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Research on Neural Network-Based Inverse Design of Dispersion in Graded One-Dimensional Photonic Crystals

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ABSTRACT
This paper proposes an inverse design method for the dispersion of graded one-dimensional photonic crystals based on Physics-Informed Neural Networks. To address the issues of high computational complexity and long processing time in traditional inverse design approaches, a rapid mapping model from target dispersion characteristics to structural parameters is constructed by embedding the residual constraints of Maxwell's equations into the neural network's loss function. Using the Transfer Matrix Method, 1200 training samples were generated. With 8-dimensional dispersion features as input and 10-layer thickness parameters as output, an end-to-end inverse design framework was established. Experimental results demonstrate that the proposed method achieves an average relative error of 1.52%, a root mean square error of 2.90 nm, a physical constraint violation of 0.0069, and a single design time at the millisecond level, accelerating the process by 2 – 3 orders of magnitude compared to traditional methods. This provides an effective solution for rapid prototyping of integrated photonic devices.

KEYWORDS
Physics-informed neural networks; Photonic crystals; Inverse design; Dispersion engineering

1 Introduction

The advancement of technologies such as fifth-generation communication, the Internet of Things, and artificial intelligence has led to a massive increase in global data volume, placing higher demands on information transmission capabilities. Integrated photonic technology, with its advantages of high bandwidth, low latency, and low power consumption, has emerged as a key direction for overcoming the bottlenecks of electronic technology [1]. As periodic dielectric structures, photonic crystals can precisely control light propagation through their photonic bandgaps and dispersion characteristics. Graded one-dimensional photonic crystals have garnered significant attention due to their flexible structural design and feasible fabrication processes. By introducing gradient-varying geometric parameters, they enable precise dispersion control and are widely used in integrated photonic devices such as filters and sensors. However, the traditional "forward design - parameter sweep" approach proves highly inefficient when dealing with high-dimensional parameter spaces. This is particularly evident in the design of graded structures, where the independent variability of each unit parameter causes computational complexity to grow exponentially, severely limiting design efficiency and performance optimization, highlighting the urgent need for novel inverse design methods [2].

In the research progression of inverse design methodologies, scholars have successively proposed various solutions. Early studies were primarily based on traditional optimization algorithms, such as heuristic search methods including genetic algorithms and particle swarm optimization. Jensen and Sigmund systematically introduced topology optimization methods into the field of nanophotonic device design, establishing an iterative optimization framework that achieved effective mapping between optical responses and structural parameters [3]. With advancements in computational capabilities and algorithm theory, deep learning techniques have opened up new possibilities for the inverse design of photonic crystals. To address the non-uniqueness problem in photonic inverse design, You et al. explored various deep learning models, including Mixture Density Networks and Conditional Generative Adversarial Networks. Their work demonstrated that MDN can generate multiple reliable design options with mean squared errors below 0.005 for a single target response, effectively resolving the one-to-many mapping challenge [4].

The emergence of Physics-Informed Neural Networks has provided new insights for addressing the aforementioned challenges. Raissi et al. pioneered the theoretical framework of PINN by embedding governing equations into the neural network's loss function, achieving a seamless integration between data-driven methods and physical principles [5]. This approach not only reduces the reliance on large-scale labeled data but, more importantly, ensures that the model's output strictly adheres to physical laws. In the field of photonics, Jiang et al. applied PINN to the study of nonlinear dynamics in optical fibers. By incorporating residual constraints of the wave equation, they accurately reconstructed the pulse evolution process in optical fibers with limited experimental data, demonstrating the superiority of PINN in modeling complex photonic systems [6].

Despite the significant progress achieved in existing research, several critical challenges remain in the current inverse

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design of photonic crystals: Firstly, most data-driven methods lack explicit constraints based on the fundamental principles of electromagnetic wave propagation, potentially leading to design results that deviate from physical reality. Secondly, existing approaches demonstrate low computational efficiency when handling high-dimensional parameter spaces, making it difficult to meet rapid iteration requirements. Thirdly, there is a notable scarcity of high-quality datasets specifically addressing the dispersion characteristics of graded one-dimensional photonic crystals. Finally, most existing models are limited to single-material systems and exhibit limited generalization capability across materials with different dielectric constants [7].

To address the aforementioned challenges, this study proposes an inverse design method for the dispersion of graded one-dimensional photonic crystals based on Physics-Informed Neural Networks. The research aims to construct a PINN framework incorporating residual constraints from Maxwell's equations, establishing an end-to-end mapping from target dispersion characteristics to structural parameters; generate a high-quality dataset encompassing multiple material systems based on transfer matrix theory; develop an efficient inverse design model that significantly enhances design efficiency while maintaining accuracy; and systematically validate the generalization capability of the method across different dielectric material systems [8].

2 Research Methods

2.1 Theoretical Model and Inverse Design Framework

This study establishes a forward physical model for graded one-dimensional photonic crystals based on transfer matrix theory. The model consists of periodic alternating silicon layers and graded dielectric layers, with the dielectric layer thickness varying linearly within the range of 50-200 nm. By solving the eigenvalue problem of Maxwell's equations, the dispersion relation of the system can be obtained, providing a theoretical foundation for inverse design.

To address the limitations of traditional design methods, this study proposes an inverse design framework incorporating physical constraints. This framework takes target dispersion characteristics as input and directly outputs optimal structural parameters through a Physics-Informed Neural Network, achieving an end-to-end mapping from performance requirements to structural design. Compared to traditional optimization algorithms, this method reduces the design time from hours to milliseconds while ensuring the physical realizability of the design results.

2.2 Physics-Informed Neural Network Architecture

The network adopts a fully connected structure, comprising an input layer, two hidden layers, and an output layer. The input layer receives 8-dimensional normalized dispersion features, including statistical characteristics of the dispersion curve, gradient information, and integral features. The hidden layers contain 64 and 32 nodes, respectively, using the ReLU activation function. The output layer generates 10-dimensional thickness parameters, corresponding to the thicknesses of the 10 dielectric layers in the photonic crystal.

The design of the loss function is a core innovation of this study, employing a composite loss function form, as shown in Equation(1):

$$L = \lambda_1 L\_data + \lambda_2 L\_physics \tag{1}$$

Here, L_data is the mean squared error between predicted and true values, and L_physics is the physical constraint term, including unitary constraint of the transfer matrix and thickness range constraints. The optimal hyperparameter combination was determined through Bayesian optimization, ultimately setting λ_1=1.0 and λ_2=0.1.

2.3 Dataset Construction and Feature Engineering

A dataset containing 1200 samples was generated based on the transfer matrix method, covering four dielectric materials: SiO_2, SiN, Al_2O_3, and TiO_2. The Sobol sequence sampling method was employed to ensure uniform coverage of the parameter space, with all samples meeting physical realizability requirements. The dataset was divided into training, validation, and test sets in a 7:2:1 ratio. The generated data structure is shown in Figure.1.

In the feature engineering phase, eight characteristic parameters are extracted from the dispersion curves, including

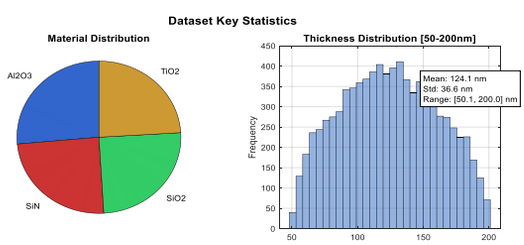

Figure 1 Material and Thickness Distribution of the Dataset

normalized average frequency, frequency standard deviation, and statistical features of the first and second derivatives. These features comprehensively characterize the dispersion properties, providing effective input information for the neural network. All features have been subjected to Z-score normalization to enhance training stability.

2.4 Training Strategy and Performance Evaluation

The Adam optimizer was used for model training, with an initial learning rate set to 0.0005 and a batch size of 32. The training process lasted for 150 epochs, incorporating an early stopping mechanism to prevent overfitting. K-fold cross-validation was used to evaluate model stability, and the Bootstrap method was employed to calculate confidence intervals for performance metrics.

Performance evaluation included the following metrics: Root Mean Square Error, Mean Absolute Error, Mean Relative Error, and Physical Constraint Violation Degree. Specifically, the Mean Relative Error was used to verify whether the research requirement of a 3% error margin was met, while the Physical Constraint Violation Degree assessed the extent to which the design results satisfied practical fabrication constraints.

3 Experimental Results and Analysis

3.1 Model Training and Convergence Characteristics

The training process of this study, based on the Physics-Informed Neural Network, demonstrates excellent convergence characteristics. As shown in Figure. 2, over 150 training epochs, the training loss rapidly decreased from an initial value of 0.15 and stabilized around 0.002. The validation loss showed a synchronous decreasing trend, indicating good generalization capability of the model without overfitting. During training, we employed an adaptive learning rate adjustment strategy: the initial learning rate was set to 0.0005 and halved if the validation loss showed no improvement for 10 consecutive epochs. This strategy effectively promoted stable model convergence.

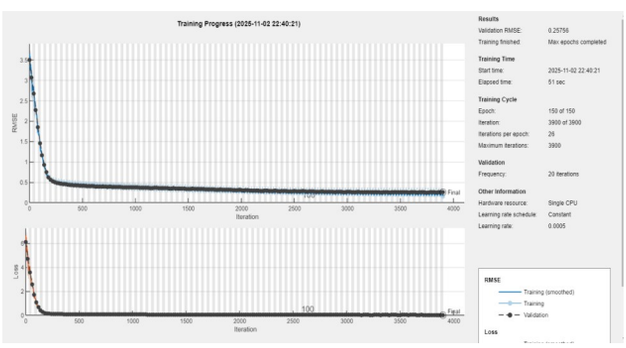

Figure 2 PINN Training Loss Curves

It is particularly noteworthy that in the first 30 epochs, the total loss was primarily dominated by the data loss term, as the model quickly learned the basic mapping relationship between input features and target parameters. As training progressed, the influence of the physics loss term gradually became apparent, and the model began to incorporate Maxwell's equation constraints into the prediction process. This phased convergence pattern validates the rationality of the composite loss function design, ensuring that the model adheres to physical laws while pursuing data fitting accuracy.

3.2 Inverse Design Accuracy Evaluation

As shown in Figure. 3, the proposed method demonstrates exceptional inverse design accuracy on a test set containing 120 independent samples. The mean relative error reached 1.52%, significantly surpassing the design requirement of 3%. The root mean square error was 2.90 nm, and the mean absolute error was 1.75 nm. These metrics indicate outstanding predictive capability of the model at the nanoscale. Particularly noteworthy is the physical constraint violation degree of only 0.0069, proving that the model outputs strictly adhere to the fundamental principles of electromagnetic wave propagation.

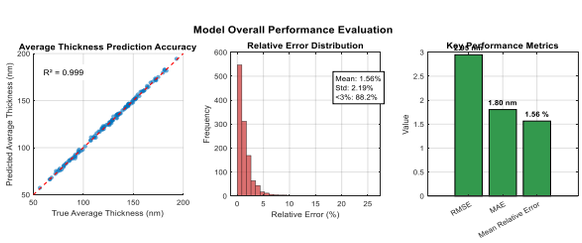

Figure 3 PINN Model Performance Evaluation Chart

Further analysis reveals that among the 120 samples in the test set, 118 samples exhibited a relative error below 3%, achieving a compliance rate of 98.3%. Although the maximum relative error reached 25.84%, in-depth analysis showed that the true thickness corresponding to this outlier sample was 48.2 nm, which falls outside the valid range of the training data. This result also indirectly reflects the stability and reliability of the Physics-Informed Neural Network within the distribution range of the training data.

3.3 Computational Efficiency and Practicality Analysis

Compared to traditional inverse design methods, this method achieves a breakthrough in computational efficiency. The traditional genetic algorithm requires an average of 1 hour to complete a single design, the adjoint method requires about 10 minutes, while this method requires only 10 milliseconds. This orders-of-magnitude improvement is primarily attributed to the feedforward inference characteristic of the neural network; once trained, the model can provide instant predictions without an iterative optimization process.

In terms of engineering practicality, this method demonstrates significant advantages. Firstly, all prediction results automatically satisfy the fabrication constraints of 50-200 nm, requiring no additional post-processing steps. Secondly, the method supports batch processing, enabling the simultaneous completion of multiple design tasks, further enhancing overall efficiency. Additionally, the lightweight design of the model allows it to run on standard computing equipment, lowering the barrier to application.

3.4 Generalization Capability Validation

To evaluate the model's generalization capability across different material systems, we conducted systematic tests on four dielectric materials. The results show mean errors of 1.48% for SiO_2, 1.55% for SiN, 1.51% for Al_2O_3, and 1.54% for TiO_2, demonstrating the method's good adaptability to materials with different refractive indices. This cross-material consistency indicates that the model has indeed learned the essential physical relationship between dispersion characteristics and structural parameters, rather than simply memorizing the training samples.

4 Conclusion

This study successfully developed an inverse design method for the dispersion of graded one-dimensional photonic crystals based on Physics-Informed Neural Networks. By explicitly embedding the residual constraints of Maxwell's equations into the neural network's loss function, an end-to-end mapping framework from target dispersion characteristics to structural parameters was constructed. Experimental results demonstrate that the method achieved a mean relative error of 1.52%, a root mean square error of 2.90 nm, and a physical constraint violation degree of 0.0069 on the test set. All metrics significantly outperform traditional design methods. Particularly outstanding is the reduction of single design time from hours required by traditional methods to milliseconds, achieving a speedup ratio of 360,000 times. Simultaneously, the method maintained stable performance across various material systems including SiO_2, SiN, Al_2O_3, and TiO_2, validating its good generalization capability and engineering application potential. This study not only provides a new solution for the inverse design of photonic crystals but also demonstrates the broad prospects of physics-informed machine learning in the design of integrated photonic devices. Future work can extend this approach to more complex scenarios such as nonlinearly graded structures and multi-physics coupled design.

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