Inverse Design of Photonic Crystal Surface Emitting Lasers is a Sequence Modeling Problem

Anonymous submission

Abstract

Photonic Crystal Surface Emitting Lasers (PCSEL)'s inverse design demands expert knowledge in physics, materials science, and quantum mechanics which is prohibitively labor-intensive. Advanced AI technologies, especially reinforcement learning (RL), have emerged as a powerful tool to augment and accelerate this inverse design process. By modeling the inverse design of PCSEL as a sequential decision-making problem, RL approaches can construct a satisfactory PCSEL structure from scratch. However, the data inefficiency resulting from online interactions with precise and expensive simulation environments impedes the broader applicability of RL approaches. Recently, sequential models, especially the Transformer architecture, have exhibited compelling performance in sequential decision-making problems due to their simplicity and scalability to large language models. In this paper, we introduce a novel framework named *PCSEL Inverse-design Transformer* (PiT) that abstracts the inverse design of PCSEL as a sequence modeling problem. The central part of our PiT is a Transformer-based structure that leverages the past trajectories and current states to predict the current actions. Compared with the traditional RL approaches, PiT can output the optimal actions and achieve target PCSEL designs by leveraging offline data and conditioning on the desired return. Results demonstrate that PiT achieves superior performance and data efficiency compared to baselines.

Introduction

Photonic Crystal Surface Emitting Lasers (PCSELs) (Hirose et al. 2014; Yoshida et al. 2019; Noda et al. 2017) are a type of nanoscale laser that combines the benefits of photonic crystals (PhC) (Quan, Deotare, and Loncar 2010) and Vertical Cavity Surface Emitting Lasers (VCSELs) (Chang-Hasnain 2000). PhCs are artificial structures that have a periodic refractive index modulation in semiconductor materials. This periodicity creates a photonic bandgap that inhibits the propagation of light in certain frequency ranges to amplify the optical resonance effect. VCSELs are lasers that emit light perpendicular to the surface of the semiconductor structure, which allows for efficient coupling to optical fibers and other optical components. PCSELs combine these two technologies to create advanced lasers that have several advantages over traditional ones and therefore enjoy the best of both worlds. PCSELs have great potential for important applications in sensing, autonomous driving, medicine, machining, and telecommunication. Fundamentally, when an electrical pumping current is injected into the active layer (that is, the core layer of PCSEL), it emits laser light which is then confined and amplified within the PhC resonant cavity (Sze, Li, and Ng 2021). Additionally, the active layer may contain quantum wells that increase the recombination rate of spontaneous photon emission (which was first predicted by Albert Einstein in his quantum mechanics papers (Hilborn 1982)) and thus substantially enhance the lasing effect (Sze, Li, and Ng 2021). So the bottom line is that the PhC layer is used to control the amplitude and direction of the emitted light, while the active layer is what actually generates the light. Therefore, proper design of the PhC layer and the active layer plays a central role in the overall quality of a PCSEL, which brings to us the critical yet challenging PCSEL inverse design problem. This problem is a combination of disciplines including physics, materials science, and quantum mechanics which generally demands prohibitively high-level domain knowledge.

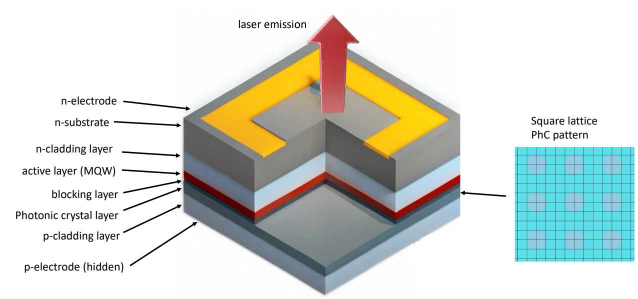

Figure 1: PCSEL structure schematic, with the active layer and PhC cavity layer shown. Based on the band-edge mode, a large area lasing resonance mode is formed within the PhC resonance cavity. Lasing arises from the evanescent coupled MQW gain medium in the active layer. The inverse design problem therefore focuses on optimizing the designs of the active layer and the PhC cavity as a whole. The size of the device is about 200 microns in side lengths and 400 microns in height and solely manufactured with semiconductor materials.

Recent developments in Transformer (Vaswani et al. 2017) architectures witness the blooming performance from prediction tasks into decision-making problems (Wen et al. 2023). This advancement, namely, sequential decision-making as sequence modeling, is notably distinct from the traditional approaches in reinforcement learning (RL), which are typically focused on learning a singular policy for a specific, narrowly defined behavior distribution. Given the broad range of successful implementations of these models, this study aims to explore their applicability to the inverse Design of PCSEL.

In this paper, we introduce a novel framework named PCSEL Inverse Design Transformer (PiT) that abstracts the inverse design of PCSEL as a sequence modeling problem. The central part of our PiT is a Transformer-based structure that leverages the past trajectories and current states to predict the current actions. Compared with the traditional RL approaches, PiT can output the optimal actions and achieve target PCSEL designs by leveraging offline data and conditioning on the desired return. Results demonstrate that PiT achieves superior performance and data efficiency compared to baselines.

Related Works

Optimzing the PCSEL through AI Overall, recent advancements in machine learning (Goodfellow, Bengio, and Courville 2016) and optimization algorithms (Wiecha et al. 2017) have propelled the progress of inverse designs in science. Early in the 90s, heuristic, evolutionary (Hegde 2019), and gradient-based (Zhang et al. 2020) optimization algorithms began to emerge prolifically. Key algorithms include simulated annealing (Bertsimas and Tsitsiklis 1993), Newton's method (Milzarek and Ulbrich 2014), Bayesian optimization (Shahriari et al. 2015), Monte Carlo method (Rubinstein and Kroese 2016), particle swarm (Ma and Li 2020) and genetic algorithm (Ren et al. 2021) etc. These algorithms provide a new way of thinking when facing hard non-convex optimization problems, which act as a solid foundation for scientific problems. However, the issue remains of heavy human involvement due to sophisticated trial-and-error iterations. To solve this, in around 2012, researchers proposed deep learning (DL) (Krizhevsky, Sutskever, and Hinton 2012; Goodfellow, Bengio, and Courville 2016) frameworks to construct a mapping relationship between input data and output targets by means of Deep Neural Networks. In particular, DL consists of supervised, unsupervised, and reinforcement learning (RL) (Sutton and Barto 2018). These DL models greatly bolstered the efficiency of inverse design in science, pushing the possibility of automated design into a new era (So et al. 2020; Jiang, Chen, and Fan 2021; Li et al. 2021; Mirhoseini et al. 2021; Li et al. 2022; Degrave et al. 2022; Li et al. 2023a; Kuprikov et al. 2022). Circa 2023, a novel framework based on RL, called Learning to Design Optical-Resonators (L2DO) (Li et al. 2023b), provides the solution for autonomous inverse design of nanophotonic chips without human intervention. With two orders of magnitude higher sample efficiency compared to supervised learning, L2DO has preliminarily realized RL-driven chip inverse design on an algorithmic level. However, to the best of our knowledge, there aren't any published results on the inverse design of PCSELs via AI methods to this day. Due to the strategic significance of PCSELs for a host of key industries, we believe there is an urgent need to develop an RL-based approach for PCSEL's rapid inverse design.

Sequential Models for Sequential Decision-Making Recent research on transformer models for sequential decision-making has revolutionized the field by pushing boundaries and introducing novel capabilities. Transformers (Wen et al. 2023) excel in capturing long-range dependencies, efficiently assigning credit, and modeling temporal dynamics. These have significantly advanced the field and hold promise for applications in reinforcement learning. Foundational works in the application of transformers to sequential decision-making include Decision Transformer (DT) (Chen et al. 2021a) and Trajectory Transformer(TT) (Janner, Li, and Levine 2021). These works have made a significant impact on the field by introducing transformative methodologies. DT, for instance, revolutionized traditional offline RL approaches by employing a transformer decoder as the backbone model. It uses (return-to-go, state) as input data, and chooses action as output. This method outperforms the offline RL baseline CQL. TT is another foundational application of transformers in sequential decision-making, which utilizes the GPT model (Radford et al. 2018) as its backbone, demonstrating remarkable performance in long-range planning tasks. Other efforts like UPDeT (Hu et al. 2021) for multi-agent planning and MGDT (Lee et al. 2022) for multi-game decision-making highlight the versatility of transformers. Looking ahead, transformer models show great promise to transform decision-making in the coming years by enabling a more nuanced understanding of situational context and more predictive recommendations.

Background

Modeling Inverse-design of PCSEL as a Sequential Decision-making problem

Sequential decision-making describes a situation where the decision-maker makes successive observations of a process before a final decision is made. In most sequential decision problems, there is an implicit or explicit cost/regret/reward associated with each observation or action. The procedure to decide when to stop taking observations and when to continue is called the 'stopping criteria'. The objective of sequential decision-making is to find a stopping criterion that optimizes the decision in terms of minimizing losses or maximizing returns, including observation costs. The optimal stopping criteria are also called optimal strategy and optimal policy, which are commonly adopted in classic RL algorithms. The inverse design of PCSEL can be modeled as a sequential decision-making problem because, just like in playing the game of Go (Silver et al. 2017) or chess, the chip designer (Mirhoseini et al. 2021; Li et al. 2023b) sets or updates the layout of PCSEL one component at a time and immediately assesses the reward/cost induced by that action. To state this more specifically, state(S) is an 8-dimension vector representing the geometric parameters in the design.

Action(a) space is discrete and consists of 16 actions. Each action represents an increase or decrease in geometric parameters by one unit according to the scale of the parameters. For example, action 0 is to increase parameter 0 by 25, and action 3 is to decrease parameter 1 by 2.5. In PCSEL, the reward is the difference between the score obtained in the current step and the score obtained in the previous step. We can calculate score from the parameters returned at each step, as in Eqn. 6. For the first step, we take the score as a reward. To analyze the composition of the score in more detail, we can examine the parameters returned by the environment and the method of calculation.

Objectives	Characteristics
Q	Q-factor
lam	lambda
$power$	power
$area$	area
div_angle	divergence angle

Table 1: Performance characteristics that determine the merit of PCSEL.

$$r_1 = \gamma * (1 - (Q_{goal} - Q)/Q_{goal}) \tag{1}$$

$$r_2 = \epsilon * (1 - |lam_{goal} - lam|/lam_{goal}) \tag{2}$$

$$r_3 = \beta * (1 - (area_{goal} - area)/area_{goal}) \tag{3}$$

$$r_4 = \alpha * (1 - (power_{goal} - power)/power_{goal}) \tag{4}$$

$$r_5 = \eta * (1 + (div\_angle_{goal} - div\_angle)/div\_angle_{goal} \tag{5}$$

$$score = r_1 + r_2 + r_3 + r_4 + r_5 \tag{6}$$

The designer continues to take actions to set/update the layout until a pre-set stopping criteria is met, which in our case is the target PCSEL performance characteristics listed in Table 1. When the target characteristics are met, one can consider the cumulative return is maximized or an optimal policy is found. Due to the high-level domain knowledge and labor intensity required by PCSEL inverse design, the authors believe modeling it as a sequential decision problem can largely alleviate human labor and accelerate the R&D of advanced PCSEL lasers.

Proposed Methods

Inverse-design of PCSEL is a Sequential Modeling Problem

The PCSEL inverse design can be conceptualized as a sequential decision model, where the goal is to maximize the score within a limited number of steps through strategic adjustments. This model is characterized by a clear reward target, a small and discrete action space, and the Markov property. Given these properties, it is naturally suited for RL algorithms.

However, unlike games that can be quickly simulated, data collection for PCSEL inverse design is challenging due to its complexity. Therefore, considering data efficiency, offline RL is a more suitable choice. Our PiT model is based

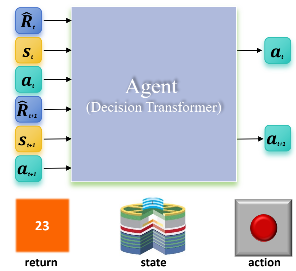

Figure 2: PiT neural network architecture.

on sequence models, for example, DT (Chen et al. 2021a) or TT (Janner, Li, and Levine 2021). Among the existing sequence models for sequential decision-making, we choose DT for its simplicity and superior performance.

Dataset

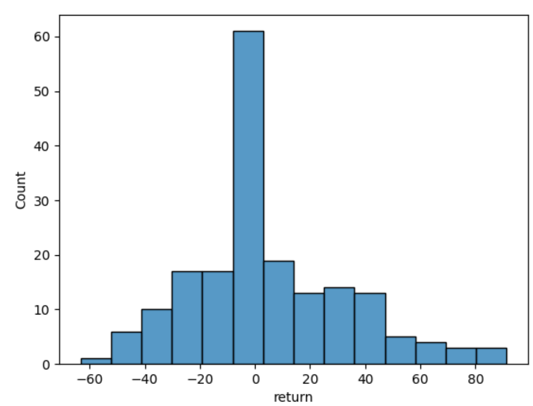

Figure 3: The frequency of the total return of the trajectories used to train PiT.

The dataset of offline trajectories for training our PiT is extracted from replay buffers that were saved during previous online RL experiments associated with PCSELs. The offline dataset contains roughly 16,057 samples (each sample includes state, action, reward, and next state). Specifically, the state is defined as a vector of design parameters of the PCSEL, the action is a change/update in the state, and the reward is defined as how close we are to the target PCSEL design. For instance, if we wish to achieve a target PCSEL design with a Q-factor of 5 million, a wavelength (lambda) of 1310 nm, a power conversion rate of 80%, a lasing area of 3.0e-13 square meters, and a divergence angle of 1.0 degrees, we would train PiT to inverse design a PCSEL that meets these target characteristics. The actual criteria is a weighted sum of these five reward of merit according to Eqn. 1-6 and is referred to as a score in the remaining text.

Imada et al. (1999)	9.19709
Ohnishi et al. (2004)	19.2290
Sakai et al. (2005)	21.23469
Hirose et al. (2014)	18.95918
Hsu, Lin, and Pan (2017)	10.01160
Chen et al. (2021b)	2.117346
Wang et al. (2021)	41.8554
Itoh et al. (2022)	20.2335
BC	71.28
PiT	73.95

Table 2: PiT's results compared to baselines in the literature.

Dataset \Method	**BC**	**PiT**
Whole	68.51	70.54
Rising	71.28	73.95

Table 3: Performance Comparison for PiT and BC under the whole and rising dataset.

Experiments

In this section, we performed a comprehensive performance comparison involving our PiT and behavior cloning. Models were trained on both the whole dataset and a subset comprising exclusively of the rising dataset, where the score at the last timestep exceeded the initial timestep.

Baseline

We choose behavior cloning as our baseline. Behavior cloning involves training a network to imitate the behavior of a demonstrated or an expert dataset. The network is an MLP with 3 layers and 256 embedding dimensions. It is a form of supervised learning where the model learns to map observations to output actions by mimicking the expert's actions.

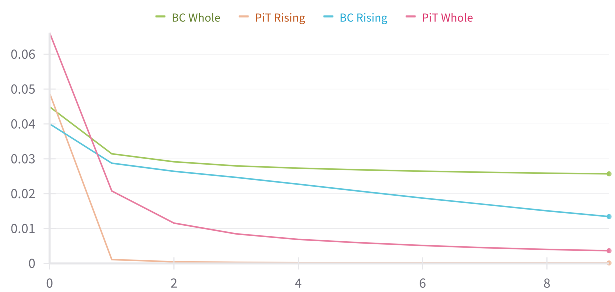

Figure 4: Training loss plot.

From Figure 4, it is evident that the PiT exhibits a lower training loss compared to baseline BC. This lower training loss indicates that PiT has a greater ability to predict the next action accurately on the training set.

Results

In Table 2, we compare PiT's results to the best literature baselines. The results are quantified by a score which is defined in Eqn. 6. Moreover, thanks to the offline RL framework, PiT obtained better data efficiency than the baselines as it doesn't require online environment interactions or labor-intensive manual optimizations by human designers. Therefore, we conclude that PiT has acquired state-of-the-art capabilities for PCSEL inverse design with consistently better performance than baselines. Nonetheless, we recognize that PiT's score is still quite some distance away from the target, which means there's room for improvement in future research.

Discussion

In this section, we conducted a performance comparison between PiT and BC trained on both the whole dataset and the rising dataset. The results are listed in Table 3.

According to the results, we can see that the offline dataset we used will determine the final results. More specifically, if we can train a better RL policy and collect a dataset with higher returns, it is possible to further improve the performance of

Conclusion

In this paper, we investigate the PSCEL inverse design problem through sequential modeling that facilitates the use of offline data and eliminates the need for online interactions. Our simulation experiments show the effectiveness of our proposed framework. We believe that our work points out promising future avenues to design advanced PSCEL lasers and photonics in general. We further analyze the impact of Transformer structure selection and highlight several potential solutions to improve the performance in the future.

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