Jacobian of Generative Models for Sensitivity Analysis of Photovoltaic Device Processes

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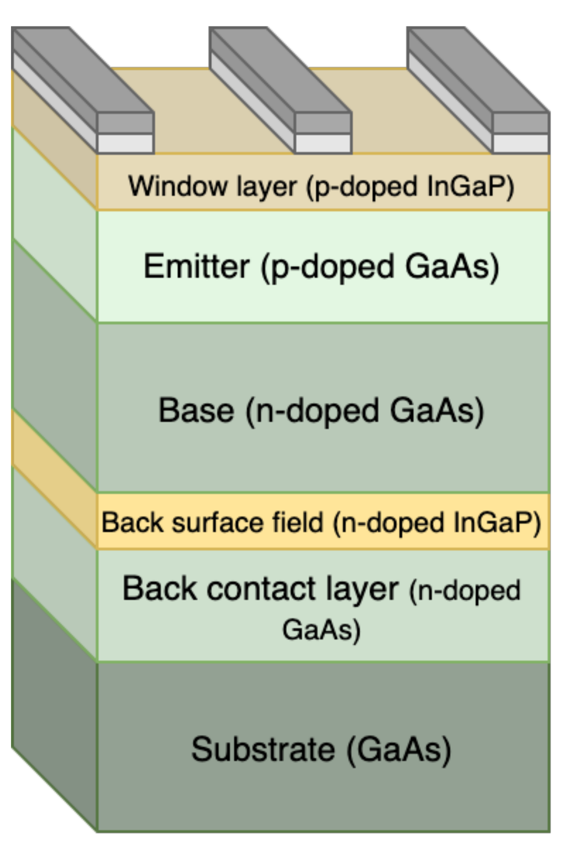
Objectives and Motivations

- With the advancements in computational methods, data availability has increased. Thus, machine learning approaches can provide a great toolbox for exploring problems in Materials engineering.
- Photovoltaic device performance depends on a series of sequential processes, each being a function of various elements that are entangled in a complicated fashion.

The main contributions of this work are:

- **Generative modeling** of the solar cell performance model conditioned on its material variables as a replacement for computationally expensive simulators.
- **Jacobian-based Sensitivity Analysis** of the solar cell performance with respect to its inputs (material variables**)**. Sensitivity analysis can provide a better understanding of the learning process and thus, from an applied view, it can give us an intuition of the engineering problem which can be potentially useful in design applications.

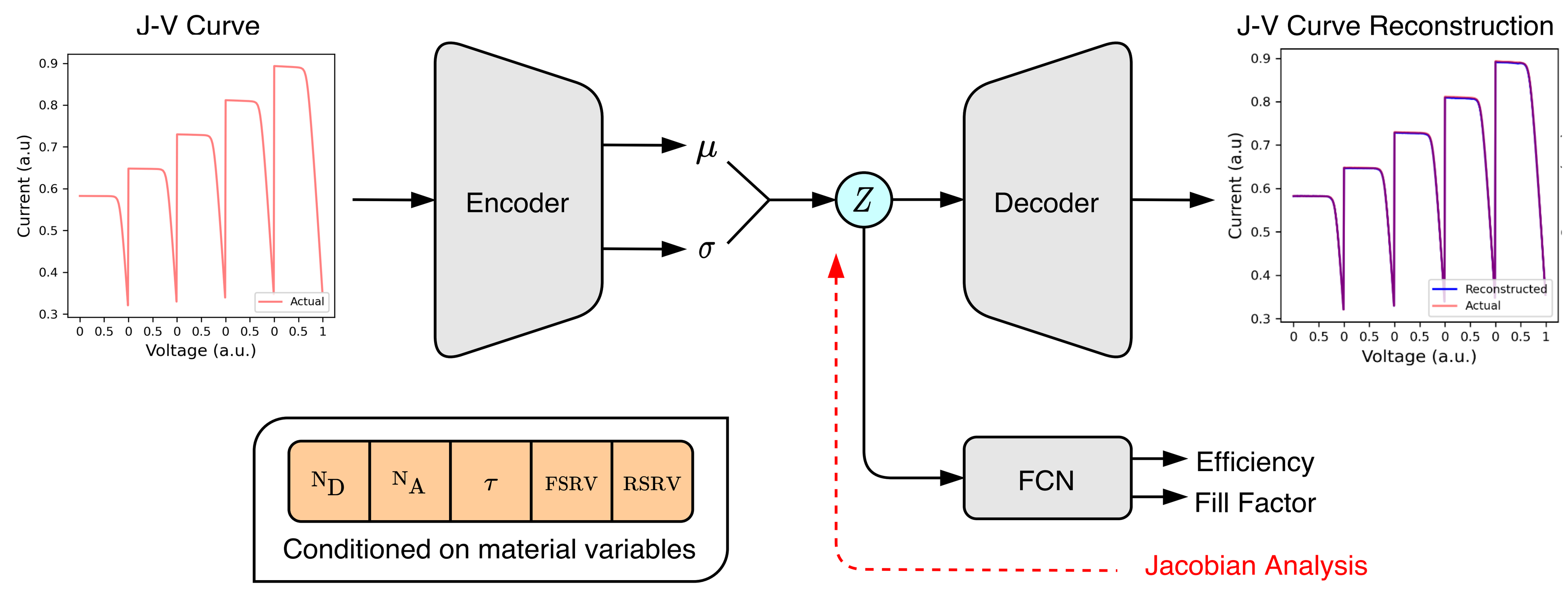
Dataset



We used a GaAs-based solar cell dataset including 20k simulated datapoints published in [1]:

- Each datapoint presents the J-V curve, current density versus voltage, based on five material variables. The J-V curve is considered as the solar cell performance measurement.
- We extend the dataset by calculating two figures of merit in solar cells namely efficiency and fill factor.

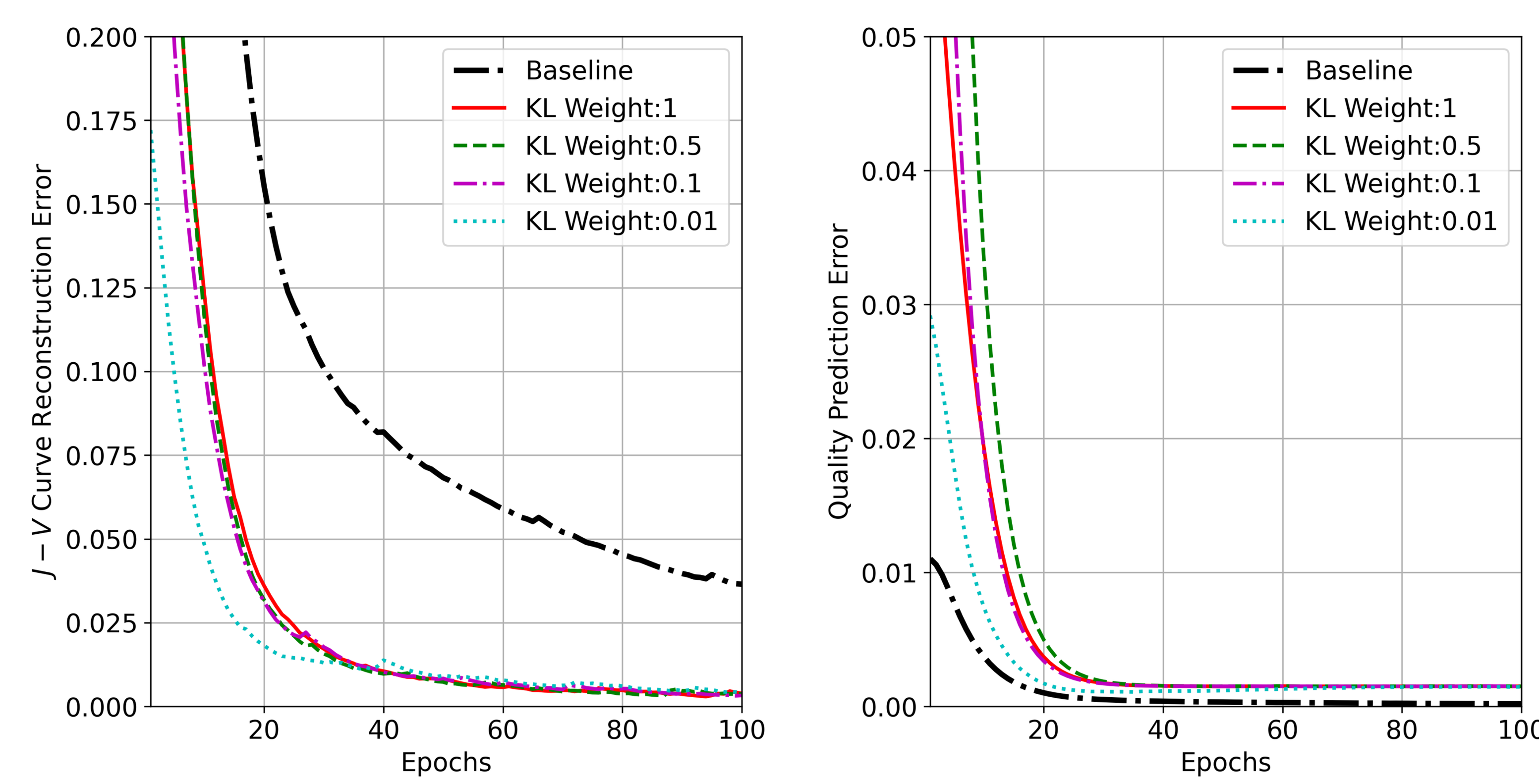
Methodology



We propose a unifying framework for learning this complex process while providing intuitive interpretations based on the sensitivity analysis:

- We train the Conditional Variational Autoencoder (CVAE) to generate J-V curves conditioned on materials variables.
- We train a fully connected network on the conditional latent space to predict solar cell quality. We compute the Jacobian of the outputs of the trained neural network with respect to the inputs for sensitivity analysis.

Results: Performance Prediction



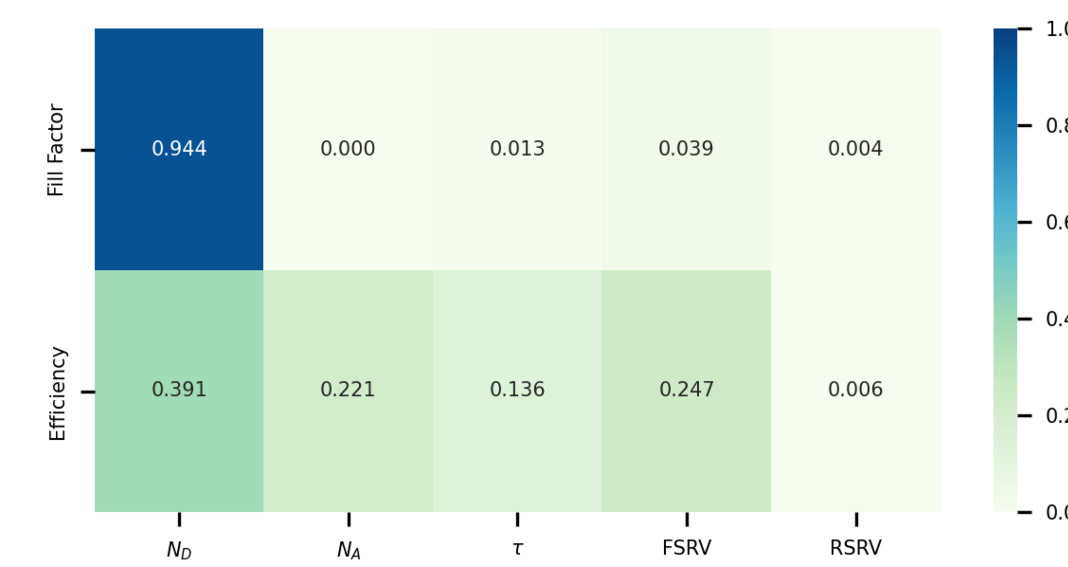
Comparison of the mean squared error (MSE) of our proposed CVAE model and a discriminative model as a baseline:

- For all values of KL weight, CVAE outperforms in J-V reconstruction which is a more important task for replacing the simulators.
- Although the baseline, MLP, slightly outperforms the quality prediction, we should note that CVAE is doing both J-V reconstruction and quality prediction together.

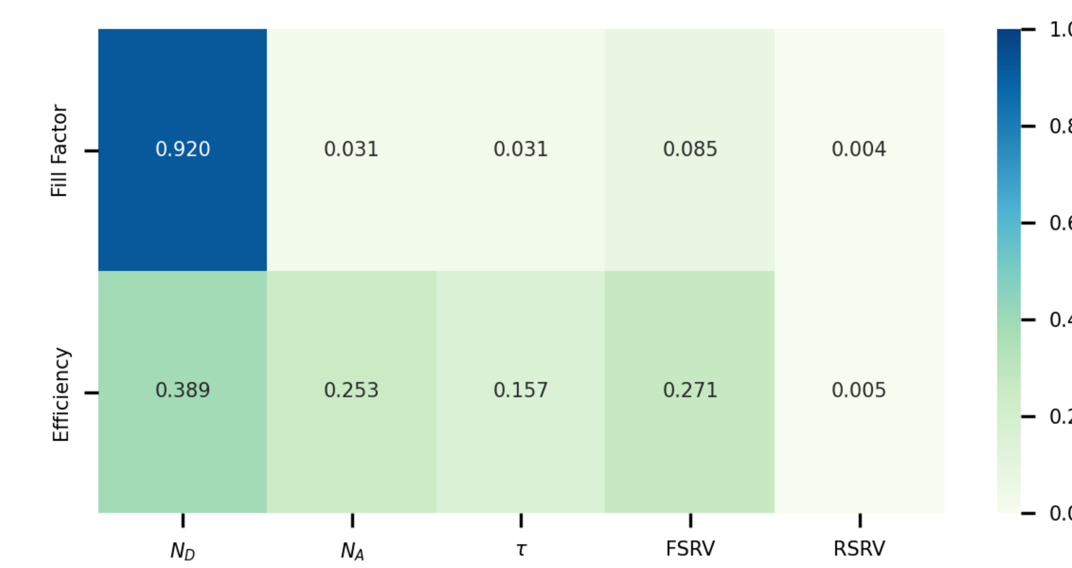
Results: Sensitivity Analysis

The visualization of sensitivity analysis is shown in the form of a heat map. We validate our Jacobian sensitivity analysis with the Sobol method, a sampling-based approach:

- The sensitivity indices obtained from the Jacobian-based approach match the indices obtained from the baseline.
- The order of effectiveness of the material variables can provide a better understanding of the underlying process.



Jacobian-based sensitivity analysis



The Sobol method

Conclusion

- Generative models can learn complex processes and can be used as a fully differentiable surrogate function for simulators.
- Sensitivity analysis gives a better intuition of engineering problems by allowing us to focus on the most effective parameters.
- The ideas used in this work can readily transfer to other design and optimization problems such as LEDs, transistors, etc.

References

[1]: Ren Z, Oviedo F, Thway M, Tian SI, Wang Y, Xue H, Perea JD, Layurova M, Heumueller T, Birgersson E, Aberle AG. Embedding physics domain knowledge into a Bayesian network enables layer-by-layer process innovation for photovoltaics. npj Computational Materials. 2020 Jan 31;6(1):1-9.

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