A “generative” model for computing electromagnetic field solutions

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Motivation

“Inverse design” problems are pervasive throughout physics, especially in photonics [1], and involve simulating electromagnetic fields within a structure at each iteration of the design process, typically with the finite-difference frequency-domain (FDFD) method. FDFD simulations can be computationally expensive and scale poorly with design dimensions, especially in 3D. In many cases, approximate field solutions are sufficient. A machine learning model to compute approximate EM fields for a structure could reduce this computational bottleneck allowing for much faster inverse design processes. [2]

Unsupervised learning: Maxwell residual

Maxwell’s equations in non-magnetic, uncharged linear material (typical environment):

$$\nabla \times \vec{H} = \vec{\epsilon}\frac{\partial}{\partial t}\vec{E} + \vec{J} \qquad \nabla \times \vec{E} = -\mu_0 \frac{\partial}{\partial t}\vec{H}$$

FDFD steady state solution $\partial_t \to \omega$, rearrange to solve for “Maxwell residual” expression:

$$\left[(\nabla \times \nabla \times) - \omega^2 \mu_0 \vec{\epsilon}\right] \vec{E} - \vec{J} = \vec{0} \equiv \vec{\mathcal{L}}_M$$

Element-wise measure of realism of predicted field $\vec{E}$

Data and features

- Given an EM source in a cavity containing arbitrary permittivity distribution, predict electric field
- Unsupervised training: arbitrarily many randomly generated permittivity structures, no labels needed
- Validation: generate unseen permittivities, compare against FDFD results calculated using `angler` [3]

References

[1] A. Y. Piggott, J. Lu, T. M. Babinec, K. G. Lagoudakis, J. Petykiewicz, and J. Vuckovic, “Inversedesign and implementation of a wavelength demultiplexing grating coupler,”Scientific Reports,2014,ISSN: 20452322.DOI:10.1038/srep07210.
[2] J. Peurifoy, Y. Shen, L. Jing, Y. Yang, F. Cano-Renteria, B. G. DeLacy, J. D. Joannopoulos,M. Tegmark, and M. Soljacic, “Nanophotonic particle simulation and inverse design usingartificial neural networks,” Science Advances, vol. 4, no. 6, pp. 1–8, 2018,ISSN: 23752548.DOI:10.1126/sciadv.aar4206.
[3] T. W. Hughes, M. Minkov, I. A. D. Williamson, and S. Fan, “Adjoint method and inverse designfor nonlinear nanophotonic devices,” Nov. 2018. [arXiv preprint]. Available:https://arxiv.org/abs/1811.01255.4
[4] Facebook AI Research, “PyTorch: tensors and dynamic neural networks in Python with strongGPU acceleration,” 2018. [Online]. Available:https://pytorch.org/.

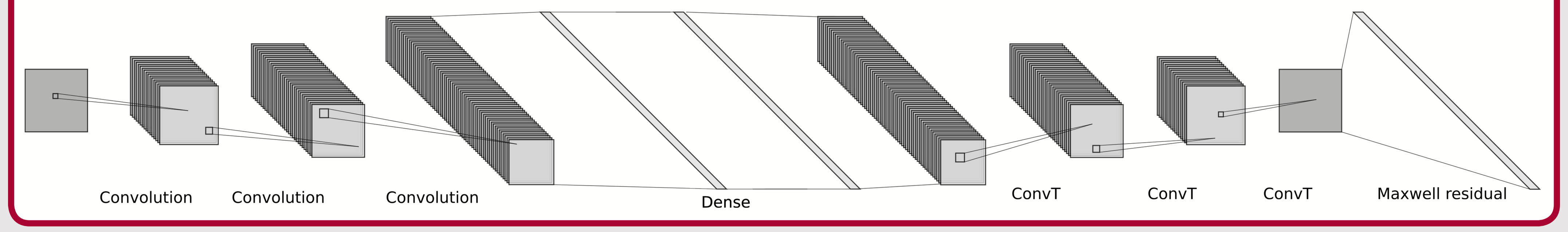
Model approach and architecture

Model learns to compute fields from structure completely unsupervised

- Inputs: permittivity structure $\vec{\epsilon}$, source location $\vec{J}$ (constant)
- “Generator” maps permittivity to predicted fields $G : \vec{\epsilon} \to \vec{E}$
- “Discriminator” (non-trainable) evaluates realism of fields $D : \vec{E} \to \vec{\mathcal{L}}_M$
- Loss is $\mathcal{L}^{(i)} = D(G(\vec{\epsilon}^{(i)}))$

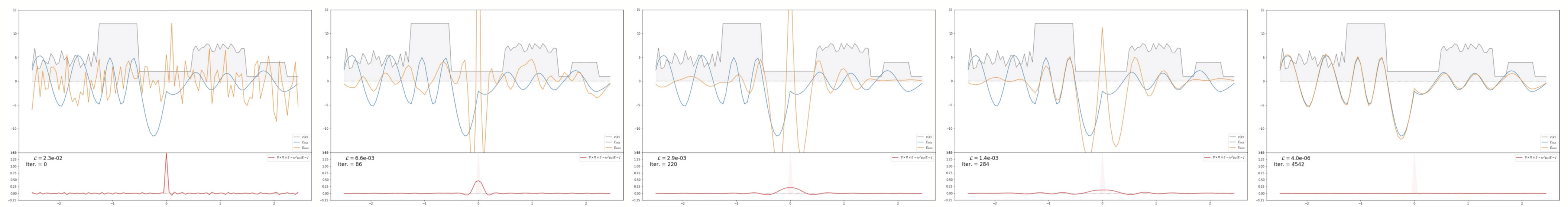
Many architectures tested, best model similar to convolutional autoencoder

- Convolutional / dense / transposed convolutional, dropout(p=0.1) and ReLU (sans last)
- Model implemented in PyTorch [4], trained on NVIDIA Tesla K80

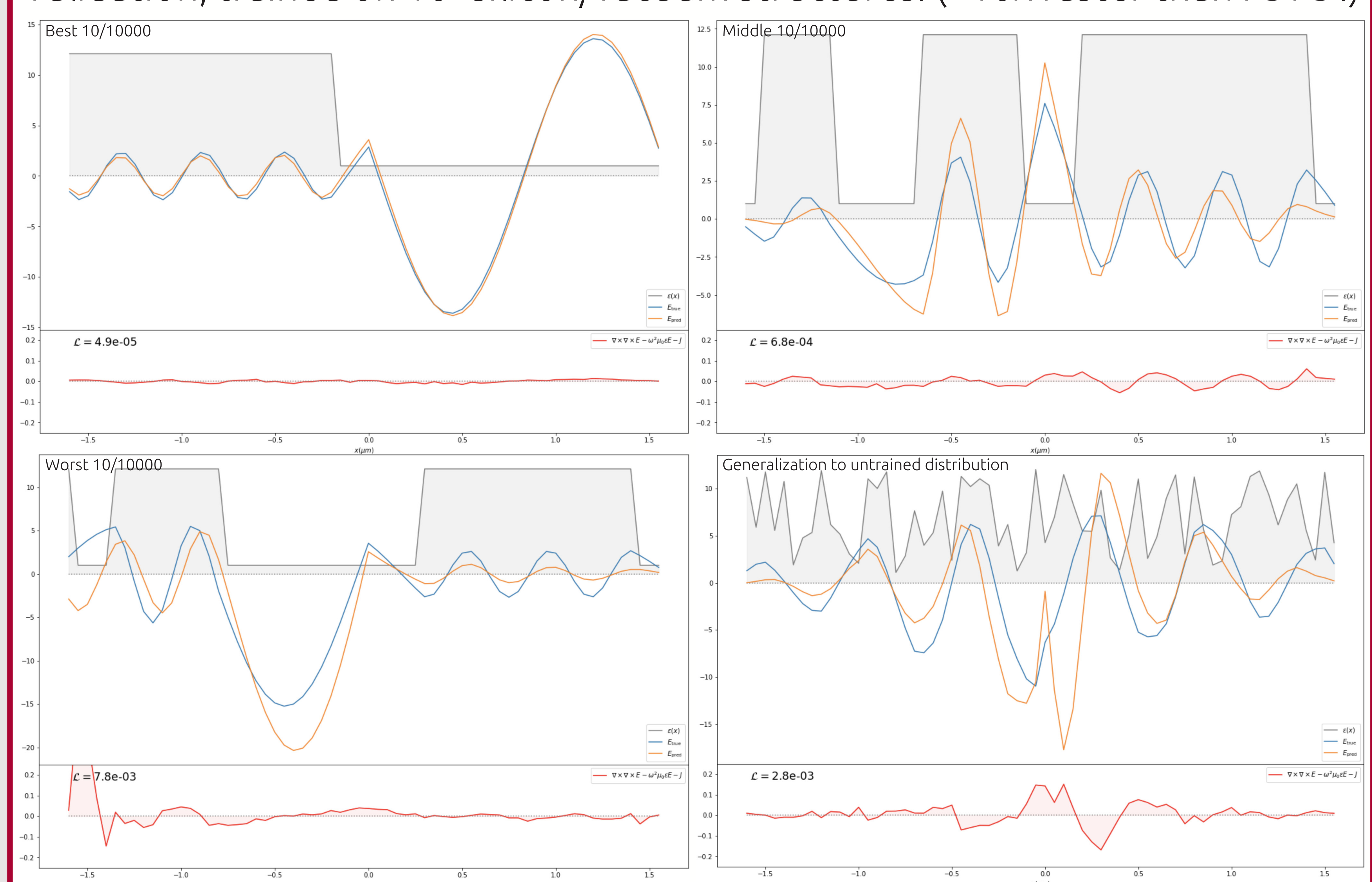


Results

Progression of training model on single permittivity input only:

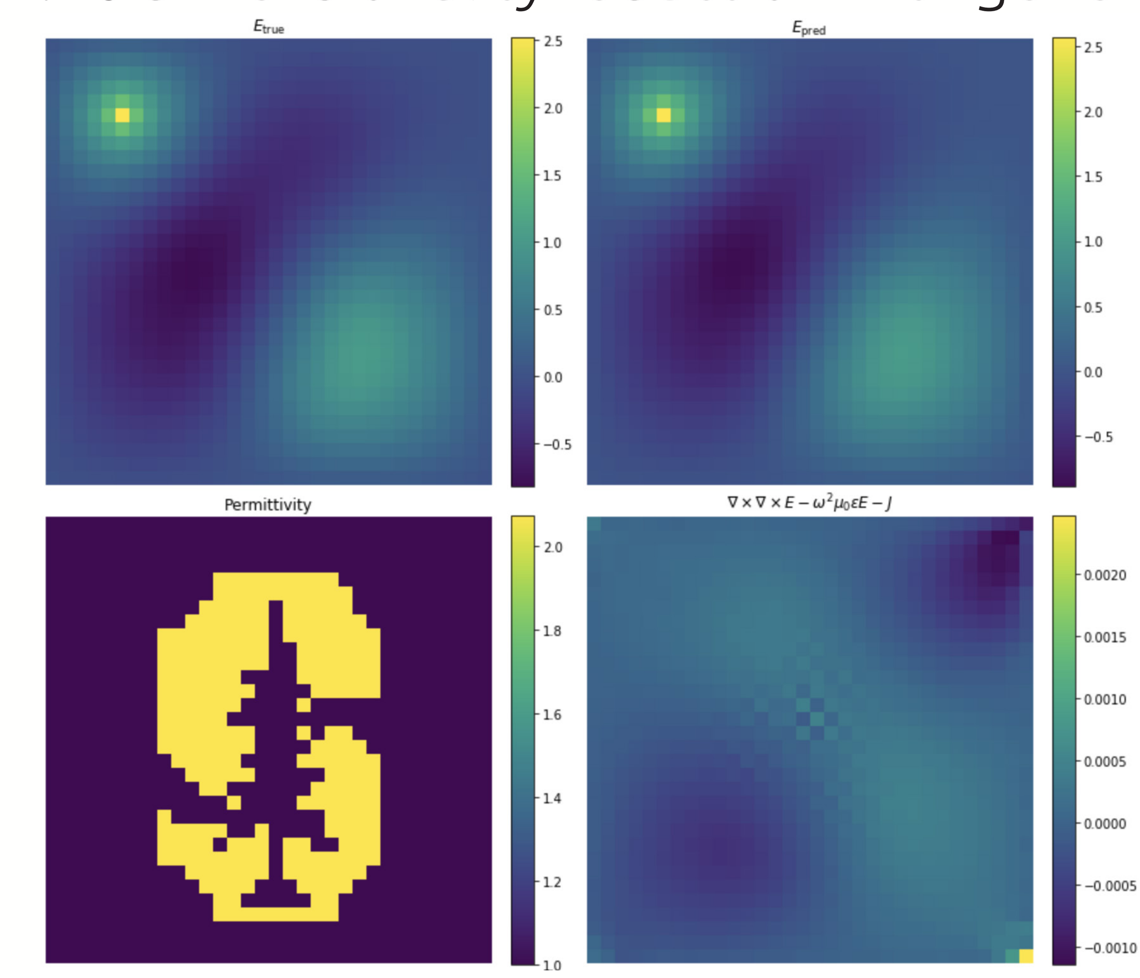


Validation, trained on 10^6 silicon/vacuum structures: (>10x faster than FDFD!)

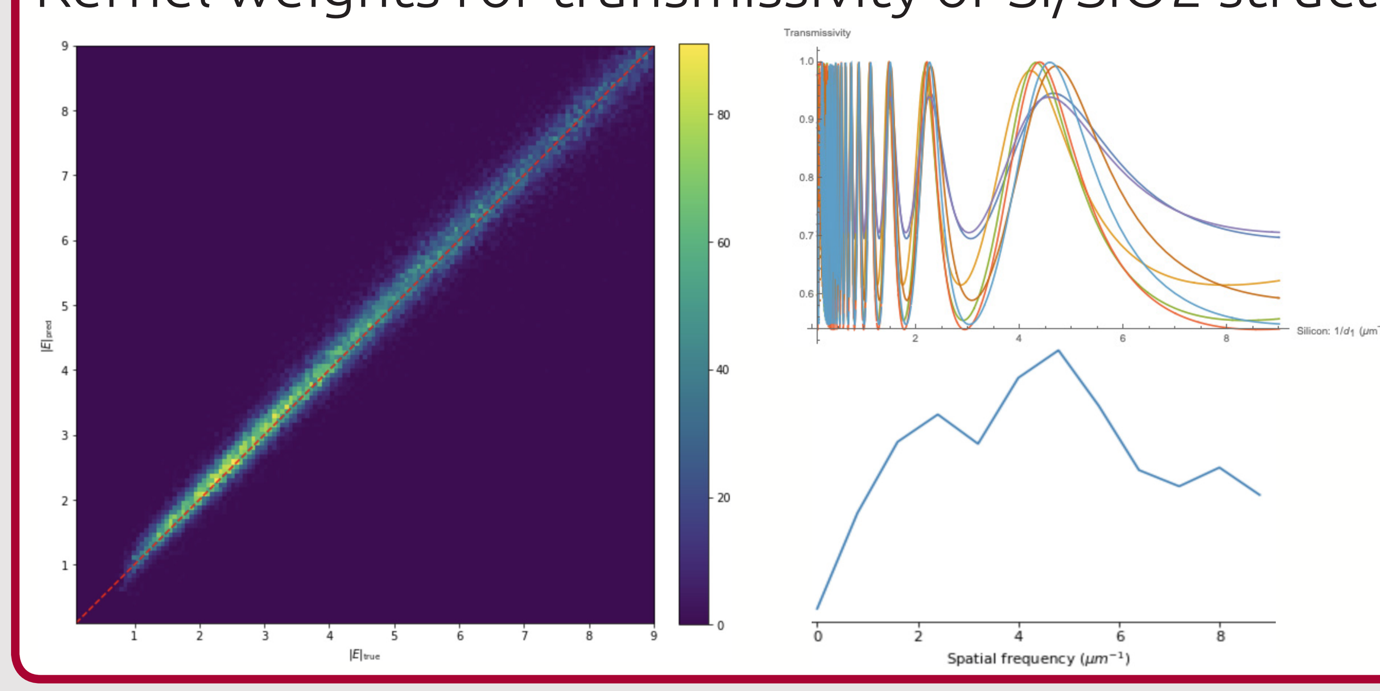


Related findings

1:16 dimensionality reduction with generative model:



Kernel weights for transmissivity of Si/SiO2 structures:



Discussion

- Training unsupervised model on single permittivity converges to FDFD results even for pathological structures
- Convolutional / dense / deconvolutional architecture ideal for cavity simulations - combines local and nonlocal factors
- Model performs well when trained on many permittivities, can generalize to permittivities outside training distribution
- More than 10x speedup over FDFD method!
- Dimensionality reduction and physical interpretability

Future work

- Predicting complex (non-cavity) fields - trickier to do
- 3D model to “seed” iterative FDFD solver, faster performance
- Generalizable dimensionality reduction for 2D/3D systems

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