyclic conditions [10], [11] or storage conditions [12], [13], various faults diagnosis [14], [15], charging management [16], and energy management [17], [18]. In summary, efficient battery management can be obtained by developing suitable data-driven methods. However, in comparison with battery management, for which mature data-driven solutions are available, research into suitable data-driven methods for benefitting battery production is still relatively limited [19].

In the limited research into battery production, great attention is being paid to designing suitable data-driven methods for predicting the properties of inter-mediate or final battery products, and carrying out sensitivity analyses of interested production parameters [20]. For example, in [21], a decision tree-based data-driven solution is proposed to forecast battery capacity and analyse the relevant production features. Turetskyy *et al.* [22] propose a multi-output method based on data-driven model to capture the effects of inter-mediate production parameters on final battery properties. Niri *et al.* [23] propose a data-driven method to capture interdependency among

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key parameters of battery production and the electrical behavior of manufactured batteries. After designing tree-based models named random forest [24] and RUBoost ensemble learning [25], the dynamical effects of production variables and material parameters on the capacities of manufactured batteries are analysed, respectively. In [26], the data-driven models are designed to enable virtual production experiment for analysing the manufactured battery behaviors.

Although the above-mentioned studies provide several promising results in designing data-driven methods to benefit battery production, there still exist lots of limitations and challenges that require to be further enhanced, especially in the sensitivity analysis of the battery production process as: 1) Most studies simply adopt conventional machine learning approaches, such as support vector machine, to make only simple predictions on the properties of manufactured battery product. There is a lack of efficient sensitivity analyses of the involved production parameters that allow engineers to better understand their production lines. 2) Although several advanced machine learning tools with interpretability have been used to analyse the battery production process, their interpretability is still worthy of further exploration. To our best knowledge, limited data-driven studies are conducted to 1) Provide both global and local interpretations of how the variations of battery early-stage production terms dynamically affect the qualities and properties of battery inter-mediate or final product. 2) Identify and rank the importance ratio of both main effect and pairwise interaction terms simultaneously when using them to predict battery properties. In real battery production, engineers are very interested in obtaining the manufactured battery properties in the early production phase and understanding how the main effects and pairwise interactions of the production terms will specifically affect the relevant battery properties.

To overcome the above-mentioned limitations, this study proposes an explainable neural network based on the generalized additive model with structured interaction (GAM-SI) to predict battery electrode mass loading and porosity in its early production phase, while the sensitivity analysis of importance ratio ranking, global as well as local interpretations of interested production terms are also performed. Some contributions could be summarized as: 1) After identifying four key production terms from mixing and coating phases, an explainable neural network is derived to provide an early-stage prediction of two key battery electrode properties. 2) Through integrating three interpretability constraints, namely sparsity, heredity and marginal clarity, the GAM-SI's interpretability for identifying how the main effects and pairwise interactions derived from four production terms affect the corresponding electrode properties is well improved. 3) The prediction and sensitivity analysis performance of the designed GAM-SI model is comprehensively evaluated for both electrode mass loading and porosity. Obviously, the designed model is capable of pursuing a satisfactory balance between prediction accuracy and interpretability of production terms of interest. This is the first known application of designing GAM-SI-based explainable neural network to predict the performance of manufactured battery and to explain how the production terms in early production phases affect the properties of the respective electrode product. This could help engineers obtain critical insight, eventually resulting in closed-loop monitoring and optimization solutions for battery smarter production.

The rest of this paper is organized as follows. Battery production fundamental and several key production terms in early production phases are specified in Section II. Section III describes the GAM-SI structure and constraints, the GAM-SI interpretability, as well as the developed GAM-SI model and performance indicator. Section IV then details the prediction results of battery electrode properties, with an in-depth sensitivity analysis of the involved battery production terms of interest. Finally, Section V summarizes this study.

II. Battery Production Fundamental

The production of Li-ion battery belongs to a complex process involving both continuous and discrete stages. In general, the entire battery production line is mainly divided into electrode production, cell assembly, and cell formation [27]. Fig. 1 shows the battery production fundamental with some key inter-mediate phases especially for the production of the battery electrode. More specifically, the prepared electrode key materials are first mixed in a mixer to produce slurry in the mixing phase. After that, a coating phase is carried out to coat slurry on the surface of mental foil (copper foil for anode, while aluminum foil for cathode) by a coating machine. Then the coating product is calendered and dried several times to remove residual matter. Afterward, the electrodes can be obtained finally by cutting them into the correct shape. During cell assembly stage, all battery components such as the anode electrode, cathode electrode, and electrolyte are then assembled together to produce basic cell. After the formation phase, in which the solid electrolyte interphase (SEI) film is produced, the battery cell can finally be used in real applications. It should be noted that due to the highly complex production stages of battery, monitoring key electrode properties in the early battery production phases (i.e., mixing and coating) and analysing the effects of related production parameters are crucial and challenging. In this context, an efficient

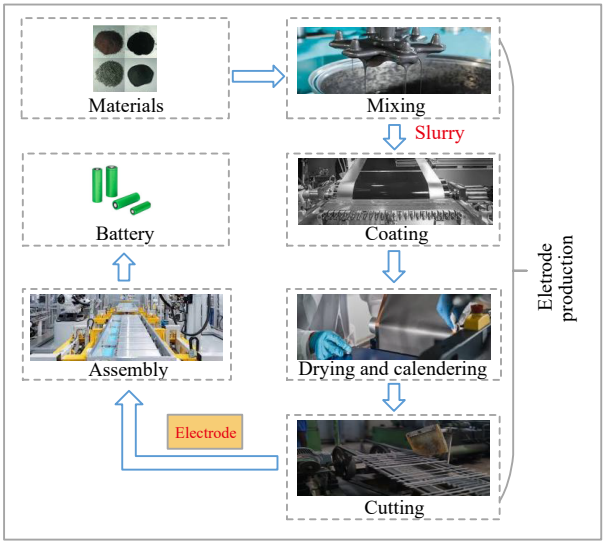

Fig. 1. Key production phases particular for battery electrode.

sensitivity analysis solution is urgently required for smarter battery production.

To design a reliable solution for achieving effective early prediction of electrode properties and sensitivity analysis of production parameters, several production parameter terms from battery key early production phases, including mixing and coating, are investigated. In addition, the sensitivity analysis of their impact on the prediction performance of the electrode properties will be performed. To be specific, the investigated production terms are three key production parameters named AM mass content, S-to-L ratio, viscosity from mixing phase and one key production parameter named Comma gap from coating phase. Here the S-to-L ratio is a ratio between the solids content of the slurry and the mass. Viscosity refers to the coating phase's shear rate. Comma gap is a gap between the comma and the coating roller. Without loss of generality, the real battery manufacturing dataset from the Franco Laboratoire de Reactivite-et-Chimie-des-Solides, whose effectiveness is well validated in [28] is explored. In the experiment, during the mixing stage, all the solid components of the slurry were blended together using a soft blender. N-methyl pyrrolidone (NMP) was then added until reaching the desired S-to-L ratio. The total mass of solid components was kept at 65 g. During the coating stage, all the electrodes were coated onto 22 μm aluminium foil, with the line speed of the Comma gap machine maintained at 0.3 m/min. Simultaneously, the size of the Comma gap was continuously adjusted to apply different shear forces during the coating process.

For the battery electrode properties, two key terms including electrode mass loading (unit is mg/cm^2) and porosity (unit is %) are explored in the study. From an engineering process perspective, both mass loading and porosity can reflect the production quality of electrodes, making them become crucial indicators to be considered in electrode manufacturing. Through the design of experiment, a total of eight sample points are obtained on each dried electrode, resulting in a raw dataset of 656 sample points. The rigorous experimental design ensures the reliability of the data set and thus provides favourable conditions for performing sensitivity analyses relevant to battery electrode production processes. For data preprocessing, after handling the outliers and missing points of the raw data collected, each set of eight samples from the same electrode is averaged to reduce random errors during the measurements, resulting in 82 observations. Besides, min-max normalization is used to eliminate scale discrepancies between different features while preserving original data distribution.

III. Methodology

This section first introduces the GAM-SI structure and related interpretability constraints. Then, three interpretable elements to perform explainable sensitivity analysis of battery production is described, followed by the elaboration of established GAM-SI model to predict electrode properties in the early battery production phase. In addition, three classical indicators to explore prediction performance are given.

A. GAM-SI Structure and Constraints

For the designed GAM-SI, it formulates a complicated functional relation by a low order representation involving non-linear main effect and pairwise interaction. Supposing S_1 is the set of main effect and S_2 is the set of pairwise interaction, the developed GAM-SI network can be derived as

$$G(E(y)|x) = \sum_{i\in S_1} f_i(x_i) + \sum_{(i,j)\in S_2} h_{ij}\left(x_i, x_j\right) + b \tag{1}$$

where b is intercept. $f_i(x_i)$ and $h_{ij}(x_i, x_j)$ are non-linear shape functions for main effects and pairwise interactions respectively, which are assumed to own zero mean as

$$\begin{cases} \int f_i(x_i)\, dF(x_i) = 0, & \forall i \in S_1 \\ \int f_{ij}\left(x_i, x_j\right) dF\left(x_i, x_j\right) = 0, & \forall (i,j) \in S_2 \end{cases} \tag{2}$$

where (i, j) and (j, i) refer to same pairwise interactions, $F(x_i)$ and $F(x_i, x_j)$are cumulative distribution functions. Here each $h_{ij}(x_i, x_j)$ is orthogonal to its main effects $f_i(x_i)$ and $f_j(x_j)$.

Fig. 2 illustrates the network structure of GAM-SI, which can be divided into two parts including the main effect module and pairwise interaction module. Based on this structure, each main effect $f_i(x_i)$ in (1) would be described through a sub-network containing an input-node, multiple hidden-layers and an output-node, while each pairwise interaction $h_{ij}(x_i, x_j)$ in (1) would be described by a sub-network containing two input-nodes. It is noteworthy that the main effects and the pairwise interaction effects do not share the weights. The main effects are trained first, followed by fitting the remaining residuals using pairwise interactions subnetworks. Then, all sub-networks will be linearly combined with an additional intercept term to capture the target output. To be more specific, the sub-networks of main effects and interactions will fit 1D curves and 2D surfaces, respectively. Here, the feedforward neural networks with a sufficient quantity of hidden nodes are utilized to approximate arbitrary curves or surfaces, while multi-layer sub-networks are adopted to capture different forms of shape functions. Moreover, one-hot encoding is utilized to preprocess categorical variables, which results in the sub-networks that capture the main effect of the categorical variable could be simplified to the multiple bias-nodes.

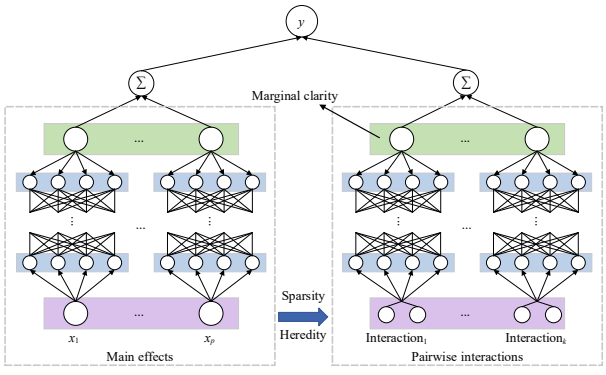

Fig. 2. Network structure of GAM-SI.

Besides, it should be noted that three interpretability constraints are assumed in the GAM-SI network, including sparsity, heredity, and marginal clarity. Here both sparsity and heredity constraints are used to improve model interpretabil-

ity, while marginal clarity constraint would be used to uniquely identify the main effect and pairwise interaction.

1) Sparsity-Constraint (S-C): Sparsity belongs to a key building block for the interpretation of well-trained GAM-SI model by removing unnecessary main and interaction impacts. Here, the importance of main effects and pairwise interactions could be quantified based on their variations. The i-th main effect's variation could be described by sample variance as

$$D(f_i) = \sum_{l=1}^{N} \frac{f_i^2\left(x_i^l\right)}{N-1} \tag{3}$$

where N refers to sample size, x_i^l is the x_i value of the l-th sample. In this study, the main effect function with small variations will be treated as trivial effect and enforced to be 0, leading to a sparse GAM-SI. Alternatively, GAM-SI selects the top s_1 main effect terms based on $D(f_i)$, as listed through the index-set S_1.

For pairwise interaction, its sparsity could be similarly obtained through selecting the top s_2 pairwise-interactions based on $D(h_{ij})$ defined by

$$D\left(h_{ij}\right) = \sum_{l=1}^{N} \frac{h_{ij}^2(x_i^l, x_j^l)}{N-1}. \tag{4}$$

Here the list of top s_2 pairwise interactions is denoted by index-set S_2. Both the indices of the sets S_1 and S_2 simply serve as representatives for each input feature to facilitate the implementation of the GAM-SI.

2) Heredity-Constraint (H-C): Apart from S-C, H-C is also important for capturing main effect as well as low to high order interactions. There generally exists two heredity principal versions including strong and weak heredities. In GAM-SI, the strong heredity and weak heredities respectively impose the constraints as

$$\begin{cases} \forall (i,j) \in S_2: & i \in S_1 \text{ and } j \in S_2 \\ \forall (i,j) \in S_2: & i \in S_1 \text{ or } j \in S_2. \end{cases} \tag{5}$$

In this way, the pairwise interactions could be contained by S_2 under conditions that both of or at least one of their parent main effects present strong heredity and are included by S_1.

3) Marginal-Clarity (M-C): In GAM-SI, main effects or pairwise interactions are assumed to own zero mean, which can cause model prediction to become unstable and affect model interpretation. In this context, M-C constraint is adopted to improve GAM-SI identifiability. Here the orthogonality condition of i-th main effect term and related pairwise interaction term (i, j) is described by

$$\int f_i(x_i) h_{ij}\left(x_i, x_j\right) dF(x) = 0 \tag{6}$$

where $F(x)$ refers to joint cumulative distribution function. Then the non-orthogonality degree could be derived by

$$\Omega\left(f_i, h_{ij}\right) = \left| \frac{\sum f_i(x_i) h_{ij}\left(x_i, x_j\right)}{N} \right|. \tag{7}$$

Here lower $\Omega(f_i, h_{ij})$ reflects that the marginal effects f_i can be separated from their child-interaction h_{ij} more clearly. In real applications, $\Omega(f_i, h_{ij})$ would be slightly larger than zero. In this context, for GAM-SI, to pursue marginal clarity, the non-orthogonality will be penalized for all $i \in S_1$ and their related child-interaction $(i, j) \in S_2$.

On the basis of all interpretability constraints, GAM-SI model can be built through handling the following optimization issue as:

$$\begin{cases} \min\limits_{\theta} \mathcal{L}_\lambda(\theta) = l(\theta) + \lambda \sum\limits_{i \in S_1} \sum\limits_{(i,j) \in S_2} \Omega\left(f_i, h_{ij}\right) \\ \text{s.t.} \int f_i(x_i)\, dF(x_i) = 0, \qquad \forall i \in S_1 \\ \qquad \int h_{ij}\left(x_i, x_j\right) dF\left(x_i, x_j\right) = 0, \qquad \forall (i,j) \in S_2 \end{cases} \tag{8}$$

where the main effects S_1 active set and pairwise interaction S_2 active set would be obtained subject to S-C and H-C respectively. The empirical loss $l(\theta)$ would be determined by the model tasks (i.e., classification or regression). The second term in (8) refers to the regularization of marginal clarity, which strength is determined by $\lambda \geq 0$.

B. GAM-SI Interpretability

For the GAM-SI network, three interpretable elements can be obtained intrinsically as:

1) Importance-Ratio (I-R): Based upon a well-trained GAM-SI model, the effects and contributions of each production term of interest to the predicted battery properties (electrode mass loading and porosity) can be quantified by I-R. Here individual variables include both individual battery production terms and their pairwise interactions. For the individual battery production terms, the I-R of each term could be quantitatively obtained by

$$IR(i) = \frac{D(f_i)}{D} \tag{9}$$

where $D = \sum_{i \in S_1} D(f_i) + \sum_{(i,j) \in S_2} D(h_{ij})$. By the same way, the I-R of pairwise interactions could be also quantified as

$$IR(i,j) = \frac{D\left(h_{ij}\right)}{D}. \tag{10}$$

Based upon the above solution, I-R for all terms can be obtained and would add up to 1. Then the importance of each term on determining battery properties can be ranked in decreasing order based on I-R values. Theoretically, the greater the I-R value, the more important the production term.

2) Global-Interpretation (G-I): Apart from quantifying the importance of each production term, the relation between individual production terms or production term pairs and the properties of interest for manufactured battery electrode can be analysed by visualizing their fitted shape function. Here, the 1D line chart and the bar chart are utilized to explain the inputs-output relationships for numerical and categorical variables, respectively. The plots would be obtained by using the final predictions of $f_i(x_i)$ for $i \in S_1$. The relationships here could be linear, monotonic and in other forms. In addition, in order to explain the joint effects of two underlying battery production terms, a 2D heatmap will be also utilized for visualizing each predicted pairwise interaction.

3) Local-Interpretation (L-I): According to the well-trained

GAM-SI model, the prediction of battery production properties can also be explained locally, resulting in a clear decision-making process. Specifically, for a sample of insterest, the GAM-SI model can output not only a prediction, but also the corresponding function form with respect to the inputs within the sample. In this way, the value of additive components, such as the effects of individual and pairwise interactions, could be quantified. Subsequently, the decision for inputs could be concretely understood by sorting the quantified effect values. Moreover, the sensitivity analyses of the predicted battery properties with respect to the small variation of the explanatory production term could be performed by visualizing the corresponding 1D line chart or 2D heat map.

C. GAM-SI Model and Performance Indicator

1) GAM-SI Model: In the battery production line, two key phases, namely mixing and coating, are crucial to determine the properties of the manufactured electrode, which in turn significantly influence the final battery performance [29]. To perform an efficient sensitivity analysis of the interested feature terms in battery production line, the GAM-SI model with a structure in Fig. 3 is developed in this study. Here the inputs include three feature terms named AM mass content, S-to-L ratio and viscosity from mixing phase, and one feature term named Comma gap from coating phase. Meanwhile, two key properties of battery electrode, namely mass loading and porosity, are used as GAM-SI model's output, respectively.

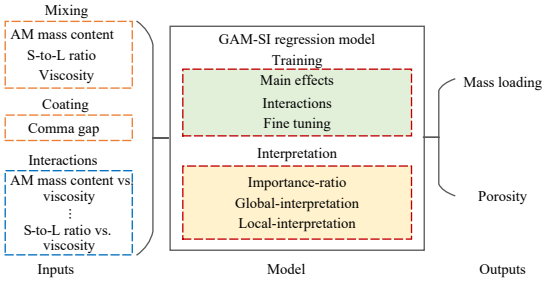

Fig. 3. GAM-SI model for the sensitivity analysis of battery production.

a) All sub-networks of main effect will be trained first for a few epochs, while trivial main effects would be pruned based upon their contribution and validation performance.

b) Then, the most K pairwise interactions will be selected for training, while trivial pairwise interactions are removed based on their contribution and validation performance.

c) After phases 1) and 2), all network parameters for some epochs will be fine-tuned.

2) Performance Indicators: To explore the performance of designed GAM-SI model for electrode properties prediction at early production stages, three efficient indicators are adopted.

a) Mean absolute error (MAE): Supposing N is the total number of electrode property points predicted from GAM-SI model, Y_n and $\widehat{Y}_n$ respectively refer to the real electrode property points and the predicted property points, then MAE could be obtained as

$$MAE = \frac{1}{N}\sum_{n=1}^{N}\left|Y_n - \widehat{Y}_n\right|. \tag{11}$$

b) Root mean square error (RMSE): Through using the same definition, RMSE can be obtained by

$$RMSE = \sqrt{\frac{1}{N}\sum_{n=1}^{N}(Y_n - \widehat{Y}_n)^2}. \tag{12}$$

For battery electrode properties prediction, when predicted property points well match real property values, the MAE and RMSE would be closed to 0.

c) Average execution time (AET): The AET is adopted to reflect the computational effort of developed model during cross-validation process. In this study, the unit of AET is second (s) for training GAM-SI models.

IV. Result and Discussion

To carry out sensitivity analysis including importance ratio quantification, global and local interpretations for the effects of early-stage production terms on electrode properties, the developed GAM-SI model is adopted to predict manufactured battery electrode mass loading and porosity in this section.

A. Analyses of Battery Electrode Mass Loading

In this test, according to the structure shown in Fig. 3, four battery production terms, including AM mass content, S-to-L ratio, viscosity, and Comma gap, are used as inputs of the GAM-SI model, while the mass loading of the manufactured battery electrode is taken as the output of the model. The detailed results, including the training and validation results, as well as sensitivity analyses of I-R, G-I, and L-I are then presented and discussed.

1) Training and Validation Analyses: Fig. 4 illustrates the GAM-SI training as well as validation losses for mass loading case. It could be noted that both these two types of losses decrease dramatically during the training stage of main effects, while they continue to reduce further by adding pairwise interactions to the GAM-SI. Specifically, there are large jumps for both training and validation losses in the first half of the tuning process, which are mainly due to the pruning of trivial pairwise interactions. It can be observed that the training loss and validation loss finally stabilize around 0.003 during the fine-tuning stage. In 20 times repeated training, GAM-SI can converge within 800 epochs consistently. Fig. 5 shows the validation loss for determining the optimal values of both main effects and pairwise interactions. Here, the x-axis refers to the number of main effects or pairwise interactions that need to be included in GAM-SI model, while the red star marks the best number value. Quantitatively, for mass load-

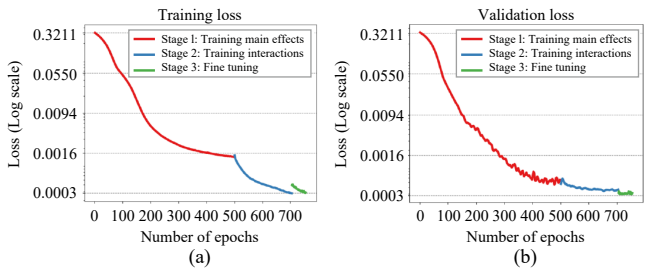

Fig. 4. GAM-SI training and validation losses for mass loading case.

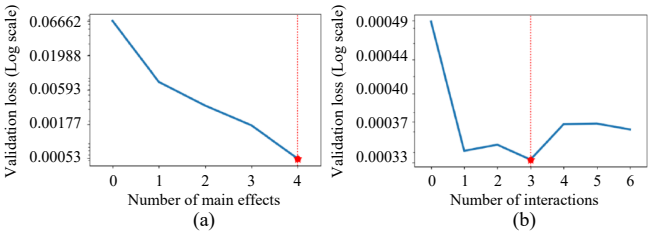

Fig. 5. Validation loss for determining s_1 and s_2 for mass loading case.

ing case, the best number are four and three for the main effect and interaction terms included in GAM-SI model, as the validation losses decrease below 0.0053 and 0.0034, respectively. Thereafter, the benefit of adding further main effects or pairwise interactions derived from battery production terms would be negligible.

2) I-R Analyses: For battery electrode mass loading prediction, after well-training relevant GAM-SI model, the quantified I-R ranking for all main effect and pairwise interaction terms could be obtained and are shown in Fig. 6. Obviously, the main effect terms make a greater contribution to the electrode mass loading prediction than the pairwise interaction terms. Specifically, for main effect terms, Comma gap presents the most important contribution, as its I-R value reaches 91.3%. This result is as expected since Comma gap has a significant influence on the weight and thickness of the coating, while these coating properties determine to a large extent the mass loading of the battery electrodes. The S-to-L ratio provides the second most important contribution with an I-R value of 4.4%, which is 62.9% and 34.0% larger than those of viscosity and AM mass content respectively. In comparison, the I-Rs of pairwise interaction terms are relatively low with a total value of 0.6%, indicating that the mass loading is mainly determined by four main effect terms.

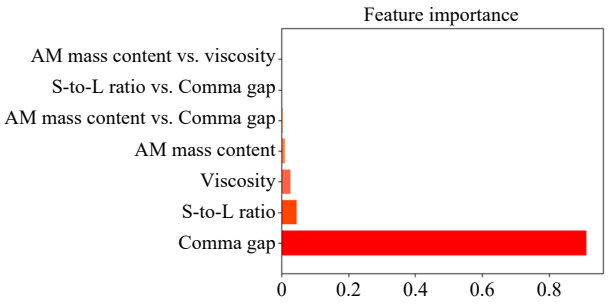

Fig. 6. Importance ratio ranking for mass loading case.

3) G-I and L-I Analyses: To provide a more comprehensive understanding of the influence of main effects and pairwise interactions on the prediction of electrode mass loading, both the global and local interpretations of the GAM-SI model for the mass loading case are depicted in Figs. 7 and 8, respectively. Leveraging the GAM structure of GAM-SI, the model captures the contribution of each feature to the output. In Fig. 7, the *x*-axis illustrates the distribution of sample data, while the *y*-axis describes the contribution of each feature. The higher the I-R value of the battery production term, the wider the range of the contribution that the term can make to the predicted electrode mass loading. It is interesting to note that for all individual main effects, increasing their term value first reduces the negative contributions and then increases positive contributions to the battery electrode mass loading. For example, for Comma gap with a largest I-R, its negative contribution initially decreases from 0.4 to 0 when its term value is increased from 100 to 200. Thereafter, the positive contribution gradually increases as the Comma gap becomes greater than 200. For AM mass content, when its value increases from 93 to 94, its negative contribution remains almost the same. In addition, the pairwise interaction effects can be also captured by pairwise interaction subnetworks. Within the features influencing mass loading, pairwise interaction effects also play a role. For example, in Fig. 7(e), AM mass content × Comma gap term demonstrates that positive contributions to the outcome occur only when both values fall within the red region in the figure. This indicates that, in the process of battery electrode production, besides main effects, the interactions between different features also need to be considered.

Next, a sample point of mass loading prediction is randomly selected for the local interpretation of the well-trained GAM-SI model, as shown in Fig. 8. The contributions of all features on this sample are displayed, with each corresponding to a subnetwork in the model. It is notable that the contributions of four main effects, three pairwise interactions, as well as the intercept are well determined, enabling the GAM-SI model to provide a satisfactory prediction result for the local mass loading point with an absolute error of 0.0095. These facts signify that electrode mass loading could be well captured by four production terms in battery early production phases.

B. Analyses of Battery Electrode Porosity

In this test, the sensitivity analyses of battery electrode porosity are performed. The inputs here are the same as those of mass loading test, while the output is electrode porosity.

1) Training and Validation Analyses: Fig. 9 shows the training and validation losses of the GAM-SI model for the case of battery electrode porosity. For the electrode porosity, both the training and validation losses reduce significantly to 0.00982 and 0.01763 when main effects are added to the network. During the training phase of pairwise interaction, the losses will be slightly adjusted. Finally, the training loss and validation loss stabilize around 0.00963 and 0.01763 respectively during the fine-tuning stage. In 20 times repeated training, GAM-SI can converge within 500 epochs consistently. Fig. 10 further shows the validation loss for the determination of s_1 and s_2 in the case of porosity. Here, the optimal number of main effects is still four, while the optimal number of pairwise interactions becomes two. Further adding more interaction terms from battery production would even cause the validation loss increase from 0.01644 to 0.01653. In this context, $s_1 = 4$ and $s_2 = 2$ are adopted in the GAM-SI model for the case of battery electrode porosity.

2) I-R Analyses: The values of the importance ratio of the main effect involved and pairwise interaction terms for the case of electrode porosity are listed in Fig. 11. The indicators show that for main effects, S-to-L ratio and viscosity here

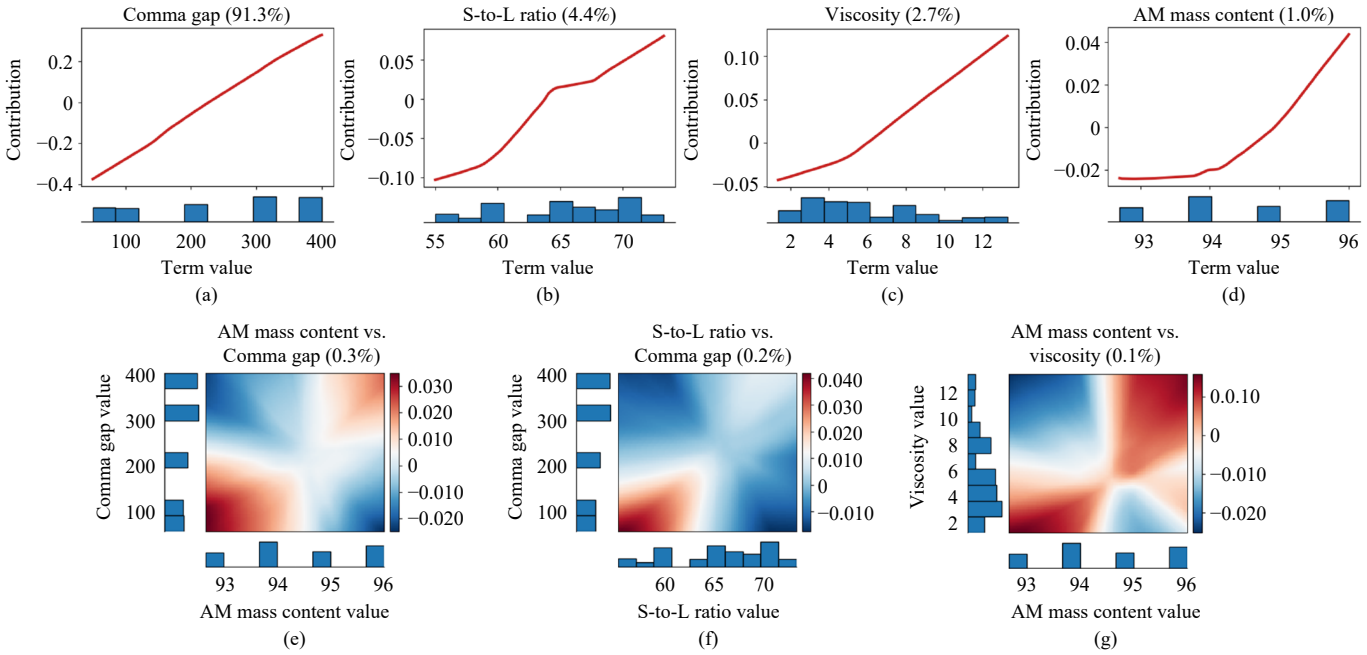

Fig. 7. Global interpretation of GAM-SI for mass loading case.

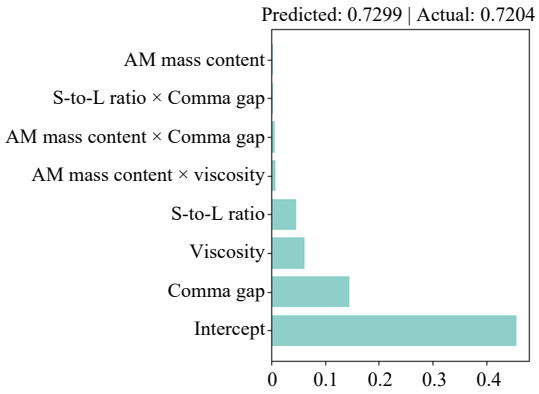

Fig. 8. Local interpretation of GAM-SI for mass loading case.

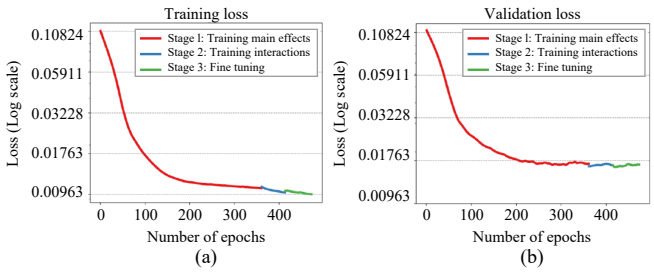

Fig. 9. GAM-SI training and validation losses for porosity case.

become the most two important terms, while AM mass content is the least important term. Theoretically, this is reasonable as the physical property of the electrode, such as porosity, is difficult to be affected by the mass content of active material. In comparison, the importance ratio values of two pairwise interaction terms are much lower than those of main effect terms, indicating that electrode porosity predictions are mainly determined by four related main effect production terms.

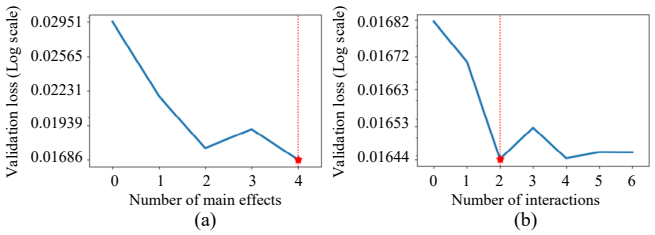

Fig. 10. Validation loss for determining s_1 and s_2 for porosity case.

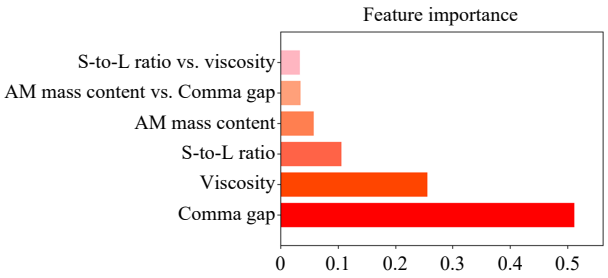

Fig. 11. Importance ratio ranking for porosity case.

3) G-I and L-I Analyses: Next, based upon the well-trained GAM-SI, the global interpretation for the case of battery electrode porosity is illustrated in Fig. 12. For the most important main effect term S-to-L ratio, an increase in its value first leads to a decrease in the associated positive contribution to 0 at 67.5 point and then to an increase in the associated negative contribution to 0.05 at 68.2 point. Thereafter, a further increase in the S-to-L ratio has little influence on the change in the contribution. Interestingly, an increase in the values for the other three main effect terms would first reduce the positive contributions and then increase the negative contributions up to the maximum points. Thereafter, the negative contributions are reduced with the increase of term values. According to the pairwise interaction diagrams shown in Figs. 12(e) and

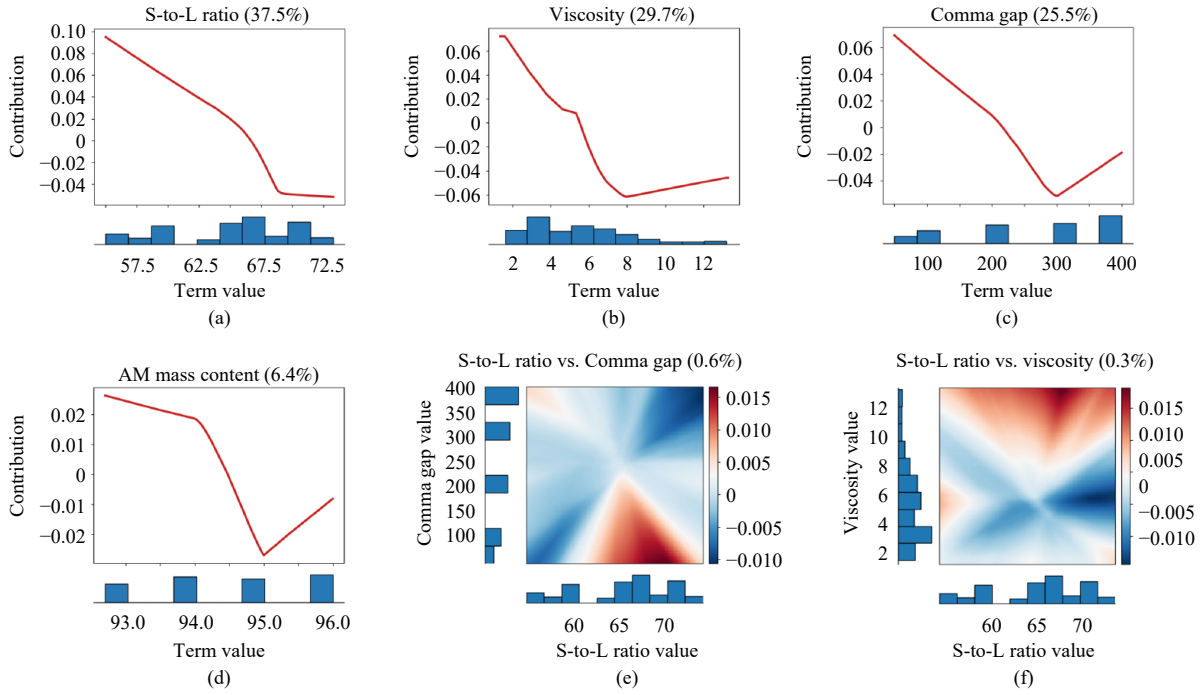

Fig. 12. Global interpretation of GAM-SI for porosity case.

12(f), high S-to-L ratio and low Comma gap, high S-to-L ratio and Viscosity could give additional positive contribution to the prediction of battery electrode porosity.

For L-I analysis, Fig. 13 illustrates a sample point of the electrode porosity prediction to perform a local interpretation of the well-trained GAM-SI model. Differently from mass loading sample point case, here the three terms including Viscosity, Intercept, and S-to-L ratio × Comma gap make positive contributions while the other four terms make negative contributions to the determination of sample point of electrode porosity. Besides, an acceptable absolute error of 0.0017 is achieved here, indicating that electrode porosity is also well predicted by the contributions of the mixing as well as coating terms in battery early production stages.

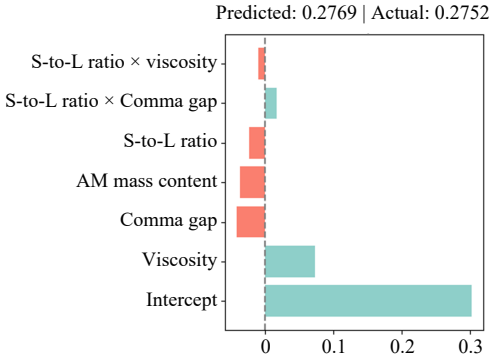

Fig. 13. Local interpretation of GAM-SI for porosity case.

C. Comparison Analysis

To further explore the effectiveness of our designed GAM-SI model for electrode properties prediction in the early stages of battery production, three other classical data-driven methods including decision tree (DT), support vector regression (SVR), and Gaussian process regression (GPR) are adopted as benchmarks for comparison analysis. To ensure a fair comparison, all these methods are derived by using a 2.60 GHz Intel Pentium 4 CPU. To be specific, DT is a classical data-driven method based on the classification and regression tree [30]. Both SVR and GPR are kernel-based methods for transferring inputs from the low-dimensional space to the high-dimensional space for regression [12], [31]. Without loss of generality, the classical and effective squared-exponential kernel is adopted for SVR and GPR in this study. To quantify the prediction accuracy and computational effort of these methods, three key performance indicators including MAE, RMSE, and AET are used in the comparison studies.

After performing a five-fold cross validation, the comparison results of these data-driven methods are summarized and shown in Table I, where bold values refer to the best results. It can be seen that DT provides the smallest AET for both electrode mass loading and porosity cases, but its MAE and RMSE values are the worst. This is reasonable as the structure of DT is the simplest to be trained but its capability to capture highly non-linear conditions like electrode mass loading and porosity is limited. In comparison, our proposed GAM-SI gives the best prediction performance for all electrode properties. For the case of mass loading, GAM-SI's RMSE is 0.09% and 2.71% better than that of GPR and SVR, respectively. For the porosity case, its RMSE is 13.26% and 15.31% better than those of GPR and SVR, respectively. This indicates that more other battery production terms are suggested to be considered for further improving prediction performance of electrode porosity. In addition, the AET of GAM-SI for both mass loading and porosity are within 8.5s, leading to a satisfactory computational effort. These facts show that our designed GAM-SI is capable of providing competent performance to efficiently predict battery electrode properties by using production terms in the battery early production phases.

TABLE I
PREDICTION RESULTS USING DIFFERENT METHODS

Mass loading			
Method	MAE (mg/cm^2)	RMSE (mg/cm^2)	AET (s)
DT	1.135	1.403	**7.5**
SVR	0.993	1.181	8.2
GPR	0.908	1.150	8.4
GAM-SI	**0.901**	**1.149**	8.1
Porosity			
Method	MAE (%)	RMSE (%)	AET (s)
DT	2.117	2.992	**7.1**
SVR	1.904	2.743	7.8
GPR	1.892	2.678	7.9
GAM-SI	**1.874**	**2.323**	7.7

V. CONCLUSION

As battery production is of great importance for determining battery performance, the efficient sensitivity analysis of battery production terms is significantly needed. This study proposes an explainable neural network named GAM-SI to not only predict battery electrode properties at battery early production phases but also carry out sensitivity analysis of four key production terms of interest. The importance ratio ranking, global and local interpretations of the main effects and pairwise interactions from four battery early-production terms (AM mass content, S-to-L ratio, viscosity, and Comma gap) on the predictions of electrode mass loading as well as porosity are performed and analysed. Illustrative results demonstrate that the developed GAM-SI is able to perform satisfactorily in predicting the electrode properties and sensitivity analysis of the production terms of interest. The developed method makes the sensitivity analyses of battery production more interpretable and provides a convenient alternative for early prediction and monitoring of manufactured battery properties, especially for the battery production chain in which there are strongly coupled mechanical, electrical and chemical parameters. This can significantly benefit the monitoring and control of the production chain to achieve smarter battery production. For example, due to the merits of data-driven nature and good interpretability, after collecting proper battery production data, engineers could conveniently adopt this GAM-SI-based method to carry out effective sensitivity analysis of the production terms of interest and monitor battery properties in the early production phases. Here to overcome the practical challenge of generating available database for battery production with low cost, the 'design of experiments' solution is suggested [32], in which the areas of the database are defined and it is ensured that there are also sufficient breakpoints between the individual control variables. Moreover, engineers can control and adjust the slurry composition or coating parameters based on the early predictions without the need for time-consuming trial and error testing, or detect defective products based on the corresponding local interpretation results from GAM-SI.

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