Modeling and Optimization of Optical Devices using a Variational Autoencoder

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Overview

Optical thin film systems are structures composed of stacked layers of different materials. They find applications in areas such as:

- Solar cell design
- Ellipsometry and metrology
- Radiative cooling
- Dielectric mirrors

The main property of interest is the transmission spectrum, which has a complicated dependence on the parameters of the thin film stack. This makes thin films a good model system for the investigation of machine learning techniques in optical device design [1].

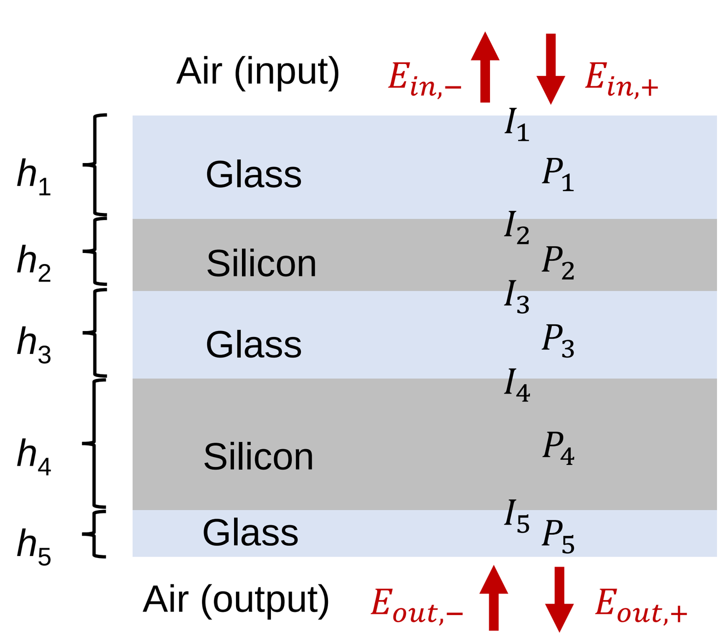
We use a variational autoencoder (VAE), which encodes a representation of data in a latent space using neural networks [2,3], to study thin film optical devices. VAEs can learn physics of thin film devices, generate new devices, and show potential for designing devices with arbitrary spectral responses.

Data

Our data consists of the parameters (layer thicknesses h_n) of a thin film optical device and its discretized transmission spectrum (T_j). 100,000 devices are randomly generated and the transmission spectra are found using transfer matrix simulations. We generate an additional 1,000 for the testing set.

The features consist of the five layer thicknesses and the 101-point discretized transmission spectrum.

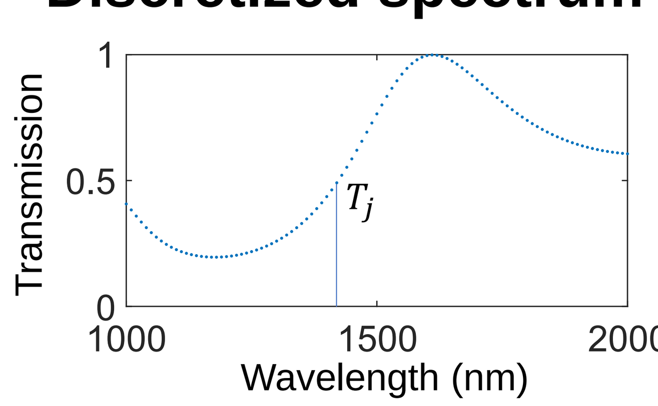
Device



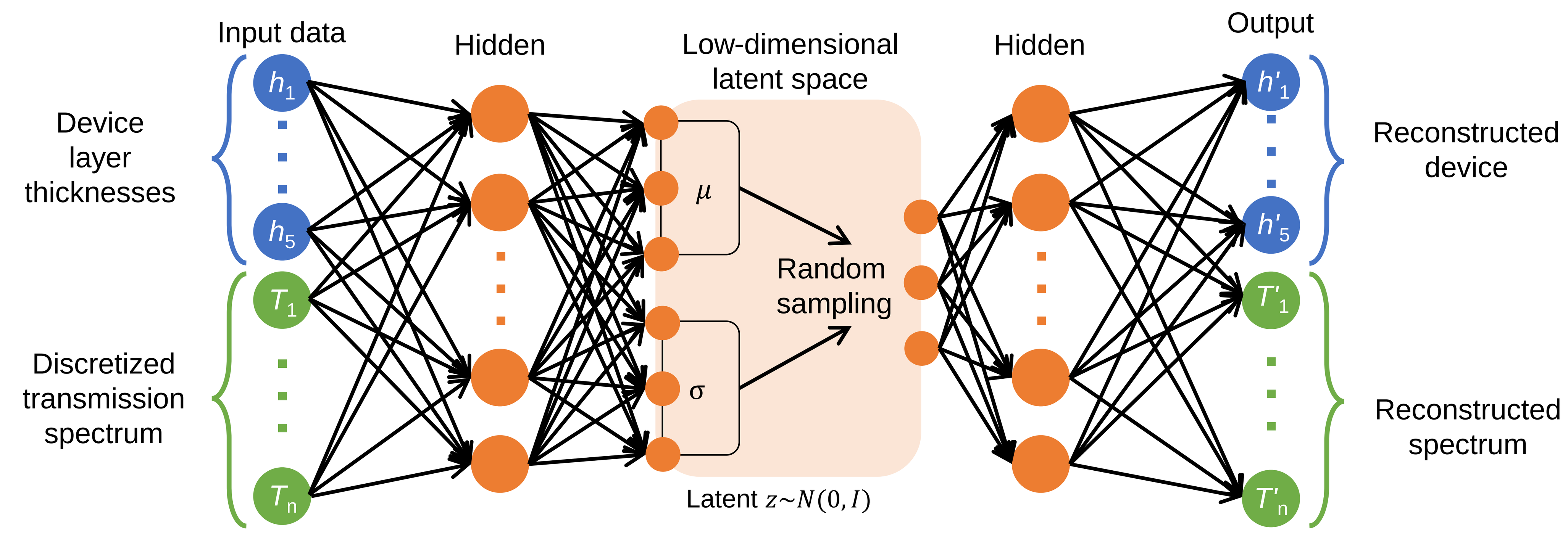
Transfer matrix model

$$\begin{pmatrix} E_{in,+} \\ E_{in,-} \end{pmatrix} = I_1 P_1 I_2 \dots P_n I_{n+1} \begin{pmatrix} E_{out,+} \\ E_{out,-} \end{pmatrix}$$

Discretized spectrum



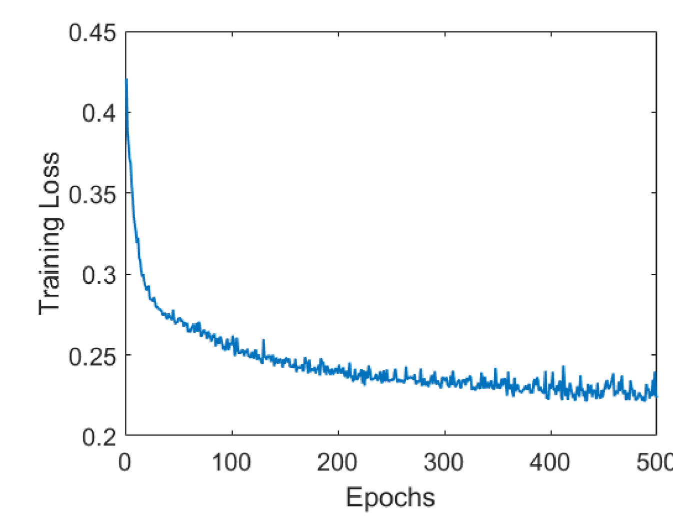
VAE Network Architecture



Our network is based on a PyTorch example by D. Kingma and C. Botha [4,5].

Encoding: 80 hidden neurons + ReLU
Latent Space: 3 dimensions
Decoding: 80 hidden neurons + sigmoid
Loss: Reconstructed MSE + KL divergence

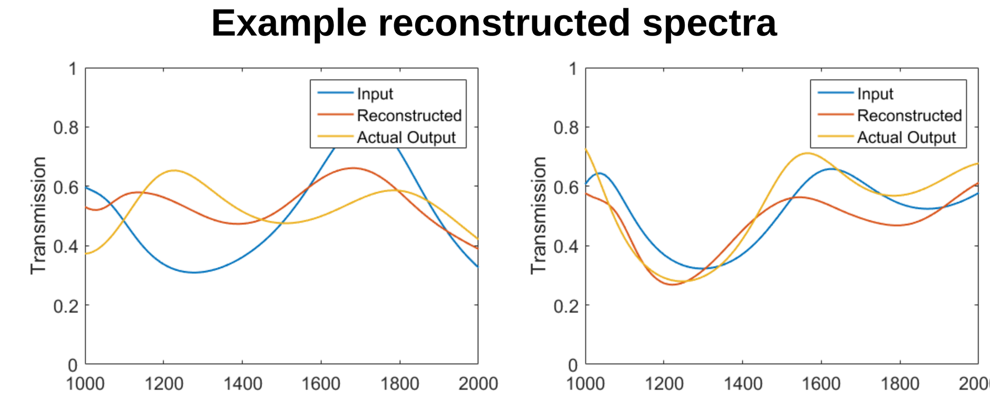
Model	Recon. MSE	Accuracy MSE
PCA	4.89	17.87
VAE	0.164	1.17



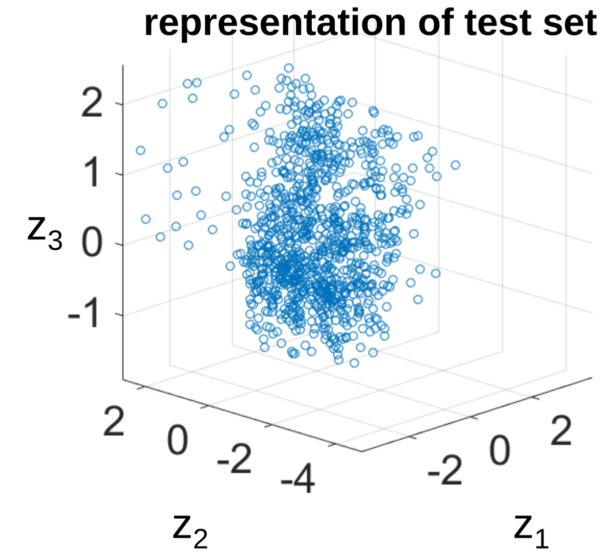
Results

Partial to full reconstruction is possible after compression to the 3-dimensional latent space. New devices and their predicted spectra can be generated by randomly sampling the latent space.

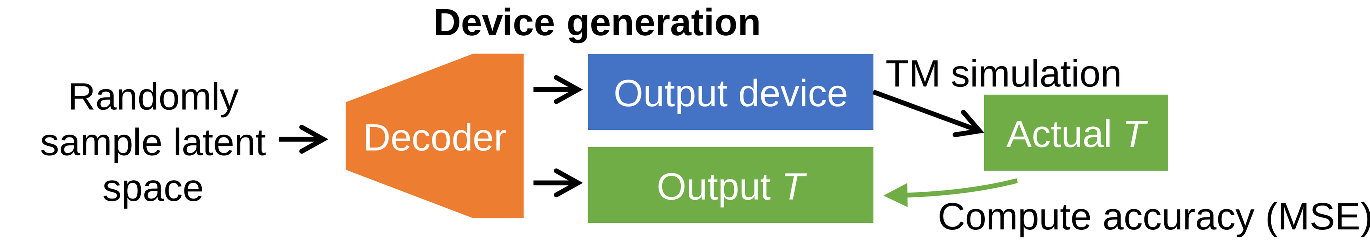
Example reconstructed spectra



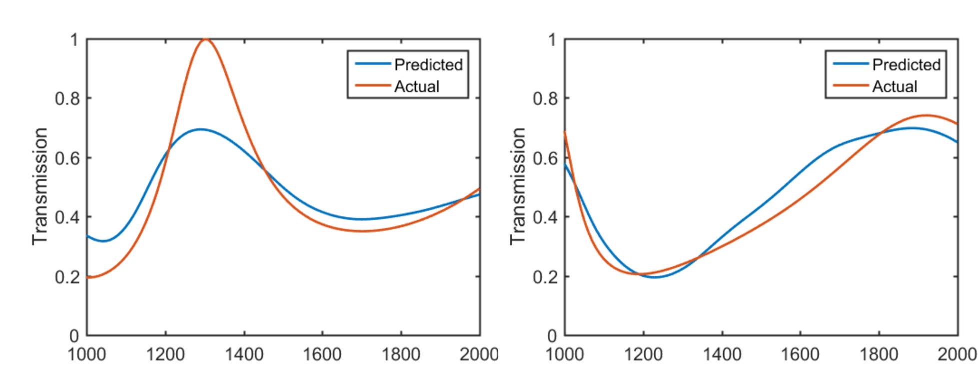
Latent space representation of test set



Device generation



Generated device examples



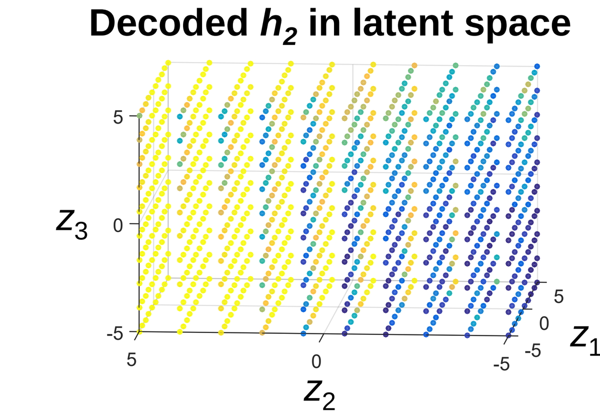
Discussion

Latent variables are strongly correlated with the most physically important parameters (thicknesses of high-refractive index layers), indicating that the network automatically learns the important physical parameters of the model.

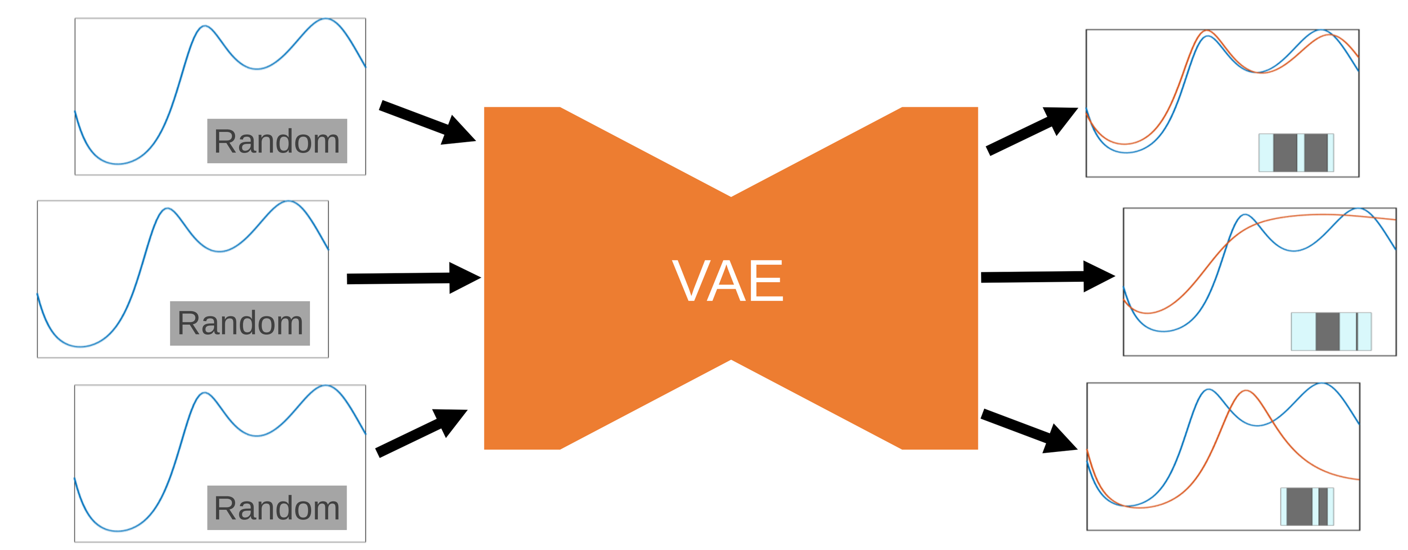
Latent z correlation with decoded thickness

	h_1	h_2	h_3	h_4	h_5
z_1	-.23	.33	.34	**.82**	-.22
z_2	-.04	**.80**	.10	-.24	.16
z_3	**-.84**	.02	-.06	-.11	-.49

Decoded h_2 in latent space



Because the VAE is robust to noise, we attempt to find optimized devices by reconstructing the target spectrum with a random device.



Future work: Continue to tune model parameters for improved accuracy, extend VAE model to more complicated optical devices

References

[1] D. Liu *et al*., "Training Deep Neural Networks for the Inverse Design of Nanophotonic Structures," *ACS Photonics,* **5,** 1365-1369 (2018).

[2] C. Doersch, "Tutorial on Variational Autoencoders," arXiv:1606.05908v2 [stat.ML], 2016.

[3] R. Gómez-Bombarelli *et al*., "Automatic Chemical Design Using a Data-Driven Continuous Representation of Molecules, *ACS Central Science*, **4**, 268-276 (2018).

[4] "Basic VAE Example", https://github.com/pytorch/examples/tree/master/vae

[5] C. Botha. Variational Autoencoder in PyTorch, commented and annotated. [online] vxlabs. Available at: https://vxlabs.com/2017/12/08/variational-autoencoder-in-pytorch-commented-and-annotated/ (2018) [Accessed 20 Nov. 2018].