Functional Response Conditional Variational Auto-Encoders for Inverse Design of Metamaterials

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Introduction

Metamaterials are macroscopic composites that contain artificial, three-dimensional, periodic (or not) unit-cell patterns engineered to produce optimized responses to a specific excitation that is unseen in natural materials. [1, 2] Like atoms forming a molecule in natural materials, **metamaterials with various microstructures can lead to different response curves**. To be concrete, for a microstructure with facility topology $\mathbf{x}$, its responses to electromagnetic wave of different frequencies form a complex response curve $\mathbf{y}$. The laws of physics determine that there exists a deterministic function $\mathbf{y} = f(\mathbf{x})$ that maps the facility topology $\mathbf{x}$ to its response curves $\mathbf{y}$.

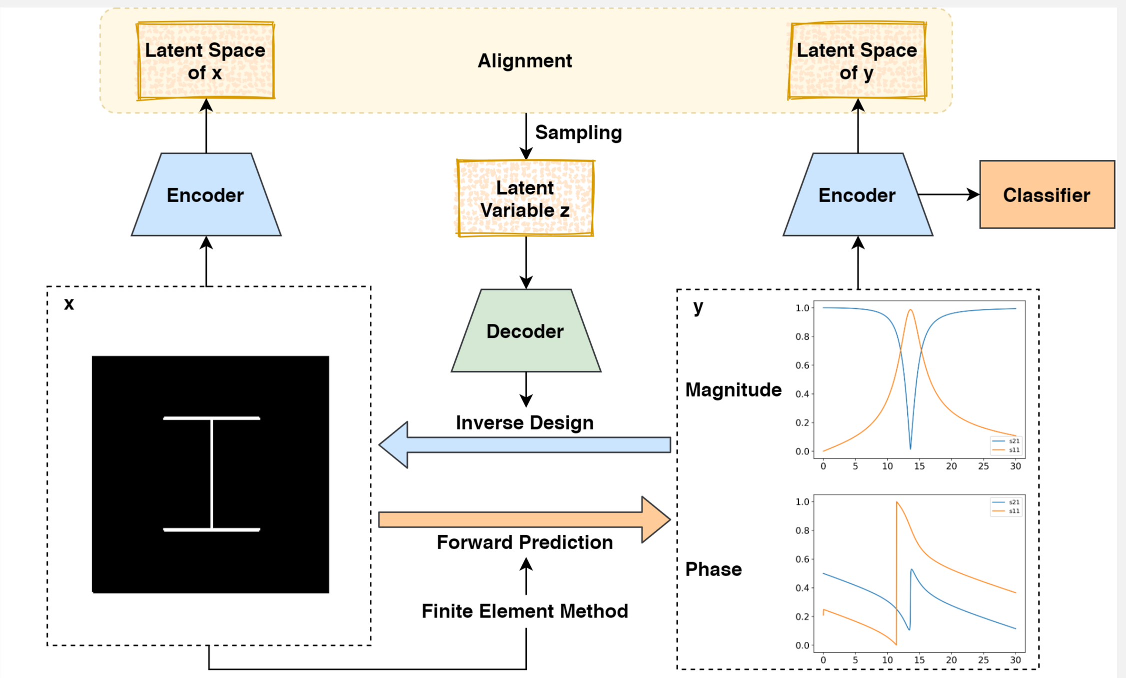
Our goal in this study is to **learn the inverse mapping function $f^{-1}(\cdot)$ from a collection of triplets $\{(\tau_i, \mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^n$**.

Leveraging on the quick development of *deep neural network* (DNN) in recent years, DNN-based inverse design via *variational auto-encoder* (VAE) [3] and *conditional variational auto-encoder* (CVAE) [4] has gained great successes in a broad range of applications.

However, available methods for inverse design based on CVAE assume that **the responses are discrete classification labels**.In this work, we fill in this gap by proposing a novel CVAE framework with functional responses as conditional input (referred to as FR-CVAE).

Method

Figure 1 demonstrates a typical microstructure of the *I*-shape and the corresponding response curves composed of four channels (two magnitude channels and two phase channels). For a collection of design points $\mathbf{x}_1, .., \mathbf{x}_n \in \mathscr{X}$, let τ_i be the topology type of $\mathbf{x}_i$ (e.g., *I*-shape, hexagon-shape and so on), and $\mathbf{y}_i = f(\mathbf{x}_i)$ being the corresponding response curves obtained via FEM simulation.



The proposed FR-CVAE

1. **an encoding network** of $\mathbf{x}$, $\phi_\alpha : \mathbf{x} \to \mathbf{z}$, that maps a design $\mathbf{x} \in \mathscr{X}$ to a lower dimension latent space representation $\mathbf{z} \in \mathscr{Z}$ ($\mathscr{Z} \in \mathscr{R}^p$), which can also be expressed as an encoding distribution $q_\alpha(\mathbf{z}|\mathbf{x}) = \mathrm{N}(\mu_z(\mathbf{x}, \phi_\alpha), \sigma_z^2(\mathbf{x}, \phi_\alpha) \cdot \mathbf{I}_p)$,
2. **an encoding network** of $\mathbf{y}$ referred to as $\phi_\beta : \mathbf{y} \to \mathbf{z}$, that embeds the functional response $\mathbf{y}$ into the same latent space $\mathscr{Z}$ via another encoding distribution $q_\beta(\mathbf{z}|\mathbf{y}) = \mathrm{N}(\mu_z(\mathbf{y}, \phi_\beta), \sigma_z^2(\mathbf{y}, \phi_\beta) \cdot \mathbf{I}_p)$,
3. **a decoding network** $\phi_\gamma : \mathbf{z} \to \mathbf{x}$, that generates an image $\hat{\mathbf{x}} \in \mathscr{X}$ from $\mathbf{z} \in \mathscr{Z}$ via a decoding distribution $q_\gamma(\mathbf{x}|\mathbf{z})$ over the design space $\mathscr{X}$,
4. **a classifier** $\phi_\psi : y \to p_\tau$, which shares the network of ϕ_β except its last layer and utilize a linear layer parameterized by ψ and softmax function to generate the classification probability p_τ.

The loss function of FR-CVAE is composed of three components.

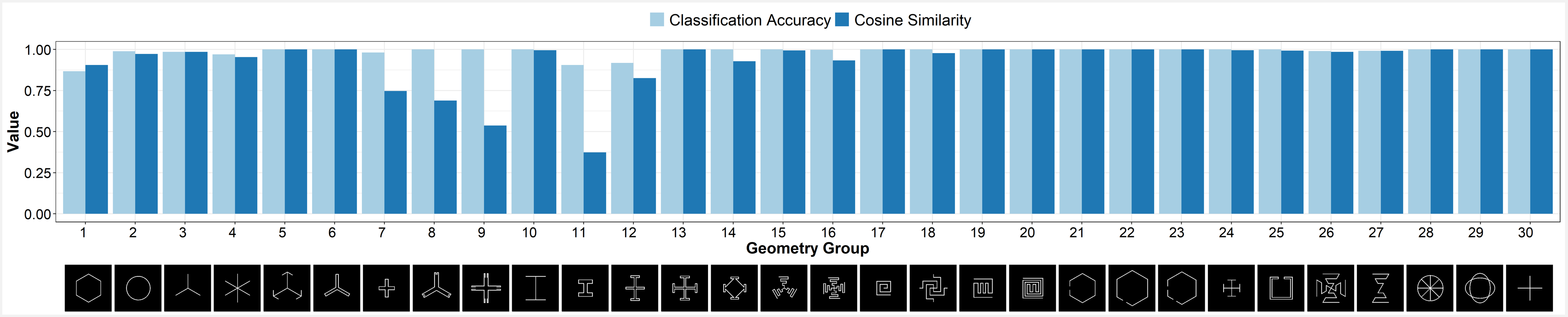
- **the reconstruction loss** $$\mathscr{L}_x(\alpha, \gamma; \mathbf{x}_i) = -\int \Big[\log q_\gamma(\mathbf{x}_i|\mathbf{z})\Big] dq_\alpha(\mathbf{z}|\mathbf{x}_i), \tag{1}$$
- **the classification loss** $$\mathscr{L}_y(\beta, \psi; \tau_i, \mathbf{y}_i) = \mathscr{L}_{CE}(\beta, \psi; \tau_i, \mathbf{y}_i) + \mathscr{L}_{Triplet}(\beta; \tau_i, \mathbf{y}_i), \tag{2}$$
- **the alignment loss** $$\mathscr{L}_{x\sim y}(\alpha, \beta; \mathbf{x}_i, \mathbf{y}_i) = w_1 \cdot KL\big(q_\alpha(\cdot|\mathbf{x}_i)||\pi_0(\cdot)\big) + w_2 \cdot KL\big(q_\alpha(\cdot|\mathbf{x}_i)||q_\beta(\cdot|\mathbf{y}_i)\big), \tag{3}$$

Assembling all these components together, we come up with the following joint loss function:

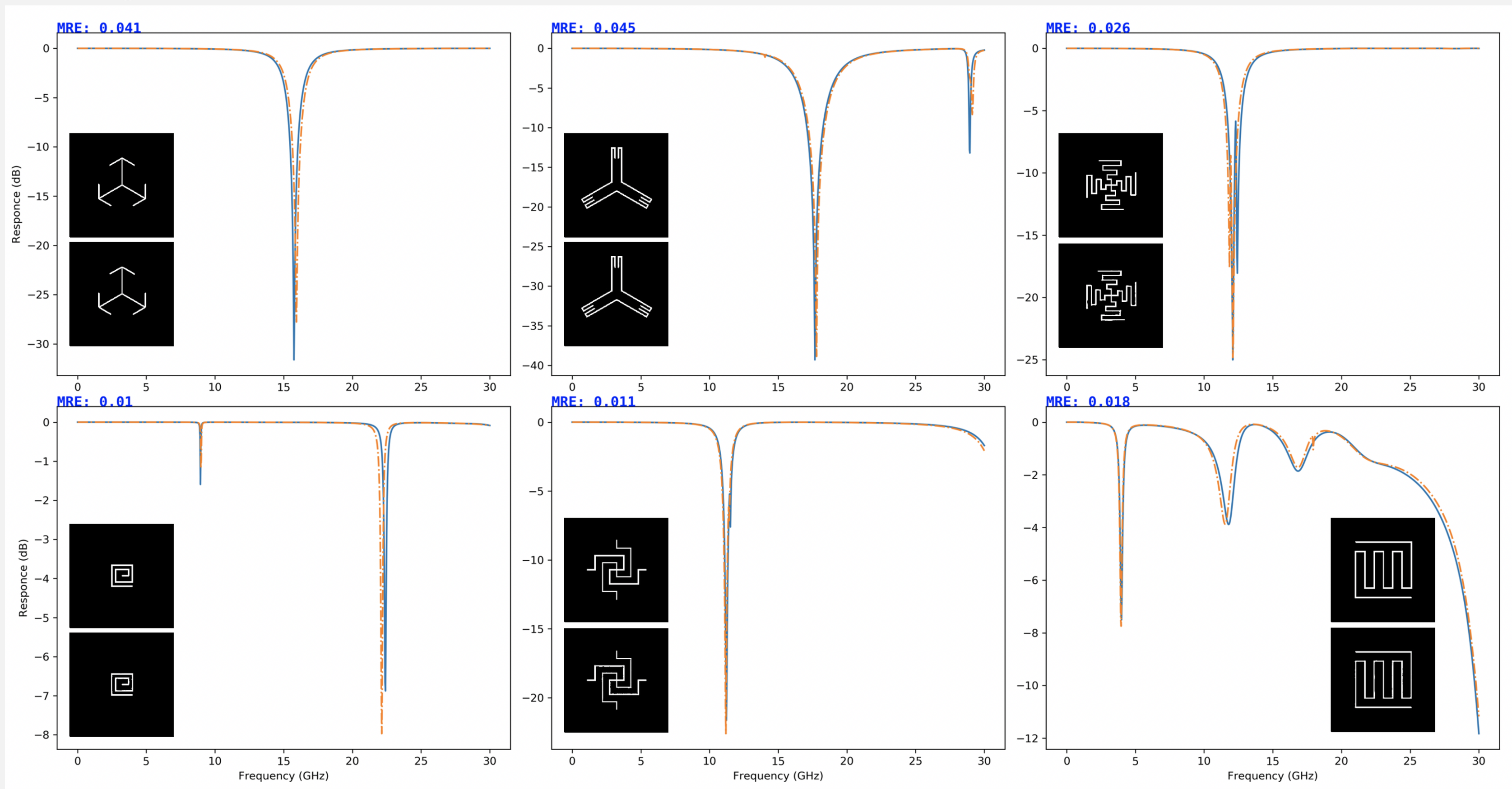
$$\mathscr{L}\left(\Theta \mid \{(\tau_i, \mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^n\right) = \sum_{i=1}^n \{\mathscr{L}_x(\alpha, \gamma; \mathbf{x}_i) + \mathscr{L}_y(\beta, \psi; \tau_i, \mathbf{y}_i) + \mathscr{L}_{x\sim y}(\alpha, \beta; \mathbf{x}_i, \mathbf{y}_i)\}. \tag{4}$$

Important Result

1. **Numerical evaluation** of the proposed model with ϕ_β being Swin-Transformer. 1-30 represent the topology types, each of which contains samples from the test data set.



2. **On-demand inverse design**. The two insets are the ground-truth design patterns (up) whose response curves are solid blue and retrieved design patterns (down) whose response curves are dashed yellow.



Experimental Setup

Dataset

- **61,992 microstructure patterns**, where the black pixels stand for substrate and the white ones are metal material, belonging to **30 topology types** and their **EM response curves** (over the frequency region of 0.1-30GHz)

Implementation Details

- 80% training set + 20% testing set
- *Adam optimizer* through minibatch gradient descent for 1,000 epochs with the batch size set to be 256, which takes about fifteen hours by using 2 Nvidia Telsa P100 16GB GPU cards

Conclusion

On a data-driven basis, the proposed novel learning framework not only can serve as a comprehensive and efficient tool that **accelerates the design**, **characterization**, and even **new discovery** in the research domain of metamaterials, but also has the potential to resolve other problems with similar structures.

- Solving the data problems of complex microstructures and complex responses
- Avoiding the time-consuming case-by-case numerical simulations

References

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