Jacobian of Generative Models for Sensitivity Analysis of Photovoltaic Device Processes

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Abstract

Modeling and sensitivity analysis of complex photovoltaic device processes is explored in this work. We use conditional variational autoencoders to learn the generative model and latent space of the process which is in turn used to predict the device performance. We further compute the Jacobian of the trained neural network to compute global sensitivity indices of the inputs in order to obtain an intuition and interpretation of the process. The results show the outperformance of generative models compared to discriminative models for learning device performance in our task. Furthermore, comparison of the results with sampling-based sensitivity analysis methods demonstrates the validity of our approach and the interpretability of the learned latent space.

1 Introduction

Process design and optimization is a key component in Materials Science and Engineering. This often requires expensive resources, equipment and time, and thus, many approaches such as design of experiments [11], Bayesian optimization [29], genetic algorithms [32] and particle swarm optimization [13] have been utilized in the field in order to efficiently minimize the number of experiments [28]. From another perspective, machine learning can be used to capture the underlying complex functions of computationally expensive simulations or real-world experiments in order to potentially replace them as a surrogate optimization function.

This work proposes a unifying framework for learning a complex process function while providing intuitive interpretations based on the sensitivity analysis of model outputs with respect to its inputs. We propose to use generative models, namely conditional variational autoencoders (CVAE)[15, 31], to learn the latent space of the solar cell device performance conditioned on the material variables. Furthermore, we use the Jacobian of the trained neural network to obtain the derivative of the model outputs with respect to the conditions and latent variables and we show that the Jacobian can be interpreted as the sensitivity index of outputs (solar cell performance) with respect to the inputs (material variables) by validating with a sampling-based sensitivity analysis approach [30, 21]. The significance of sensitivity analysis is that it gives a better intuition of the underlying engineering process that can further help to understand or design the real-world experiments. Figure 1 shows an overview of our method.

We focus on solar cells, a photovoltaic device, whose performance depends on a series of sequential processes, each being a function of various material properties mainly governed by manufacturing parameters, intrinsic characteristics and solar cell architectures. In addition, from the device-design point of view, solar cells can consist of a different number of layers; as these processes and layers are entangled in a complicated fashion, predicting the outcome is only feasible through high fidelity and expensive simulators [9, 1]. However, given a substantial amount of simulated data, machine

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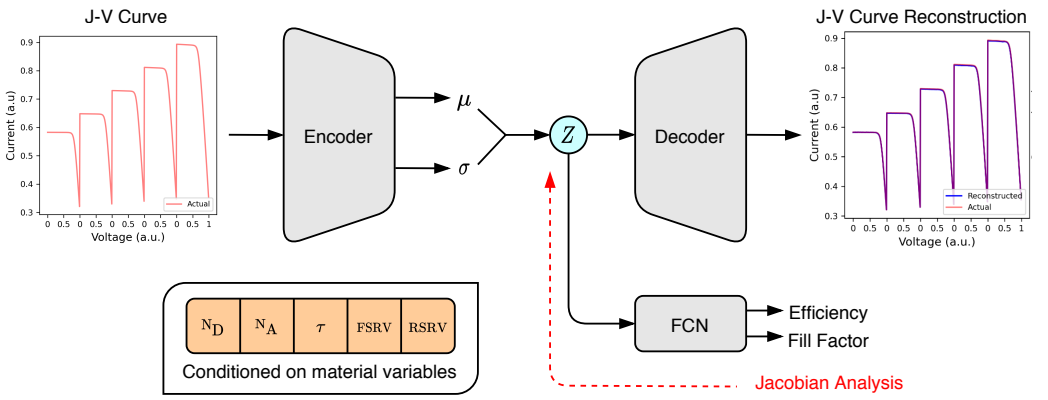


Figure 1: Diagram of our proposed learning framework. The conditional variational autoencoder (CVAE) is trained to reconstruct *J-V* curves conditioned on the material variables. A fully-connected neural network is also trained simultaneously to predict the quality of the solar cell given the latent variables and conditions. Finally, the Jacobian of its outputs are computed with respect to its inputs to obtain the sensitivity indices.

learning models can learn a generative model of the simulation that, in principle, can substitute the simulator as a faster and more efficient tool.

We develop and evaluate our approach on a publicly available simulated dataset of Gallium arsenide (GaAs) based solar cells[24]. The knowledge and methodology in solar cells can be easily translated to other multi-layer energy materials and semiconductors, such as light-emitting diodes, power electronics, batteries, and transistors [24]. Therefore, we believe that our machine learning based sensitivity analysis method can be generalized to their respective design and optimization processes as well. Thus, the main contributions of this work are:

- **Generative modeling** of the complex process model of solar cell device performance for learning a meaningful latent space. We show that generative models have better performance compared to discriminative models for this task.
- **Jacobian analysis** of neural networks for sensitivity analysis of process models with respect to the input parameters (materials variables). We further demonstrate that Jacobian analysis through the latent space can provide reliable sensitivity indices which can be used to get a better intuition about the process for efficient process design.

2 Related Work

Machine Learning for Energy Materials Design. Machine learning has received considerable attention in the process design and optimization of energy materials. Stability prediction [17, 2], chip placement [19], material properties (e.g., bandgap) identification [23, 8], and performance prediction [24, 12, 22] are a few examples. In addition to the application of machine learning in design and optimization, it has been employed in material characterization for image-based identification of material structures [5, 33] and defect detection [4]. This is particularly useful in the field of semiconductors where defect engineering is a crucial component of manufacturing.

An application of Bayesian inference networks coupled with a surrogate neural network function for optimization of GaAs-based solar cells has been studied in [24]. The surrogate function is a discriminative model followed by a denoising autoencoder and is trained on the simulated data. However, our method learns a conditional generative model of the dataset and instead of optimizing the device performance, we use the Jacobian of the trained model for sensitivity analysis and improved interpretability.

Sensitivity Analysis. Sensitivity analysis evaluates the contributions of the inputs of a model to the uncertainty of its outputs [26]. Global sensitivity indices can be obtained using sampling-based methods [30, 26, 3] that are coupled with carefully designed sampling schemes [25, 21]. However,

it has been established that the partial derivative of a function, while local, can be interpreted as a sensitivity index if averaged over a range of the input variables. [16]. In neural networks, sensitivity analysis can provide a toolset for interpreting and understanding the learning process [7, 20, 27] and thus, from an applied view, it can give us a more intuitive explanation of the engineering problem.

3 Methods

We present a learning framework for the generative modeling of design processes in engineering domains and further show how the Jacobian of the neural network computed from its outputs with respect to the latent space can provide reliable sensitivitiy indices. This section describes the underlying methods.

3.1 Generative Modeling of Engineering Processes

Generative latent variable models learn the joint probability of distribution of the data $\mathcal{X}$ and the unobservable latent variables $\mathcal{Z}$ in the form of $p_\theta(x, z) = p_\theta(z)p_\theta(x|z)$ where $p_\theta(z)$ is the prior on the latent variable and $p_\theta(x|z)$ is the conditional distribution. The marginal likelihood of the data can be obtained by integrating the joint distribution $p_\theta(x, z)$ over the latent space $\mathcal{Z}$ as:

$$p_\theta(x) = \int p_\theta(z)p_\theta(x|z)dz. \tag{1}$$

However, since the integration and the true posterior $p_\theta(z|x)$ are intractable, variational autoencoders (VAE) [15] use the inference network $q_\phi(z|x)$ as an approximation to the true posterior. Thus, rewriting the marginal likelihood gives us the evidence lower bound (ELBO) as:

$$\text{ELBO}(x) \triangleq -\text{KL}(q_\phi(z|x)||p_\theta(z)) + \mathbb{E}_{q_\theta(z|x)}[\log\, p_\theta(x|z)], \tag{2}$$

where the first term is the Kullback-Leibler divergence between the true and approximate posteriors and the second term denotes the reconstruction loss. VAE models are trained via minimizing the ELBO loss.

Since the processes in engineering are often defined based on certain conditions, we propose to use conditional variational autoencoders (CVAE) [31] to essentially condition the ELBO loss as:

$$\text{ELBO}(x|c) \triangleq -\text{KL}(q_\phi(z|x, c)||p_\theta(z|c)) + \mathbb{E}_{q_\theta(z|x,c)}[\log\, p_\theta(x|z, c)], \tag{3}$$

where c is the condition. In this paper, as depicted in Figure 1, the inputs to the CVAE model are the *J-V* curves of solar cell simulations and the conditions are the material variables.

3.2 Regression on the Latent Space

Increasing the efficiency[1] and to a lesser extent the fill factor[2] of solar cells are the main objectives in their design and optimization. These two figures of merit can be obtained from the *J-V* curve. However, instead of predicting these values directly from the high-dimensional data of the *J-V* curve, we use the conditional latent space of the CVAE which has a compact, lower-dimensional representations of the curves. Thus, we train a fully connected neural network whose inputs are the latent variables concatenated by the conditions (material variables) and its outputs are solar cell efficiency and fill factor, as shown in Figure 1.

3.3 Sensitivity Analysis of Neural Networks

Sensitivity analysis studies how the uncertainty in the output of a model can be apportioned to its inputs [30]. To obtain the sensitivity indices of material variables in the process model, here we use

[1] Power efficiency or energy conversion efficiency is defined as the fraction of the output power to the input power. Usually the reported efficiencies are conducted under Air Mass of 1.5 input illumination intensity.

[2] Fill factor is defined as the fraction of the maximum power point to the power obtained from multiplication of open circuit voltage and short circuit current. It represents the quality of p-n junctions and resistances within solar cell devices and can be driven from the *J-V* curves.

the Jacobian of the trained neural network [7, 20] which is defined as the partial derivative of its outputs with respect to its inputs evaluated at datapoint x^* as:

$$J_{ij}(x^*) = \frac{\partial}{\partial x_j} f_i(x)\Big|_{x^*}. \tag{4}$$

In other words, $J_{ij}(x^*)$ measures the sensitivity of output i with respect to the input j in the local vicinity of x^*. This method is more efficient compared to sampling-based sensitivity analysis, since the Jacobian of neural networks is readily available through automatic differentiation. However, the Jacobian matrix only gives local sensitivity analysis, therefore, to obtain a global sensitivity index, we measure the mean of the square of the Jacobian matrices evaluated over all points during the training and testing of the network. We further validate that, as shown in [16], the derivative-based sensitivity indices are well-aligned with sampling-based global indices.

In this work, we perform the Jacobian analysis to obtain the sensitivity of solar cell efficiency and fill factor with respect to material variables on the fully connected network that was trained on the latent space of the CVAE.

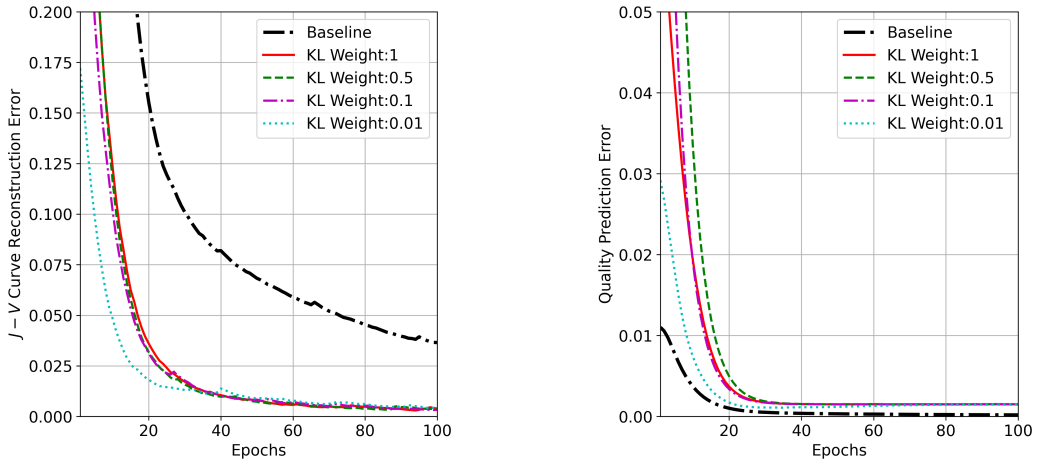
4 Evaluation

This section describes our experimental setup for evaluation of the proposed methodology for learning generative models and analyzing the sensitivity of synthesis processes.

4.1 Experimental Setup

Dataset. We use the simulated GaAs-based solar cell dataset published in [24]. The dataset consists of the current density versus voltage (*J-V*) curves of randomly sampled five material variables—donor doping concentration in the bulk (Si as the dopant, N_D), acceptor doping concentration in the emitter (Zn as the dopant, N_A), bulk lifetime (minority carriers lifetime, τ), and front and rear recombination velocities (FSRV and RSRV)—common in solar cell design. The dataset has been generated using the PC1D simulator [9] designed for studying photovoltaic device characteristics.

We further extend the simulated dataset by obtaining the efficiency and fill factor of each data point from the *J-V* curves using physics-based equations [6]. As these values are often used to describe the overall quality of a solar cell device, the sensitivity analysis is carried out with respect to them. The



(a) Reconstruction error of solar cell *J-V* curves.

(b) Prediction error of solar cell qualities.

Figure 2: Comparison of mean squared error (MSE) of CVAE and a discriminative model for learning solar cell process functions obtained on the validation dataset. The baseline in both plots is an MLP trained for regression of the output. (a) Reconstruction error of solar cell *J-V* curves conditioned on material variables. (b) Prediction error of solar cell qualities (fill factor and efficiency) using the conditional latent space of the CVAE.

Table 1: Comparison of mean squared error (MSE) of CVAE and MLP for *J-V* reconstruction and quality prediction obtained on the final epoch on the validation dataset.

KL Weights	CVAE 0.01	CVAE 0.1	CVAE 0.5	CVAE 1	MLP
***J-V* Reconstruction Error** $(\times 10^3)$	3.825	3.748	3.746	**2.807**	36.07
Quality Prediction Error $(\times 10^3)$	1.452	1.529	1.478	1.487	**0.178**

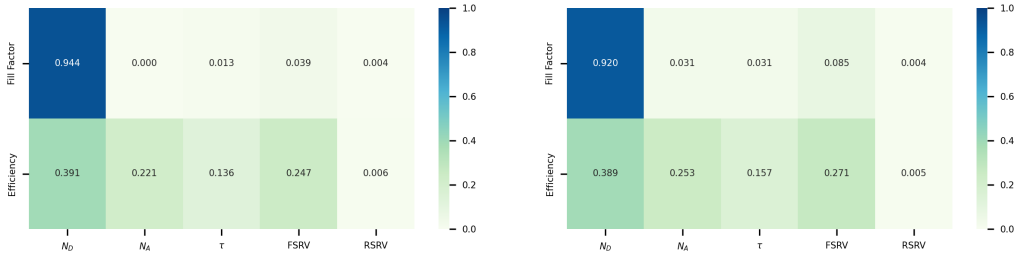
dataset is composed of 20,000 datapoints from which 80% have been used for training and the rest for validation.

Implementation Details. We implemented our models in PyTorch and took advantage of its automatic differentiation [22] to compute the Jacobian matrices. The encoder and decoder architectures in the CVAE model are 256×256 fully-connected networks and the latent space has 4 dimensions. To keep the baseline method, multilayer perceptron (MLP) for regression, consistent with the CVAE model, we used an MLP network with 256×256 hidden layers. We trained all models using the Adam optimizer [14] with a learning rate 0.001 and batch size 64. Finally, we used the Python library SALib [10] for sampling-based sensitivity analysis for the validation of our results.

4.2 Prediction Performance

We compare the performance of our method in terms of *J-V* curve reconstruction and solar cell quality prediction with the baseline. The baseline model is a multiplayer perceptron (MLP) that gets material variables as inputs and is trained simply as a discriminative model. Figure 2a shows the evaluation of CVAE models with different weights for the KL term in the loss function. The results show that the conditional generative modeling of the process function significantly outperforms the baseline in predicting the *J-V* curves by jointly learning the latent space. This shows that, in this study, the generative latent variable models have better performance and generalization compared to discriminative models in learning complex process functions.

Our proposed framework simultaneously trains a fully-connected network on the latent space for predicting solar cell quality. Figure 2b compares its quality prediction with the baseline model. Although the baseline is learning a much simpler task of mapping the material variables (5 dimensional data) to solar cell qualities (2 dimensional), our model provides a competitive performance, thus demonstrating the interpretability of its latent space. It is also worth mentioning that the *J-V* reconstruction is a much more important task for the model to achieve good performance since that essentially enables it to replace the simulator as a surrogate function. Table 1 presents a quantitative comparison of the CVAE models with different KL weights and the MLP baseline model.



(a) Jacobian based sensitivity analysis.

(b) Sampling based sensitivity analysis.

Figure 3: Normalized sensitivity indices of solar cell fill factor and efficiency with respect to the material variables. The values are normalized across each row to have a summation of 1. (a) Sensitivity indices obtained from the Jacobian of the trained CVAE on the test dataset. (b) Sensitivity indices obtained from the Sobol method using the Saltelli's sampling scheme.

4.3 Sensitivity Analysis

We obtain global sensitivity indices of the problem under study. As a validation of our approach, we compare the obtained values with the global sensitivity indices computed using the Sobol method [30] coupled with the Saltelli's sampling scheme [25]. Figure 3 presents the results obtained from the two methods normalized across each row. The results suggests that the Jacobian-based analysis has successfully computed very similar global sensitivity indices. This essentially validates our approach.

As seen in figure 3, both methods show that the donor doping level in the bulk (N_D) has the most effect on both efficiency and fill factor. From the materials science point of view, doping concentrations are generally important engineering parameters which affect many of solar cells processes, namely charge excitation, drift and diffusion currents and charge separation. They are directly related to the thermodynamics (built-in voltage of the p-n junction, fermi energies, etc.) and kinetics (mobility, series resistance, the radiative and Auger recombination, etc.) of solar cell devices. Since the results from our Jacobian analysis is aligned with our theoretical expectation, we can conclude the importance of donor doping level in the bulk with more certainty.

5 Conclusion

We presented a framework based on conditional variational autoencoders (CVAE) for learning the process model of solar cell characteristics and showed its improved performance compared to discriminative models. We further proposed to train a neural network on the latent space to predict solar cell qualities, such as fill factor and efficiency, and carried out a Jacobian-based sensitivity analysis for obtaining sensitivity indices of these values with respect to the model inputs. Comparison of the sensitivity indices with sampling based global methods demonstrates the validity of our approach. As sensitivity analysis in general can give us an insight into the problem, it can allow for further improvements in terms of process design and optimization. Finally, although we evaluated our methodology in terms of solar cell devices, the ideas can be readily transferred to other experimental design and optimization problems in material science and engineering as we did not make any assumptions on the problem itself in our methodology. Future work will study the application of the sensitivity analysis for optimization and design purposes.

Broader Impact

The research presented in this paper could potentially result in the development of more energy efficient solar cell and photovoltaic devices. At a minimum, the adoption of this machine learning approach would help to focus experiments on the variables that have the largest impact. Ultimately we can build self-driving laboratories based on iterative function of computational screening, automated synthesis and automated characterization [18].

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