

# Multiple-Input Neural Networks for Improved Photovoltaic Device Parameter Predictions

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**Abstract** — With the recent surge in AI popularity, neural networks have been used in a number of solar cell applications, including for materials discovery, processing optimization, and high-throughput characterization. One such implementation involves using neural networks to predict the physical parameters of solar cells. Researchers have employed simple device parameters, such as current-voltage characteristics, to estimate more complex materials parameters, such as carrier mobility. In this study, we propose a novel approach to data input for neural networks. Compared to the conventional practice of utilizing a single current-voltage curve as the predictive input, our novel approach involves the integration and layering of multiple experimental curves. This introduces heightened dimensionality to the data and thereby improves the overall performance of predictive models for solar cell optimization and non-destructive rapid characterization.

## I. INTRODUCTION

The increasing popularity of machine learning and artificial intelligence has led to increased usage of neural networks within photovoltaics research. Applications include using neural networks to map and characterize defect regions, assist in the device optimization/design process, as well as in device physics modeling/simulation [1-3]. Another application is the use of neural networks for the prediction of materials parameters. The purpose of this is threefold: to reduce the cost of characterization, to expedite the characterization process, and to gain insights in the patterns that emerge from investigations into the structure of the network themselves. Parameter prediction algorithms typically use simple parameter inputs, such as current-voltage curves, to predict more complicated, and therefore more-costly-to-measure, parameter outputs such as carrier mobilities, electronic trap state density, and carrier lifetimes, to name a few.

In terms of experimental inputs for machine learning algorithms, solar cell current-voltage (JV) curves have the advantages of measurement simplicity and ubiquity; another important advantage is that they naturally contain all of the physics of the device. According to Nelson (2003) [4], the short circuit current for a p-n junction under illumination is given by Equation 1.

$$j_{sc}(E) = -j_n(E, -w_p) - j_p(E, w_n) - j_{gen}(E) \quad (1)$$

Even just one of these terms contains a wealth of information. For example, The electron current ( $j_n$ ) is given in Equation 2, where  $w_p$  is the depth of the depletion region into the p layer,  $R$  is the reflectivity,  $L_n = \sqrt{\tau D_n}$  is the electron diffusion length,  $D_n$  is the diffusion coefficient,  $S_n$  is the surface recombination velocity,  $\alpha$  is the probability of photon absorption, and  $b_s$  is the flux density of photons [4]. What this equation illustrates is that the JV curve of a photovoltaic device is dependent on all of the relevant physical properties of that device.

$$\begin{aligned} j_n(E, w_p) &= \left[ \frac{qb_s(1-R)\alpha L_n}{(\alpha^2 L_n^2 - 1)} \right] \\ &\times \left\{ \frac{\left( \frac{S_n L_n}{D_n} + \alpha L_n \right)}{\frac{S_n L_n}{D_n} \sinh \frac{(x_p - w_p)}{L_n} + \cosh \frac{(x_p - w_p)}{L_n}} \right. \\ &\quad - \frac{e^{-\alpha(x_p - w_p)} \left( \frac{S_n L_n}{D_n} \cosh \frac{(x_p - w_p)}{L_n} + \sinh \frac{(x_p - w_p)}{L_n} \right)}{\frac{S_n L_n}{D_n} \sinh \frac{(x_p - w_p)}{L_n} + \cosh \frac{(x_p - w_p)}{L_n}} \\ &\quad \left. - \alpha L_n e^{-\alpha(x_p - w_p)} \right\} \end{aligned}$$

In addition to the physics motivation, the relatively fast acquisition speed, ease of measurement, and ubiquity of this characterization method in the field make JV curves an ideal candidate for applications involving large amounts of experimental data.

## II. METHODS

This section outlines a new method of integrating several JV curves as inputs into neural networks for materials parameter extraction and prediction. To demonstrate this method, we fabricated PbS colloidal quantum dot (CQD) solar cells, characterized them in a custom multi-modal optoelectronic scanning setup [5], and trained custom-designed neural networks on the collected data from multiple devices.

### A. Physical Experimental Setup

PbS CQD solar cells were chosen as they are relatively easy to manufacture, enabling high-throughput device production, and have complicated and not fully understood electronic transport physics that may not conform to the standard solar cell diode models used in the field. This is advantageous as neural networks generally require large amounts of training data, and could potentially be used to elucidate novel transport physics. PbS CQDs were synthesized [6] and solar cells were fabricated [7] using slight modifications of standard procedures. A custom optoelectronic characterization setup [5] was used to measure spatial maps of JV curves, photoluminescence, transient photovoltage, and transient photocurrent values. The system utilizes a 520 nm laser and white LED which is collimated onto the device. The device is mounted on a 3-axis translation stage allowing for the collection of multiple data points as well as the creation of parameter maps.

### B. Network

The performance of the new layering technique was assessed by comparing several neural networks, each with distinct hyperparameters but subjected to identical training conditions. The neural networks employed in this study were based on the encoder model from Ren, et al.'s denoising autoencoder [8]. In total, 3 networks were trained and evaluated: Network 1 utilizes a fully connected architecture with three hidden layers, Network 2 has three hidden layers, but with 1D convolution layers, and Network 3 has three hidden layers, but with 2D convolution layers. Network 3 is the network that utilizes the new layering scheme.

### C. Layered Input

The illuminated current voltage curves are measured at 28 different biases. Therefore, the inputs into Networks 1 and 2 are single 28x1 vectors. In contrast, the input into Network 3 is a 28x9x2 "image." The new layering method, depicted in the bottom left of Figure 1, involves selecting eight surrounding points for a given central point (green) and stacking them together. The surrounding points (magenta) are at a distance  $n$  from the central point. This new variable adds an additional hyperparameter for the network. Layering these curves creates a new 28x9 input matrix with 2 channels: one representing voltage and the other the current. This new input can be treated as an image, and 2D convolutions and other conditions typical of image-based networks can now be applied, which allows for more robust and enhanced training features.

## III. DISCUSSION/RESULTS

Table 1 contains the mean absolute percentage error between the measured and predicted network values for various materials parameters: photoluminescence (PL), transient photovoltage ( $\Delta V$ ), and transient photocurrent ( $\Delta Q$ ). The results in this table show that regardless of the depth or

complexity of the network, the training error is improved when employing the new layered input method.

|           | PL     | $\Delta V$ | $\Delta Q$ |
|-----------|--------|------------|------------|
| Network 1 | 31.30% | 32.19%     | 15.73%     |
| Network 2 | 33.74% | 23.66%     | 17.78%     |
| Network 3 | 27.76% | 18.12%     | 10.28%     |

Notably, the training error is lowest with the new method even across several different parameters. This affirms the capability of the new method to enhance neural network performance. Qualitative results of network performance are provided in Figure 1 through the measured and predicted parameter maps. The key factor contributing to the improved performance of the new method is the existence of points with similar JV curves but vastly different material parameters across large areas of the devices. This phenomenon creates a challenge for the network because it leads to an averaging effect: the network must balance between the similar points as the weights of the network will move in opposite directions during gradient descent. The new method resolves this issue by introducing extra dimensionality and more variation so that the network can distinguish between these points.

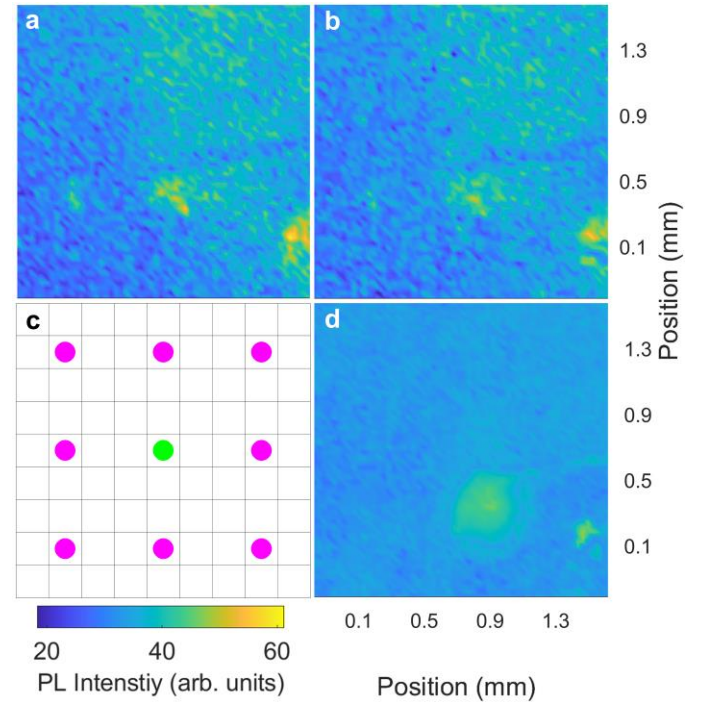


Fig. 1. a) Experimentally measured relative PL intensity map. b) Network prediction of the PL intensity map from a using the new layering technique. c) Layering of JV curve inputs with spacing size  $n = 3$ . d) Network prediction of the PL intensity map without the new layering technique applied. Figures a, b, and d use the same scale bar, which is located on the bottom left.

#### IV. CONCLUSION

In conclusion, this study introduced a novel layered input method for neural networks, specifically applied in the context of materials parameters prediction in solar cells. The methodology involves treating the JV curve input as an "image" with two "color" channels, enabling the application of 2D convolutions and other conditions typical of image-based networks. The results, as summarized in Table 1, demonstrate superior training error performance regardless of the depth or complexity of the neural network. The enhanced robustness of the new layered input method signifies its potential to improve predictive accuracy in materials parameter estimation. This research can be applied as a strategy for various neural networks in different photovoltaic applications, paving the way for further advancements in predictive modeling and analysis.

#### V. ACKNOWLEDGEMENTS

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#### REFERENCES

- [1] H. Chen, et al. "Solar cell surface defect inspection based on multispectral convolutional neural network." *Journal of Intelligent Manufacturing*, vol. 31, pp.453-468, 2020.
- [2] B. Yılmaz and R. Yıldırım, "Critical review of machine learning applications in perovskite solar research," *Nano Energy*, vol. 80, p. 105546, Feb. 2021.
- [3] S. Bhatti *et al.*, "Revolutionizing Low-Cost Solar Cells with Machine Learning: A Systematic Review of Optimization Techniques," *Advanced Energy and Sustainability Research*, vol. 4, no. 10, p. 2300004, 2023.
- [4] J. Nelson, *The Physics of Solar Cells*. London: Imperial College Press, 2003, pp. 165.
- [5] Y. Lin, et al. "Local Defects in Colloidal Quantum Dot Thin Films Measured via Spatially Resolved Multi-Modal Optoelectronic Spectroscopy." *Advanced Materials*, vol. 32, no. 11, 2020.
- [6] M. A. Hines and G. D. Scholes, "Colloidal PbS Nanocrystals with Size-Tunable Near-Infrared Emission: Observation of Post-Synthesis Self-Narrowing of the Particle Size Distribution," *Advanced Materials*, vol. 15, no. 21, 2003.
- [7] L. Liu, S. Z. Bisri, Y. Ishida, D. Hashizume, T. Aida, and Y. Iwasa, "Ligand and Solvent Effects on Hole Transport in Colloidal Quantum Dot Assemblies for Electronic Devices," *ACS Appl. Nano Mater.*, vol. 1, no. 9, pp. 5217–5225, Sep. 2018
- [8] Z. Ren et al., "Embedding physics domain knowledge into a Bayesian network enables layer-by-layer process innovation for photovoltaics," *npj Computational Materials*, vol. 6, no. 1, Jan. 2020.