A Quantum-Inspired Probabilistic Model For the Inverse Design of Meta-Structures

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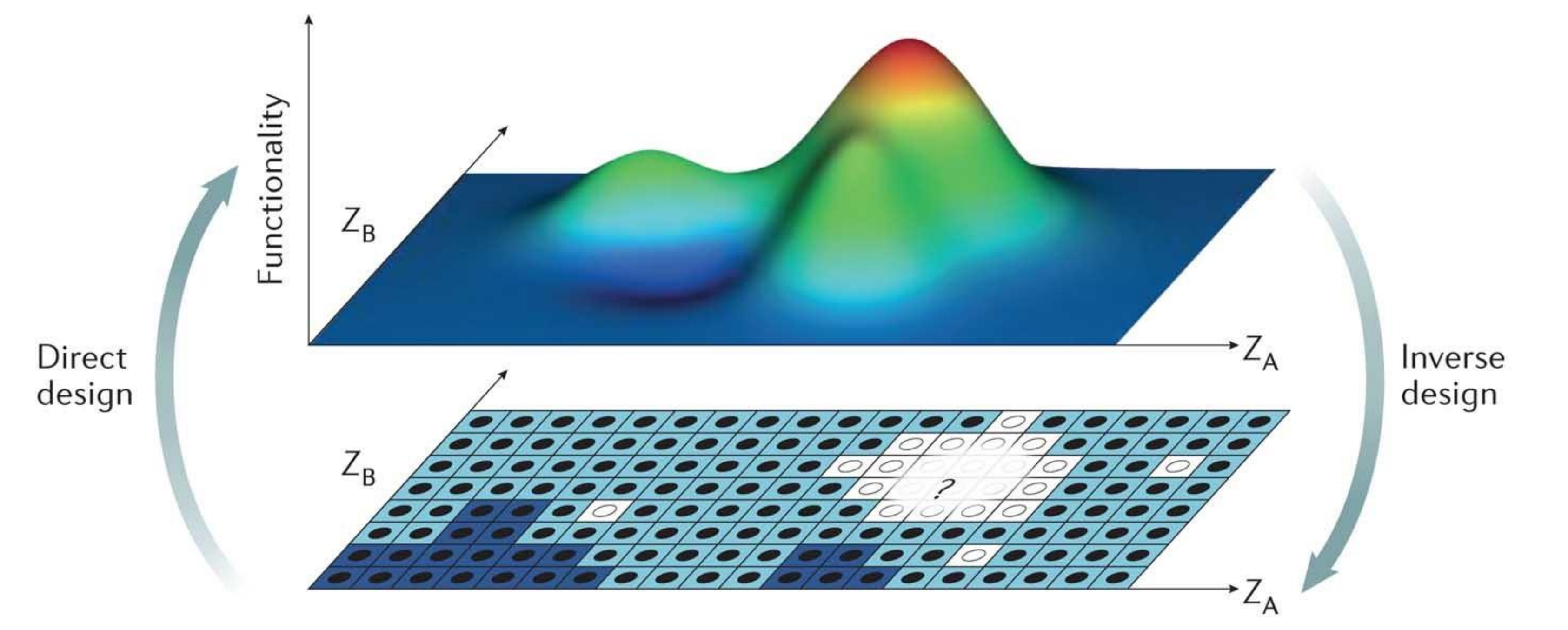
Inverse Design



Contributions

We propose a quantum-inspired model for marginal density recovery, which traces over other particles to attain marginal values of a joint density. Alternatively, we propose a *probability-density-based network (PDN)* for the multivalued inverse design to provide all plausible structural design solutions for desired functionality. We show that PDN leads in all the three qualities: *accuracy, efficiency, output variety*, outperforming VAE & TNN.

Methodology

In quantum theory, we can recover the marginal density matrix via trace operation.

$$\rho_{S_1} = tr_{S_{2,\dots,n}}(\rho_S) = \sum_{j=1}^{n} {}_{S_{2,\dots,n}}\langle j|\rho_S|j\rangle_{S_{2,\dots,n}}$$

This allows us to recover single result mixed in a joint density matrix. In inverse design, we can optimize a joint density for a multivalued physical relation and get each result. PDN views output as quantum superposition of eigenstates, i.e. Gaussian distributions.

$$|\Psi\rangle = c_1|\Psi_1\rangle + c_2|\Psi_2\rangle + \dots + c_m|\Psi_m\rangle + \dots = \sum_m c_m|\Psi_m\rangle$$

In von Neumann measurement scheme, quantum states of an open quantum system evolve with environmental states, so that interference terms can be considered as 0

$$p(x) = |c_1|^2|\Psi_1(x)|^2 + \dots + |c_m|^2|\Psi_m(x)|^2, \qquad \sum_m |c_m|^2 = 1$$

Following maximum likelihood estimation, PDN is proved to be equivalent to a linear superposition of ANNs and each only fits to a single label. The output layer of PDN is a class of gaussian distributions parameterized by weights, means, and deviations that

$$y \sim \sum_{i=1}^{m} \pi_i(x) N(\mu_i(x), \sigma_i(x)), \qquad \sum_{i=1}^{m} \pi_i(x) = 1$$

where x denotes the desired transmission (input), y denotes corresponding structure (label), $\pi_n(x)$ denotes normalized weight of the nth distribution, N denotes the Gaussian distribution density. The maximization of $p(y|x)$ defines the optimization objective.

$$\theta^{MLE} = argmax_\theta \prod_{i=1}^{n} p_{model}(y_i|x_i;\theta)$$

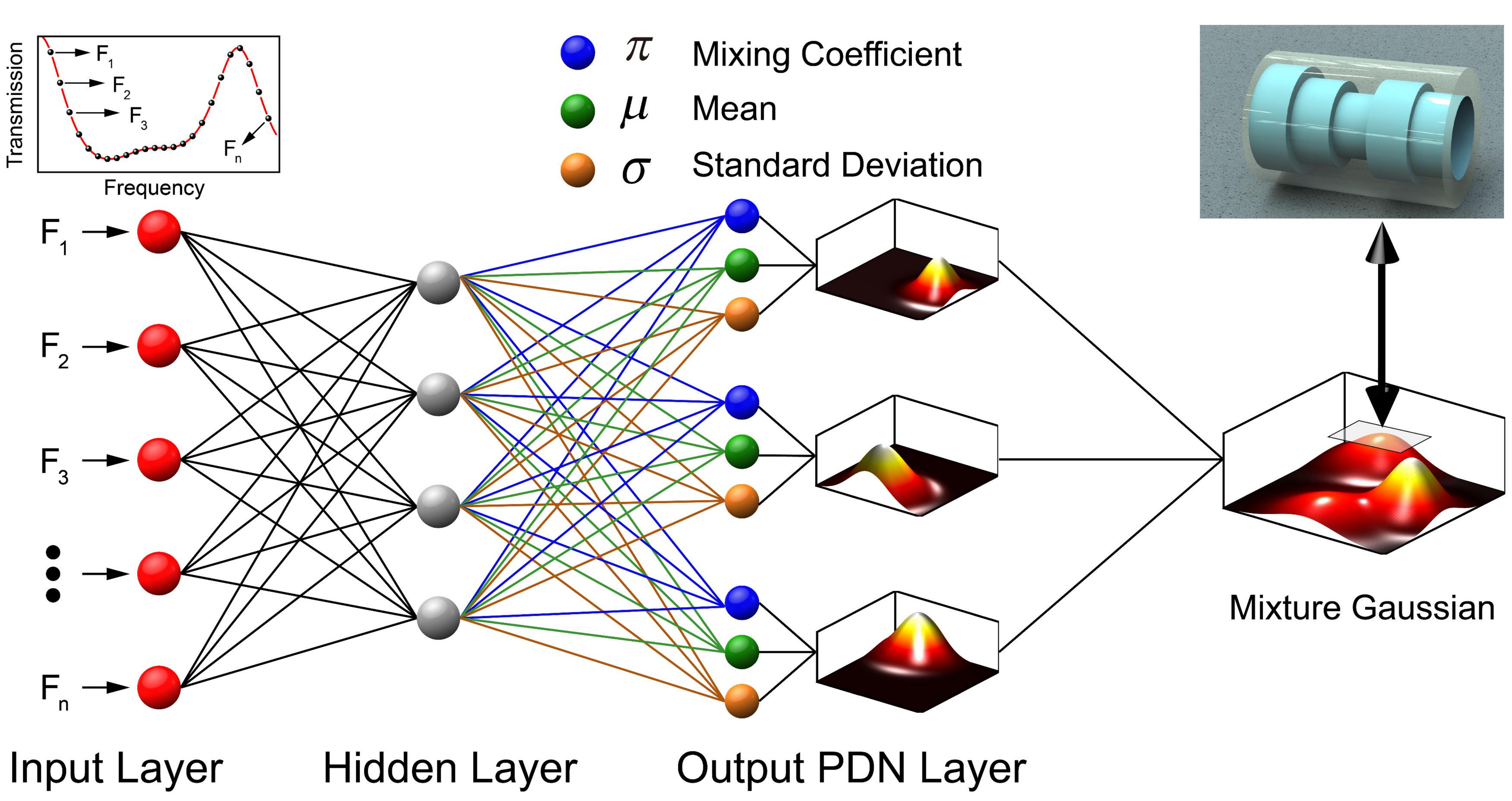


Fig. 1. The architecture and mechanism of proposed PDN.

Results

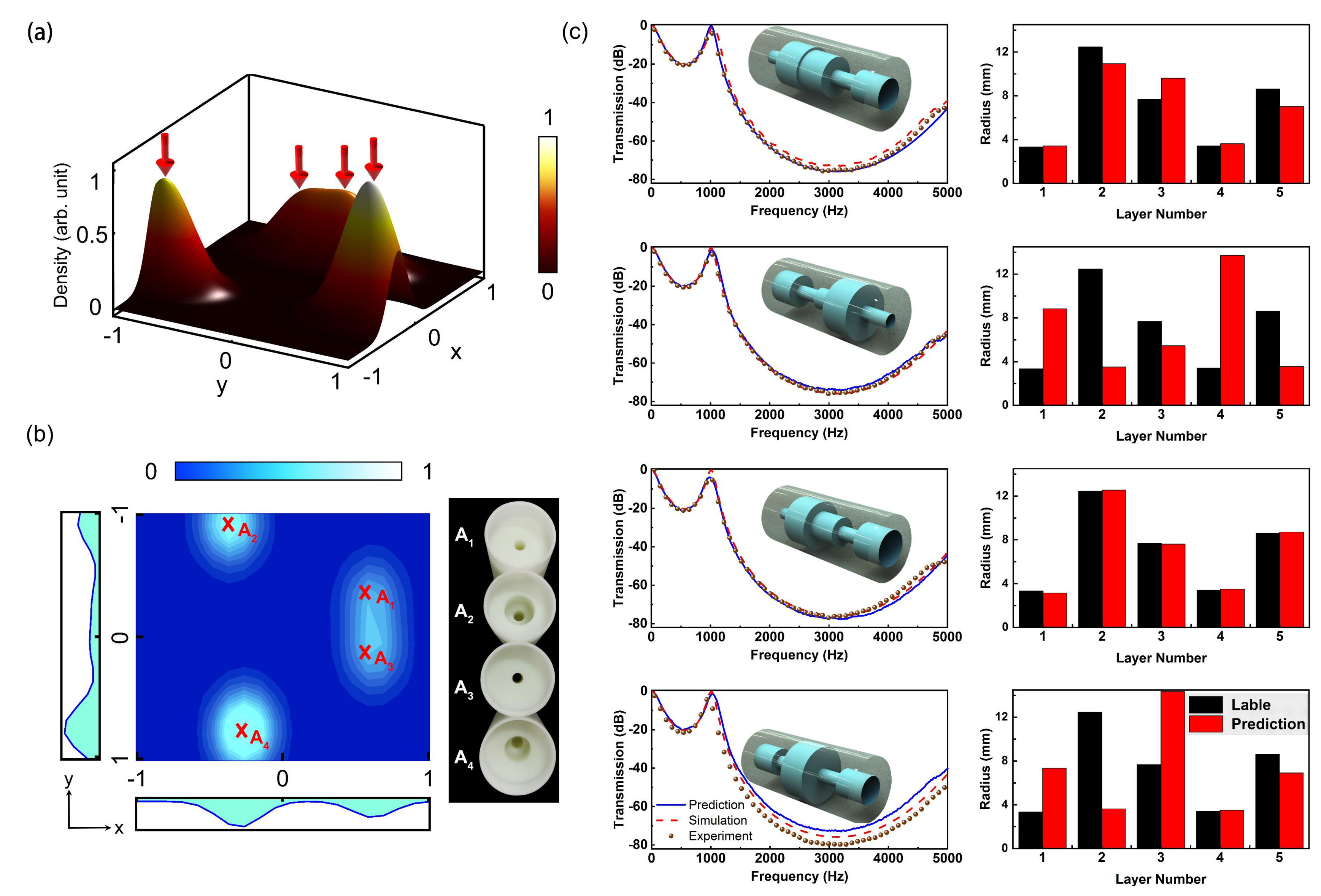


Fig. 2. Evaluation of the first samples predicted by PDN. (a) Four structures were sampled from the mixed Gaussian. (b) The position of samples and the photo of materials. (c) Comparison of transmissions/structures of all the four samples. Here, 'prediction' refers to predicted transmission or structure, 'simulation' refers to the desired transmission, 'experiment' refers to the measured transmission of the predicted structure. Four different structures all produce very similar transmissions close to the desired transmission as a result of multivalued prediction.

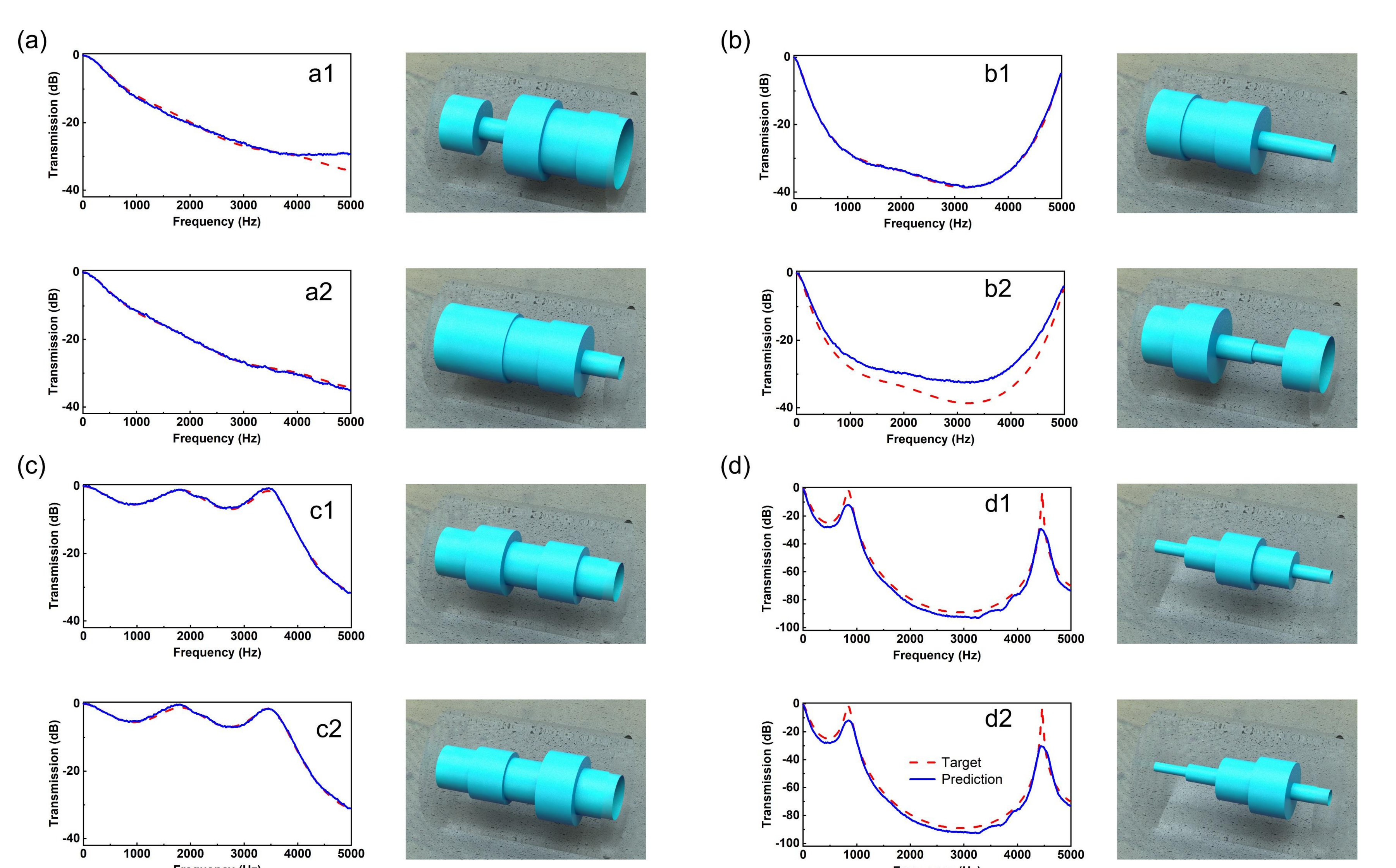
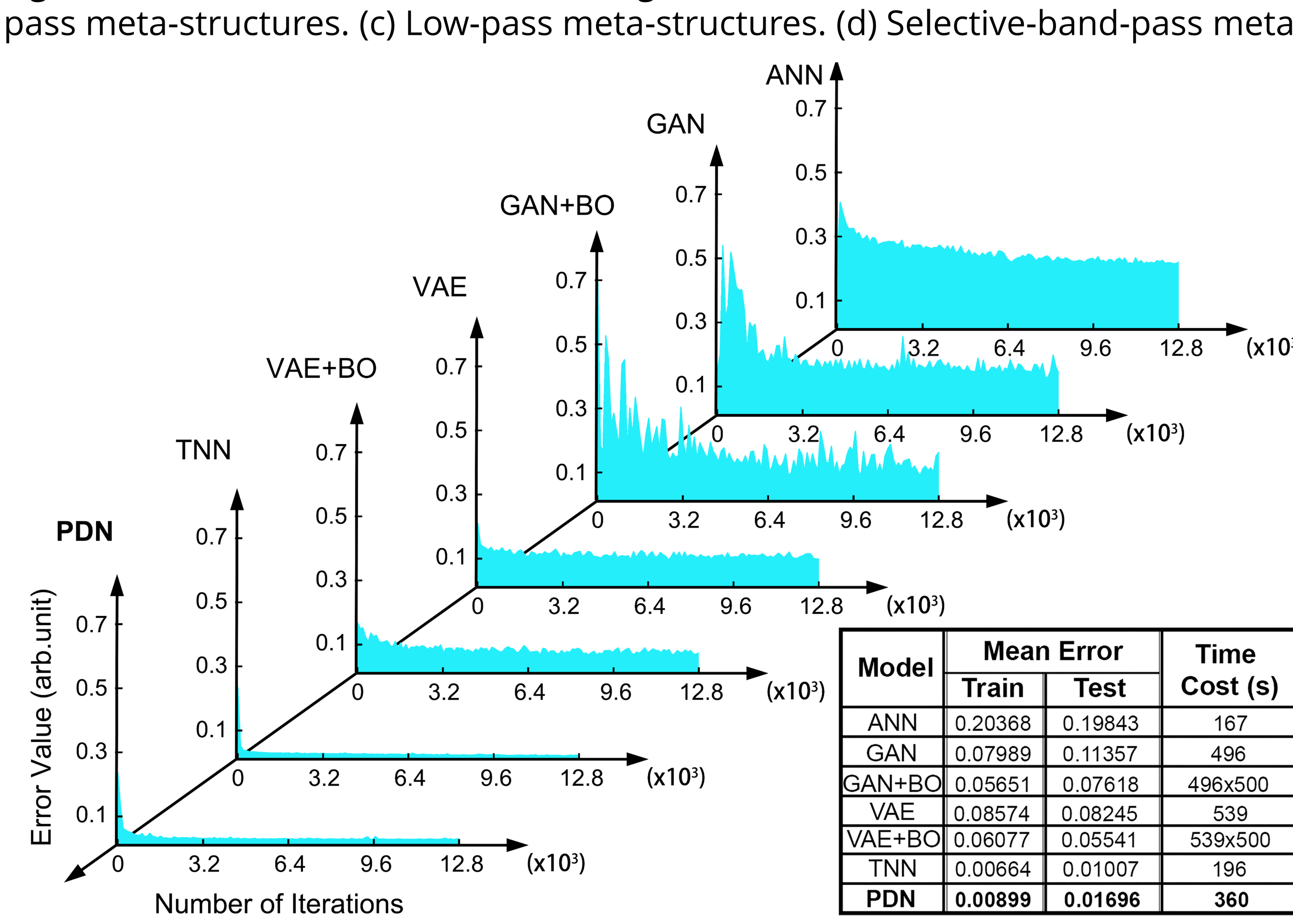


Fig. S2. Additional PDN on-demand design instances. (a) Anechoic meta-structures. (b) High-pass meta-structures. (c) Low-pass meta-structures. (d) Selective-band-pass meta-structures.



Model	Mean Error		Time Cost (s)	Output Variety
	Train	Test		
ANN	0.20368	0.19843	167	×
GAN	0.07989	0.11357	496	√
GAN+BO	0.05651	0.07618	496x500	√
VAE	0.08574	0.08245	539	√
VAE+BO	0.06077	0.05541	539x500	√
TNN	0.00664	0.01007	196	×
PDN	**0.00899**	**0.01696**	**360**	√

Fig. 4. Comparison of different deep learning models for inverse design.