Accelerating Inverse Design of Nanostructures using Manifold Learning

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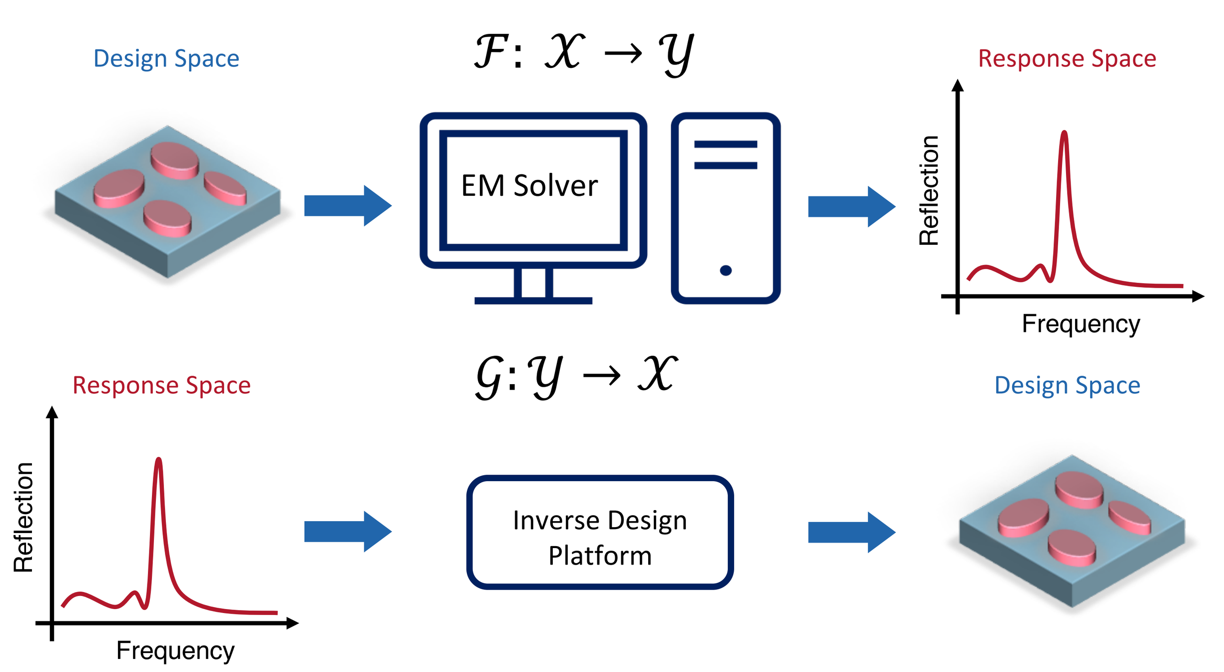
Motivation

Photonic nanostructures have widespread applications in lens design, biosensing, computing, imaging, etc. These structures can manipulate light and control the optical responses temporally, spatially, and spectrally. **Inverse design** of these structures can become challenging due to the limitation in computation resources, **large number of free parameters**, **non-uniqueness**, and **non-convexity** of the problem. Deep learning and machine learning have recently attracted remarkable attention in the inverse design of nanostructures. However, limited works have used these techniques to reduce the **geometrical design complexity** of structures.

In this work, we present a method based on manifold learning for knowledge discovery and inverse design of nanostructures with **minimal** geometrical design complexity.

Forward and Inverse Problem

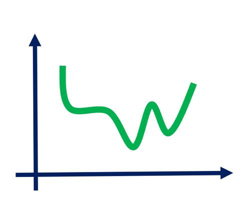


Challenges:

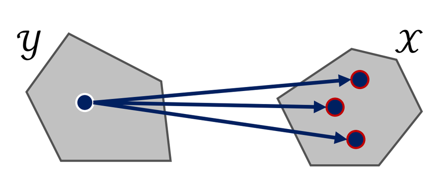
- No closed-form solution

$y = f(\cancel{x})$

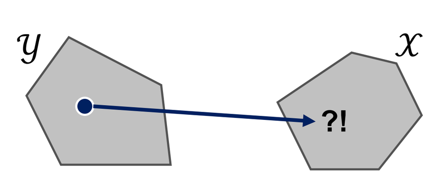
- Non-convexity



- Non-uniqueness



- Existence of the solution

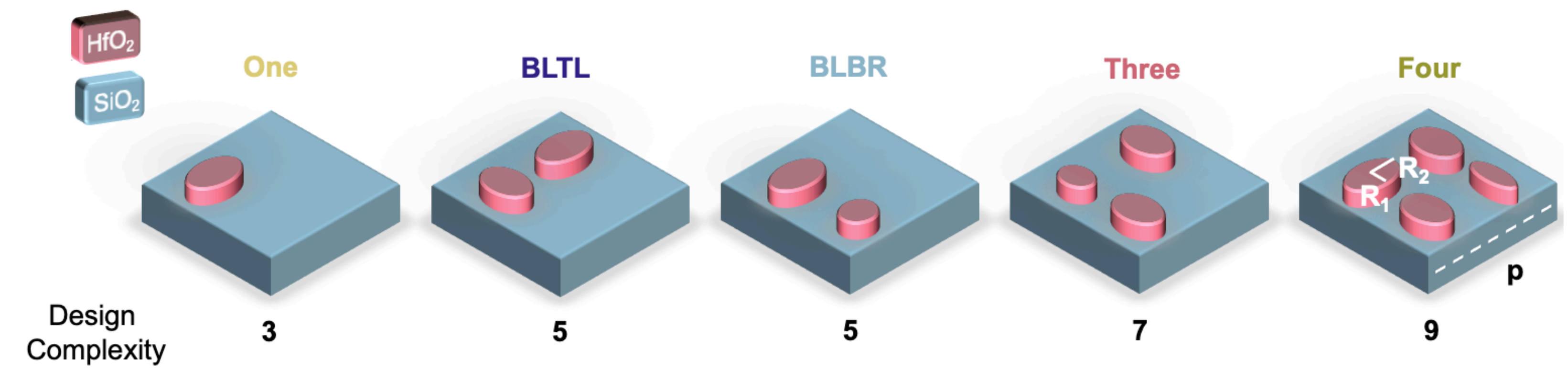


Limitations of the Previous Methods

- Time consuming
- Sub-optimal solutions
- Highly sensitive to initial guess
- Not considering existence of the solution
- Lack of interpretability and intuition

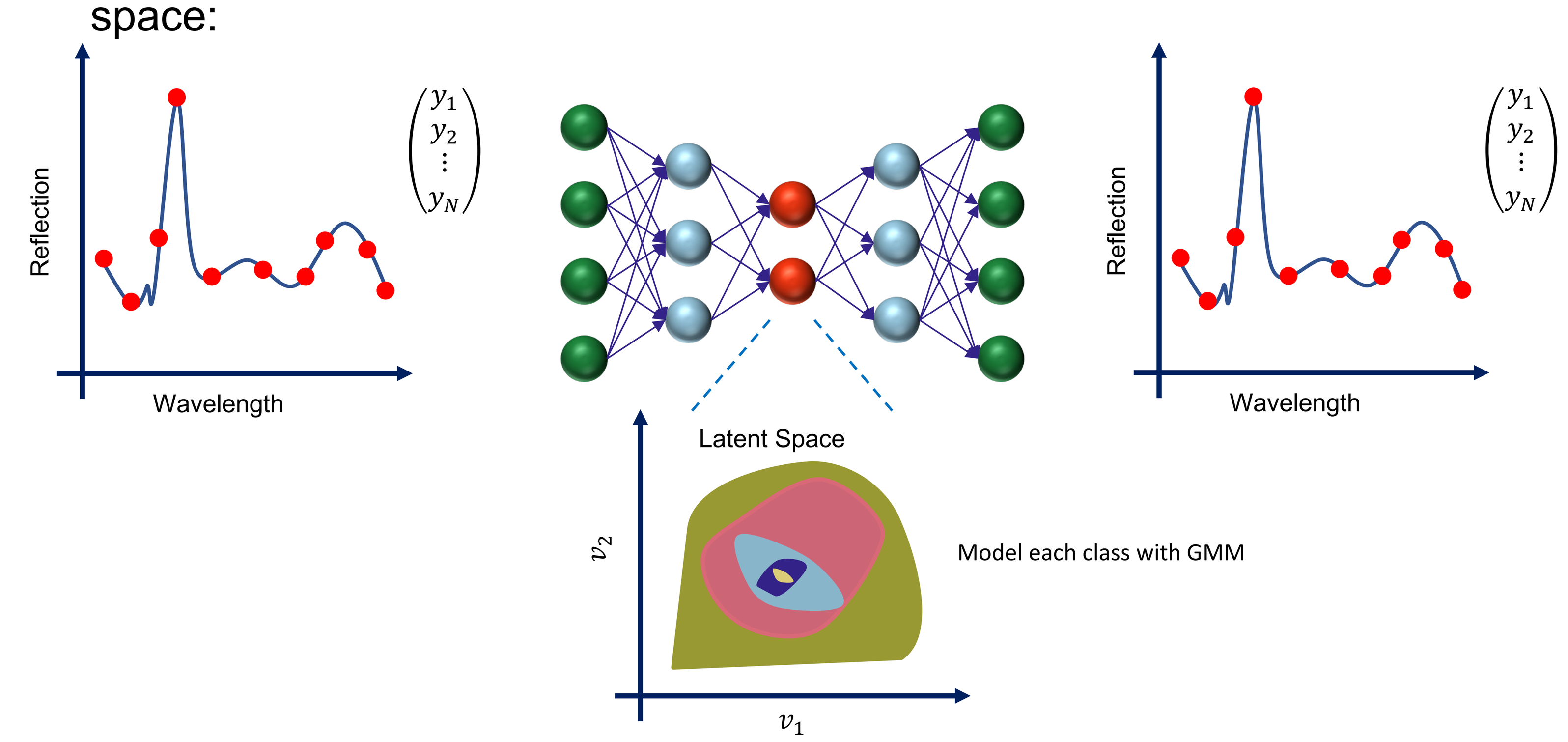
Manifold Learning for Inverse Design

1) Generating random samples from nanostructures with different geometrical complexities:



Unitcell of nanostructures with different geometrical design complexities. The design parameters are the periodicity ($p \in [500, 900]$nm) of the unitcells and the radii of the ellipsoids ($R_i \in [60, 200]$nm). The responses are simulated for wavelengths $300 < \lambda < 850$ nm.

2) Forming the feasible region of responses for each class in the latent space:

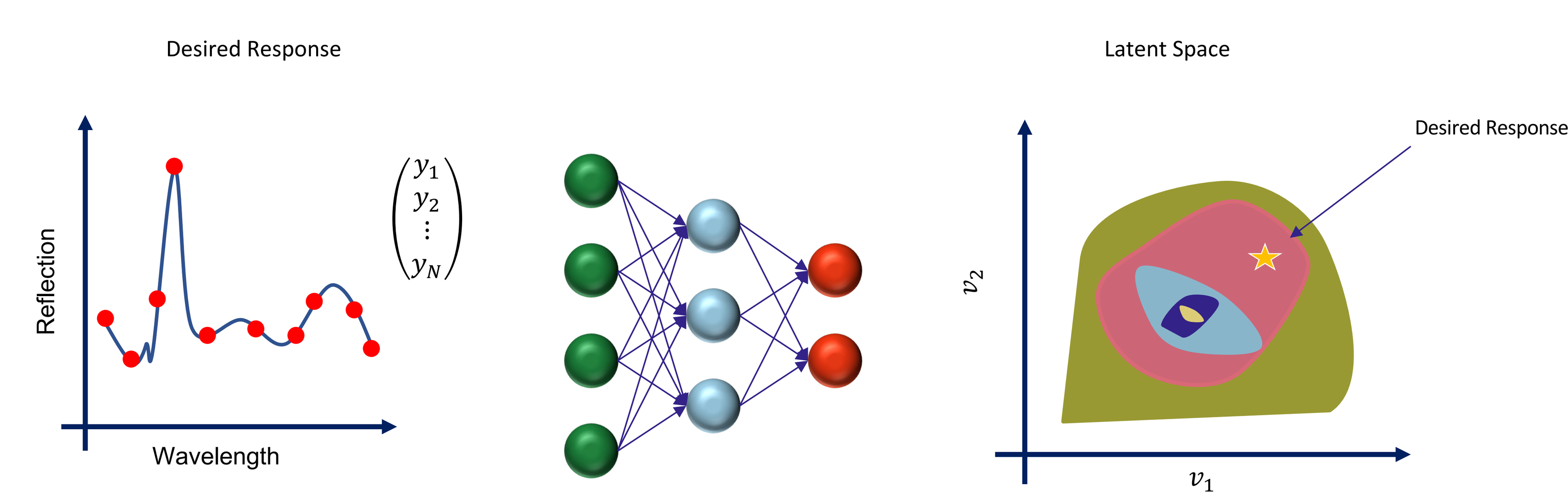


The responses generated from randomly selected sets of design parameters will be mapped into the latent space by training an autoencoder. Then the sub-manifold of the feasible regions for each class is modeled using GMMs.

3) Search for the solution using manifold learning Inverse design algorithm:

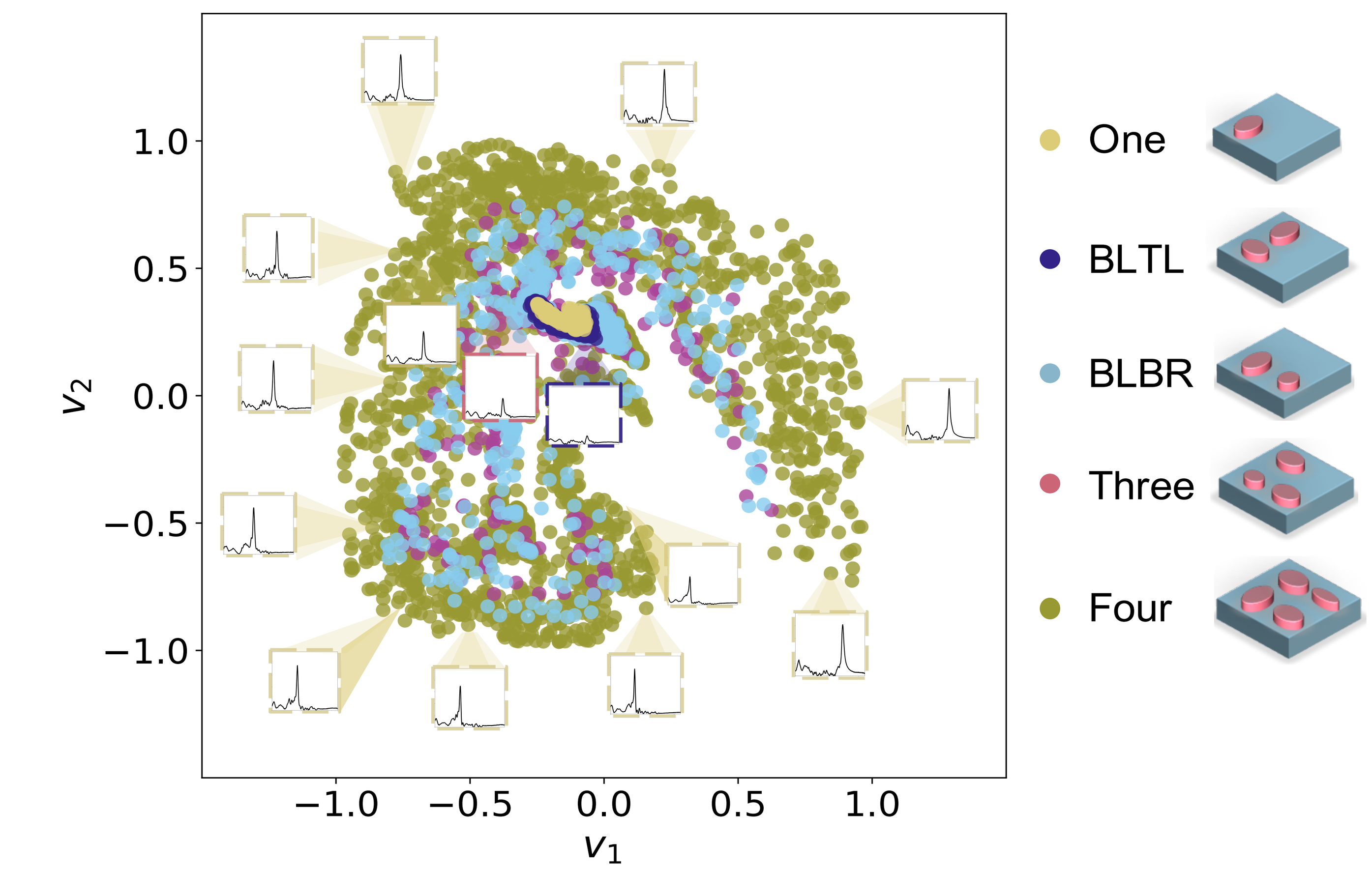
Algorithm 1: Evolutionary Design Algorithm

Result: Optimum Design with Minimal Complexity
Step 1: Map the desired response into the latent space using the trained AE
Step 2: Find the log-likelihood of the feasibility of the response for each design complexity and select design candidates with higher log-likelihoods
Step 3: Use feed forward DNN to search over the design space of the candidates and find the optimal solution



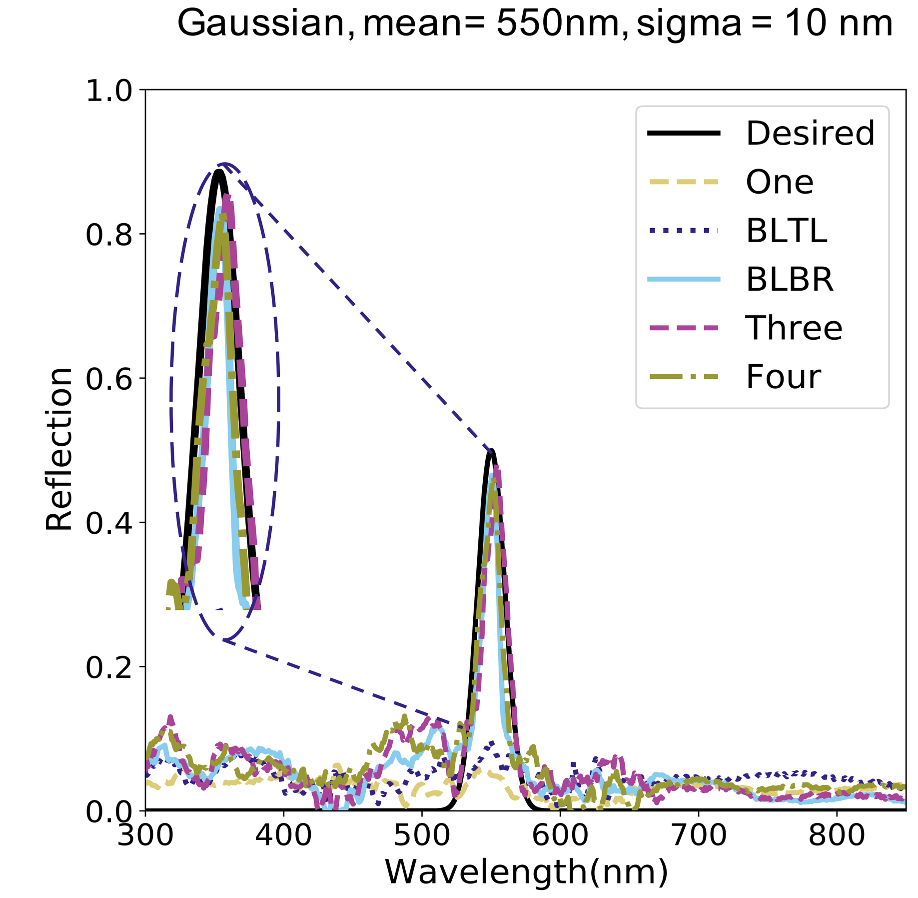
For a desired response, we reduce the dimensionality using the trained encoder and find the feasibility log-likelihood of each class of structures.

Results



Representation of the responses in the latent space. The largest feasible region corresponds to the structure with four ellipsoids. Movement around the margin results in blue/red shifts in the resonances. Movement from margins to the center, results in low-Q resonances.

Gaussian, mean= 550nm, sigma = 10 nm



- For a desired response we provide different solutions with different geometrical complexities based on the log-likelihoods of GMMs for each design complexity.
- We used a feed forward NN that maps the design space into the response space to search for the optimal solutions, which significantly reduces the time required for solving the inverse problem.

Table 2: Design parameters (in nm), NMSE, and log-likelihood for responses in Fig. 3(b). T, B, L, and R refer to Top, Bottom, Left, and Right, respectively. R_1 is the radius along x-axis and R_2 is the radius along y-axis for each ellipsoid.

	Design Parameters										
Structure	p	R1BL	R2BL	R1BR	R2BR	R1TL	R2TL	R1TR	R2TR	NMSE	$\log(p)$
One	683	64	64	0	0	0	0	0	0	0.892	-434.96
BLTL	882	787	111	0	0	174	89	0	0	0.880	-133.34
BLBR	736	132	121	132	132	0	0	0	0	**0.378**	-5.59
Three	700	168	121	168	98	121	98	0	0	0.411	-8.00
Four	700	823	823	823	160	121	121	160	121	0.416	-2.69

References

[1] Kiarashinejad, Yashar, et al. "Knowledge discovery in nanophotonics using geometric deep learning." *Advanced Intelligent Systems* 2.2 (2020): 1900132.

[2] Kiarashinejad, Yashar, et al. "Deep learning reveals underlying physics of light–matter interactions in nanophotonic devices." *Advanced Theory and Simulations* 2.9 (2019): 1900088.