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TRIAL-AND-ERROR LEARNING FOR MEMS STRUCTURAL DESIGN ENABLED BY DEEP REINFORCEMENT LEARNING

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ABSTRACT

We present a systematic MEMS structural design approach via a "trial-and-error" learning process by using the deep reinforcement learning framework. This scheme incorporates the feedback from each "trial" to obtain sophisticated strategies for MEMS design optimizations. Disk-shaped MEMS resonators are selected as case studies and three remarkable advancements have been realized: 1) accurate overall performance predictions (97.9%) via supervised learning models; 2) efficient MEMS structural optimizations to guarantee targeted structural properties with an excellent generation accuracy of 97.7%; and 3) superior design explorations to achieve one order of magnitude performance enhancement than the training dataset. As such, the proposed scheme could facilitate a wide spectrum of MEMS applications with this data-driven inverse design methodology.

KEYWORDS

Artificial Intelligence, MEMS Design, Design Space Exploration, Deep Reinforcement Learning.

INTRODUCTION

Artificial intelligence (AI) has shown prodigious success in solving complex real-world problems in interdisciplinary fields, such as Google's AlphaGo program [1], drug designing and development [2], material discoveries [3], protein engineering [4], and robotics [5]. In recent years, there has been an increasing interest in applying artificial intelligence to MEMS structural designs due to the complicated multi-physics coupling nature. The goal of such design methodologies is to improve or substitute the conventional time-consuming and compute-intensive design approaches such as finite element analysis (FEA) modeling. Several prior works have shown that artificial intelligence can be applied to predict the properties of MEMS structures accurately through deep neural networks [6, 7] and to customize MEMS devices based on targeted properties using conditional generative adversarial networks (CGAN) [8]. However, these methodologies are focusing on extracting underlying geometric features within the given training dataset and it is very challenging to explore and discover new designs with better performances out of the distributions of the training data.

On the other hand, it has been shown that humans can learn from the "trial-and-error" process [9]. Based on current knowledge, humans can develop strategies to make attempts that are most likely to result in success. By analyzing and summarizing the feedback obtained after each trial, humans can learn how to modify the strategies to improve the probabilities of success. Such a trial-and-error step can be repeated, and the corresponding knowledge is accumulated according to previous experiences. Finally, a sophisticated strategy can be established adaptively to handle the practical problems encountered by humans. Inspired by the "trial-and-error" scheme, a similar principle for MEMS structural design problems to explore the high-dimensional design space can be realized by using the deep reinforcement learning (DRL) algorithm.

In this work, case studies of disk-shaped MEMS resonators are used to demonstrate this trial-and-error-inspired methodology. Supervised learning (SL) is adopted to train several models, namely SL-based analyzers, which can predict the performance of arbitrary MEMS structures accurately (97.9%) and quickly (more than 10^4 times faster than FEA). Equipped with the SL-based analyzer, the DRL agent explores the design space efficiently and achieves a high generation accuracy of 97.7% based on prespecified targeted properties. The proposed DRL algorithm can also be used to find new MEMS designs with extreme physical properties that are out of the distribution of the training dataset for optimal performance, such as quality factors. Results show that MEMS resonators with remarkably high quality factors of one order of magnitude higher than those of both the training dataset and the CGAN approach [8] can be discovered through the proposed DRL scheme. Such methodology could be extended to other MEMS device design problems to open a new approach of using the DRL algorithm for data-driven inverse structural design.

SYSTEM ARCHITECTURE

The proposed DRL framework is illustrated in the flow chart as shown in Fig. 1. The step-by-step optimization strategy enabled by the DRL algorithm represents the core component of this framework. To overcome the low-sample-efficiency nature of reinforcement learning and accelerate the collection process of design-property pairs, supervised learning is utilized to train models that can capture the underlying essential physics for MEMS resonators and predict them accurately. The model is developed via deep residual neural networks as shown in the enclosed region in Fig. 1 and is adopted as the learning environment within which the reinforcement learning agent operates. Disk-shaped MEMS resonator devices [10] with three vibrational modes of interest as shown in Fig. 2 are chosen for case studies. MEMS resonator designs are translated into pixelated images with a resolution of 100 times 100 as free-form design representations while maintaining key geometric features. Over 100k cases of qualified pixelated images are initialized randomly from a topology generator with the depth-first-search (DFS) algorithm as the training data and topological constraints are always satisfied. Finite element analysis is used to numerically analyze these random designs for modal analysis to characterize their vibration responses and extract the associated parameters such as mode shapes, natural frequencies, and quality factors. The designs are subsequently labeled with the calculated vibrational characteristics. After sufficient training iterations in the form of the deep residual neural network, SL-based analyzers are obtained and they can be utilized to predict vibration responses with good accuracy and remarkably less amount of time.

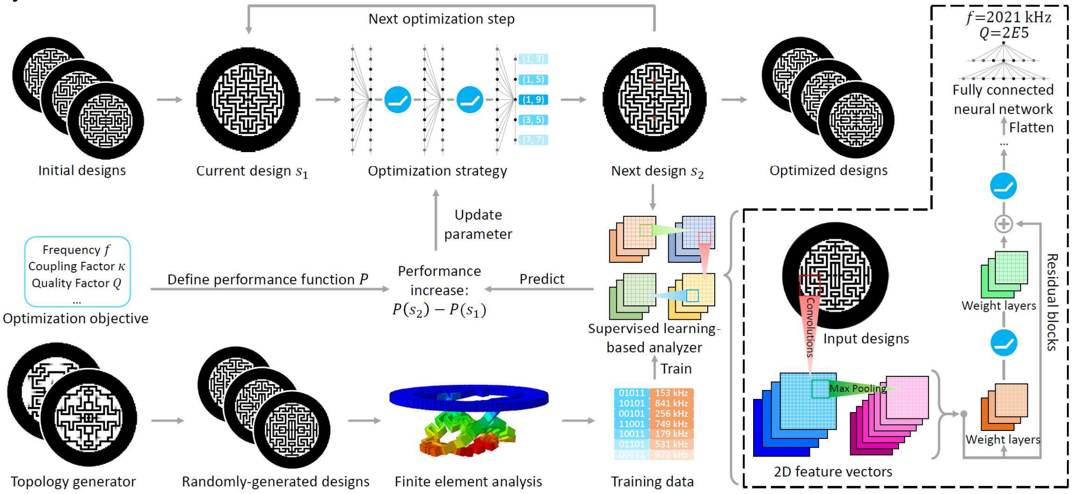

Figure 1: The architecture of the reinforcement learning framework for MEMS structural designs. The region enclosed by dashed lines represents the architecture of the supervised learning-based analyzer to predict the properties of interest. After the design initialization, the proposed DRL agent starts to change the topologies of current designs by an optimization strategy to constitute new designs. The optimization strategy is updated by incorporating feedback (i.e., performance increases according to the optimization objectives, which are predicted from supervised learning-based analyzers) for implementing the design changes. The new optimization strategy is applied to new designs in the next cycle.

With the fast prediction obtained from the SL-based analyzer, the DRL agent utilizes an optimization strategy (represented by the deep neural networks) to constitute new designs to achieve the optimization objectives through a step-by-step, trial-and-error manner. The optimization objective can be specified according to certain design tasks and a corresponding performance function that scores every design candidate from the whole design space can be subsequently determined by analyzing the relative distance between the current design and the desired designs with targeted performance. The reward criterion is defined as the performance value improvement after applying the design modification from the optimization strategy at the pixel level.

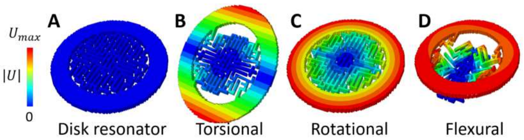

*Figure 2: **A**) Geometry and **B**-**D**) three vibrational modes of interest of a representative MEMS disk resonator.*

The operation pipeline for our reinforcement learning framework can be summarized as follows: In the first step, the MEMS resonator designs are initialized randomly to feed into the trial-and-error processes. Secondly, given the initial design as the current observation, the agent will change the properties (i.e. solid or void) of one set of specific pixels determined by the current optimization strategy to constitute a newly generated design as the next observation. Next, the newly created design is processed through a pre-trained SL-based analyzer to predict the overall performance of targeted properties. Afterward, the optimization strategy for the next iteration is updated by incorporating the reward signal (i.e., performance increment) from the environment as the feedback for implementing the previous modification decision. After several training iterations, a sophisticated optimization strategy would be produced, from which optimized designs with improved properties would be discovered after sufficient optimization steps.

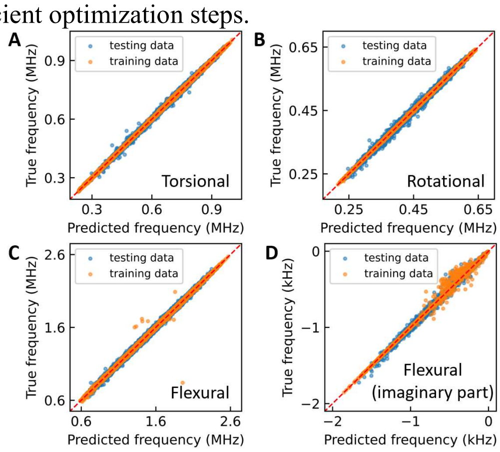

*Figure 3: Predicted frequencies derived by the SL-based analyzer with respect to true frequencies for **A**) torsional mode, **B**) rotational mode, **C**) flexural mode, and **D**) the imaginary part of the frequency for the flexural mode.*

RESULTS AND DISCUSSION

The SL-based analyzers are examined to predict frequencies (real part) for three modes of interest and the imaginary part of the frequency of the flexural mode for the disk-shaped MEMS resonators. The FEA simulation results are treated as ground truths and are compared with predictions from the SL-based analyzers. The accuracy is defined as how close the agreements between simulation results and the residual neural net outputs are. It is observed that all resulting points are located extremely close to the 45-degree line as shown in Fig. 3, indicating that high consistency has been achieved. Table 1 also shows that prediction results highly agree with FEA simulations with an averaged accuracy of 97.9%. For model validation purposes, SL-based analyzers are tested to show great agreements of ~99% with a previously published work [10]. Additionally, the SL-based analyzers are about 4×10^4 faster than that of the traditional FEA approaches, which is consistent with our previous results [6].

Table 1: The performance of the SL-based analyzers.

	Training error	Testing error	Accuracy
Torsional	0.2%	0.8%	99.2%
Rotational	0.1%	0.9%	99.1%
Flexural	0.5%	1.1%	98.9%
Flexural (Im)	2.3%	5.6%	94.4%

Two optimization objectives are further tested to demonstrate the feasibility of the DRL framework to discover MEMS structures with: 1) the multiple targeted modal frequencies (e.g., 0.51 MHz in rotational mode and 2.02 MHz in flexural mode); and 2) the highest quality factor in terms of anchor loss (e.g., in the flexural mode).

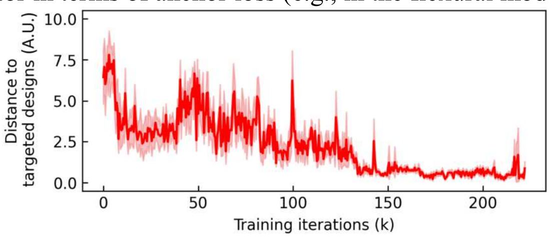

Figure 4: The relative distance to the targeted design with multiple desirable properties versus the training iterations. The red shaded areas represent the uncertainties of generated designs.

For the first optimization objective, it is important to show that the DRL agent can gradually learn how to find the desirable designs through the "trial-and-error" process by minimizing the relative distance to the targeted point. The relative distance, d, is defined as

$$d = \left(f_{flex} - f_{flex}^{*}\right)^2 + \left(f_{rot} - f_{rot}^{*}\right)^2 \qquad (1)$$

where f_{flex} and f_{rot} represent the frequencies of flexural and rotational modes of the current design, respectively, and f_{flex}^{*} and f_{rot}^{*} represent the targeted frequencies of flexural and rotational modes of the desired design, respectively. The performance function is defined to be the negative of the relative distance to the targeted value. Afterward, the DRL agent explores non-trivial decisions for performance improvements in the global design space. After adequate parameter updating steps, a desirable optimization strategy is established which can put forward a series of effective modification steps toward the targeted natural frequencies (0.51 MHz, 2.02 MHz in this example). Figure 4 shows the learning curve of the optimization strategy for modifying designs toward the combination of targeted natural frequencies. The trained optimization strategy is evaluated by measuring the averaged deviation between the natural frequencies of generated designs to that of the targeted designs. Initially, the optimization strategy is far from effective and precise as it always has large fluctuations during the learning process. Gradually, the DRL agent discovers the underlying pattern behind the optimization problem and finally converges to a stable model that can minimize the relative distance to the desired design. Figure 5A shows the distribution evolutions of optimized designs after each optimization step in terms of two targeted variables. Initially, the pre-optimized designs are randomly produced such that they spread over a wide range of natural frequencies with a mean of (381.27 kHz, 1090.98 kHz) and a standard deviation of (60.80 kHz, 229.75 kHz). After applying the first optimization step, the resultant data points advance collectively towards the targeted point with a mean of (399.73 kHz, 1198.27 kHz) and a reduced standard deviation of (58.49 kHz, 261.66 kHz). By the same token, the corresponding mean values will further approach the targeted values and the data points will become less dispersed for every step. After being modified by three successive steps, the optimized designs start to be concentrated near the targeted values. With a seven-step optimization process, the majority of data points reside within the neighboring zone of the targeted location while some outliers that may contain some impeditive features remained to be further improved. After a 10-step optimization process, nearly all data points congregate within a tiny region centered at (513.88 kHz, 2030.90 kHz) with a standard deviation of (12.73 kHz, 42.20 kHz) which represents a high generation accuracy of 97.7%. This step-by-step optimization process verifies the effectiveness of every decision that our powerful DRL-based optimization strategy put forward at each step and further validates the feasibility of deep RL approaches for supervising the design process. A representative design satisfying the objectives of the targeted combination of natural frequencies is exhibited in Fig. 5A. Figure 5B shows the FEA simulation results of the optimized design. The calculated natural frequencies are very close to the targeted combination at 510.08 kHz and 2020.71 kHz, indicating our DRL approach is very effective at precisely achieving the targeted optimal designs.

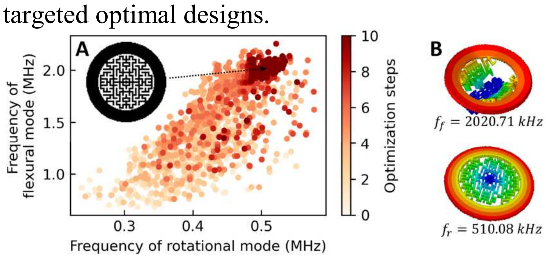

*Figure 5: **A)** The optimization steps (color map) for multiple targeted frequencies (the flexural and rotational modes) and an optimized design example. By applying the optimization strategy, the generated designs collectively move toward the targeted points after each optimization step to result in high generation accuracy of 97.7% after 10 steps. **B)** Flexural (f_f) and rotational (f_r) mode frequencies and the shapes of the optimized design.*

It is also important to show that the proposed DRL framework can be used to discover designs with high quality factors. High quality factor is highly desired for MEMS resonator devices since it represents the low dissipation rate of energy for high efficiency. The quality factor, Q, can be calculated as $Q = -f_r/2f_i$, where f_r is the real part of frequency (i.e. natural frequency), f_i is the corresponding imaginary part. In this study, design optimization of the flexural-mode quality factor is utilized to illustrate the essential ideas of the proposed methodology. The performance function is defined as the predicted quality factor based on SL-based analyzers. Figure 6 shows the learning process curve for the quality factor versus the training iterations, in which the DRL agents gradually produce high-performance designs with the resultant average quality factor at the order of 10^5.

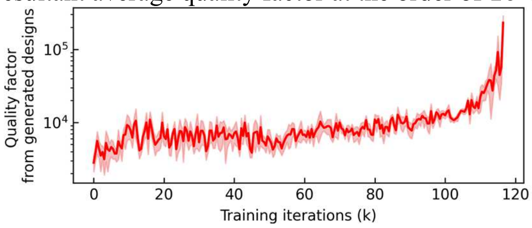

Figure 6: The obtained quality factor versus training iteration plot showing the optimization process. The DRL agent can learn the essential strategy to optimize quality factors which are progressively enhanced with respect to training iterations. The red shaded areas represent the uncertainties of generated designs.

Figure 7 shows the statistic distribution comparison between randomly generated designs and the high-performance designs produced from the RL algorithm. Most of the original designs reside in the lower performance range with the mean value of quality factor around 1.77×10^4 , whereas most of the optimized structure designs obtained by our DRL method reside in the higher performance range, whose mean quality factor can be as high as 2.54×10^5, representing more than one magnitude performance improvement against the initial random designs and the CGAN scheme [8]. This shows that the DRL algorithm has indeed learned the underlying patterns of the top-ranked designs as well as how to improve them in an effective manner. As an application of our high-performance DRL algorithm, the trained neural networks can be served as a top-performed design generator, with much lower computational costs than those of traditional exhaustive approaches.

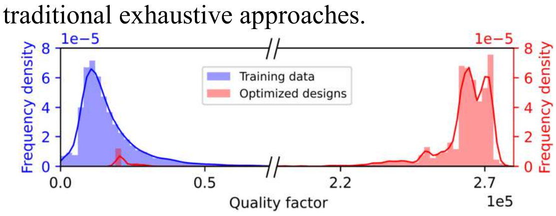

Figure 7: Performance distributions of training data and optimized designs with the high-quality factor objective. The performance of optimized designs can be one order of magnitude higher than that of the training data on average.

CONCLUSION

The framework for using deep reinforcement learning to optimize MEMS structural design in a free-form manner has been proposed and demonstrated. With a sufficient number of training iterations, the proposed DRL-based design methodology can successfully generate MEMS circular disk resonator designs with natural frequencies close to targeted frequencies for multiple modes and with small natural frequency standard deviations. Furthermore, the quality factors can be successfully optimized, being more than one order of magnitude larger than the original randomized resonator designs. The results show great promise in demonstrating that DRL algorithms can be considerably helpful in designing MEMS devices that satisfy all design constraints and parameter requirements while being extremely time and energy efficient. We believe that with reasonable modifications, a similar approach can be developed for the automated design and optimization of other types of MEMS devices in the future.

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