A General Framework Combining Generative Adversarial Networks and Mixture Density Networks for Inverse Modeling in Microstructural Materials Design

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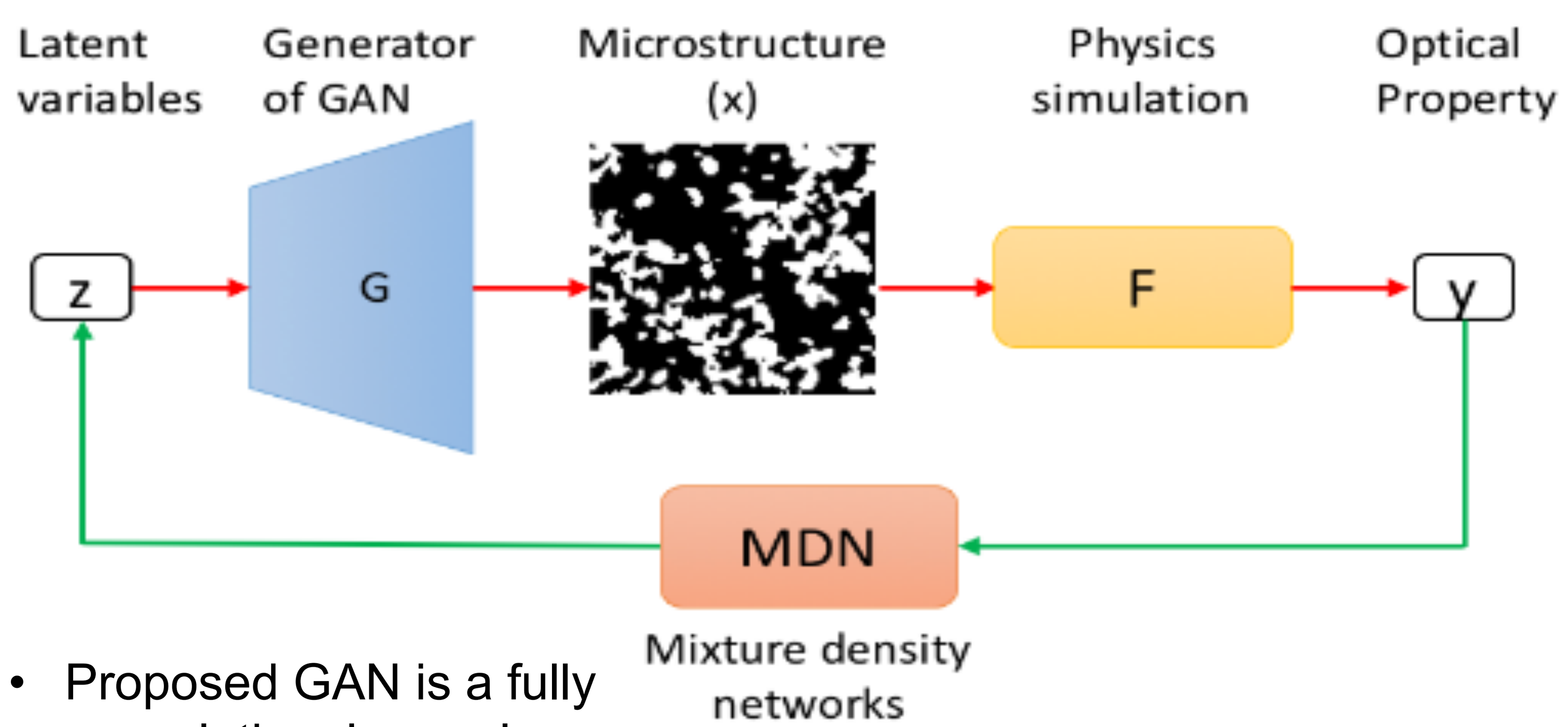
NEURAL INFORMATION PROCESSING SYSTEMS

Motivation

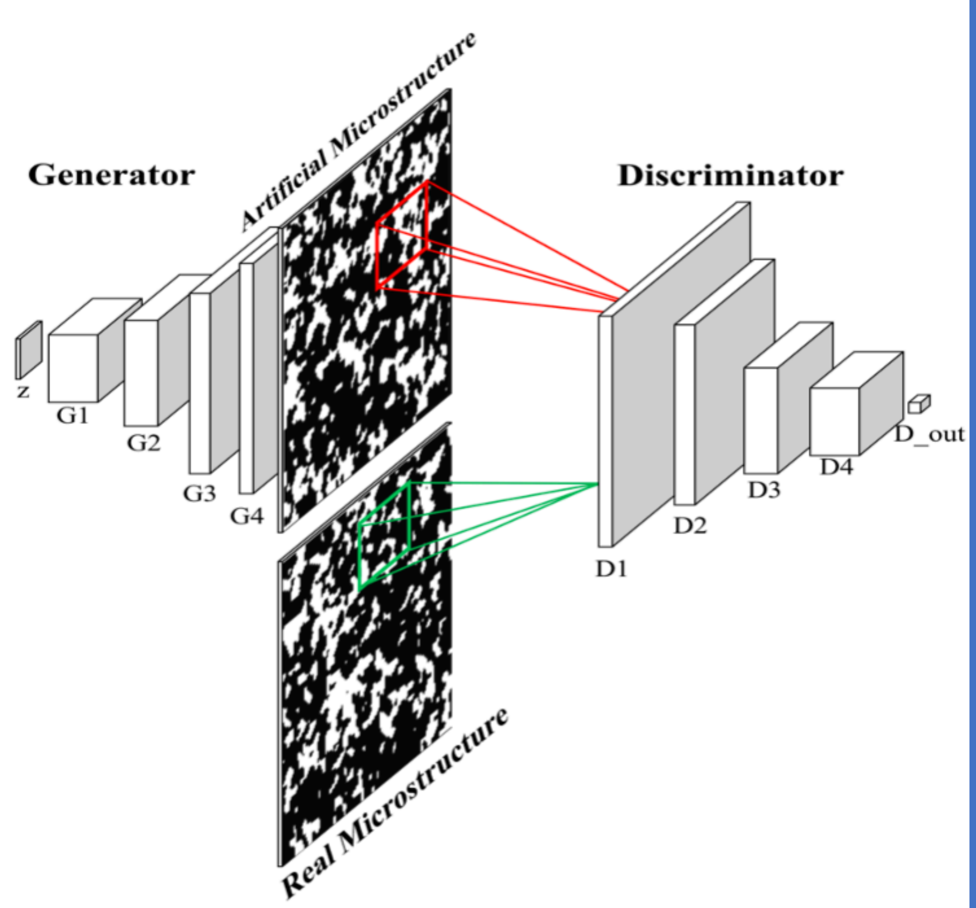
- **Challenges in inverse modeling**
  - Inverse modeling usually requires learning a one-to-many non-linear mapping.
  - Inverse models usually need to learn a mapping from low-dimension inputs to high-dimension outputs, which means important missing information needs to be recovered from less informational inputs to produce high informational outputs.
  - Traditional optimization based method is time consuming, and can only produce limited solutions.
- **Solution**
  - A framework combining generative adversarial networks (GAN) and mixture density networks (MDN)

Method

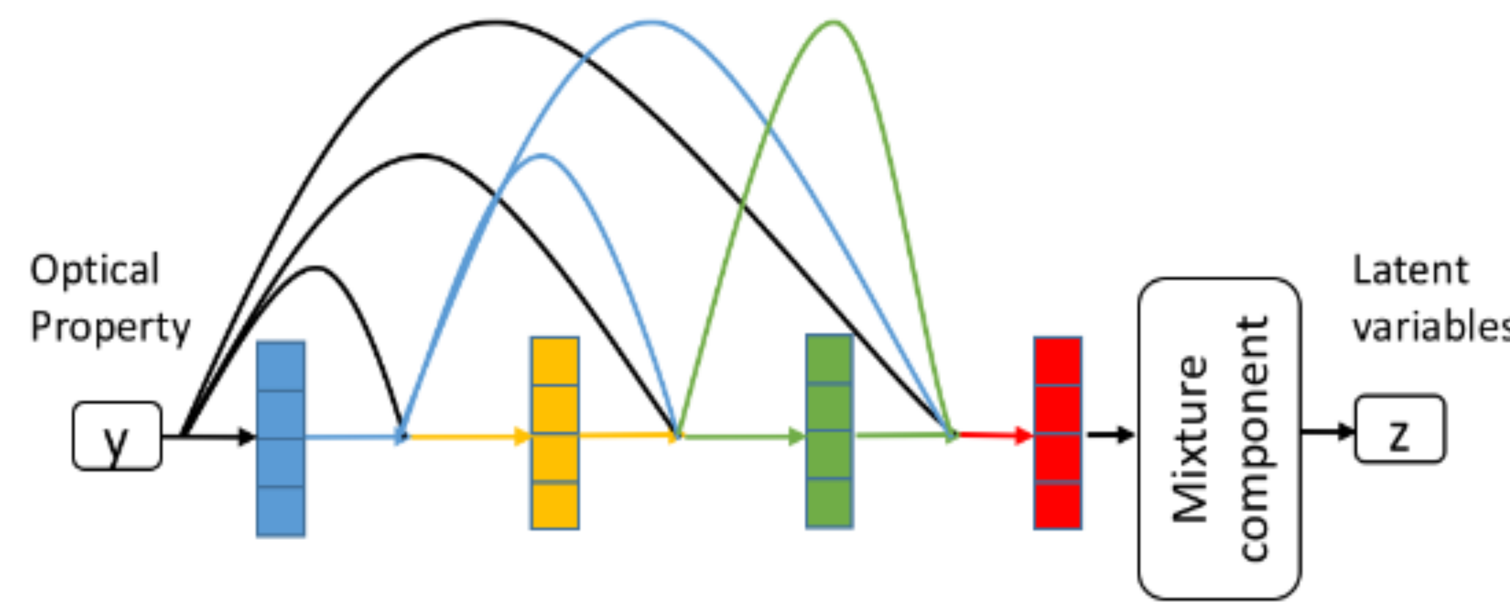
- The proposed method consists of GAN and MDN.
  - GAN is used to obtain the low-dimensional design representations (i.e. latent variable vector) of the microstructure images.
  - MDN models the mapping between latent variable vector and design objective.



- Proposed GAN is a fully convolutional neural network.
- Generator consists of four (de-convolutional)-batch normalization-ReLU layers, and a (de-convolutional)-tanh layer to produce images.
- Discriminator consists of four convolution-batch normalization-leaky ReLU layers, and a convolutional-sigmoid layer to classify images.



- Mixture density networks (MDN)
  - The goal of MDN is to predict an entire probability distribution for the output based on input.
  - MDN in this work is constructed by four densely connected fully connected layers and a mixture component that models a mixture of Gaussian distributions.



Baselines

- **Optimization based inverse modeling**:
  - A meta model-based Bayesian optimization is conducted to optimize the latent variable space to achieve the desired materials optical absorption property.
- **MDN based deep learning inverse modeling**:
  - A deep learning inverse modeling solely based on MDN as another baseline. More specifically, MDN takes materials optical absorption property as input and directly produces microstructural images.
- **PCA and MDN based inverse modeling (referred as PCA-MDN method)**:
  - PCA is used to replace GAN and combined with MDN to produce microstructure images given a desired materials optical absorption property.

Evaluation Metric

Residual error percentage (REP) is used to evaluate the performance of models, which is defined as

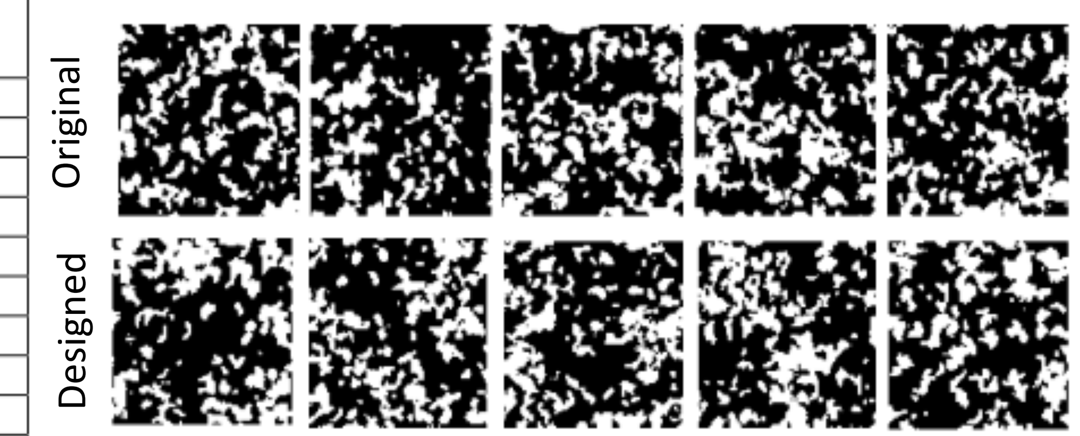
$$REP = \frac{|\hat{y} - y|}{y} \times 100\%$$

where $\hat{y}$ and y are the optical absorption property of generated microstructure and target optical absorption property, respectively.

Results

Dataset No.1:
The size of microstructure image and the latent variable vector are 96×96 and 3×3.

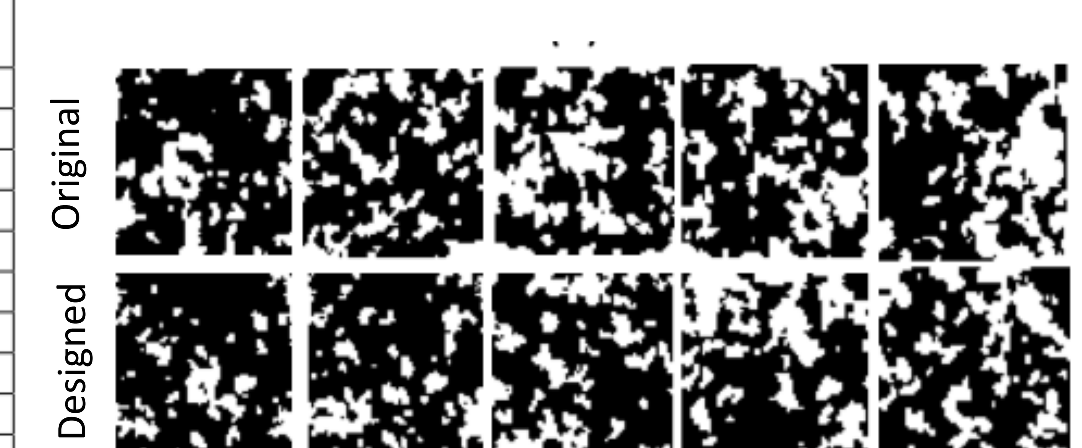
Value	Min REP	Average REP	Standard deviation of REP	Running Time
The proposed method				
0.55	0.65%	15.68%	8.40%	9.75s
0.60	0.18%	9.15%	5.97%	9.50s
0.65	0.22%	5.80%	3.93%	9.67s
0.70	0.13%	5.29%	3.86%	9.62s
0.75	0.20%	7.83%	3.91%	9.50s
Baseline: PCA-MDN method				
0.55	5.05%	17.67%	7.84%	7.22s
0.60	0.50%	10.89%	6.48%	7.30s
0.65	0.17%	5.92%	4.00%	7.20s
0.70	0.40%	8.81%	5.27%	7.20s
0.75	2.95%	18.34%	5.54%	7.36s
Baseline: MDN based deep learning inverse modeling				
0.55	0.84%	9.07%	3.14%	175.27s
0.60	4.70%	14.40%	4.08%	187.86s
0.65	9.35%	20.04%	4.06%	177.60s
0.70	12.29%	25.18%	4.21%	147.23s
0.75	17.73%	26.81%	3.55%	178.70s
Baseline: Optimization based inverse modeling				
0.55	-	-	-	4.4h
0.60	1.08%	-	-	3.6h
0.65	3.38%	-	-	5.8h
0.70	-	-	-	10.6h
0.75	-	-	-	8.9h



- The average REPs of the proposed method are the lowest for most target values. Moreover, min REPs are much less than 1%, which is much lower than baselines.
- It only takes around 10 seconds to produce designed microstructural images.

Dataset No.2:
The size of microstructure image and the latent variable vector are 64×64 and 2×2.

Value	Min REP	Average REP	Standard deviation of REP	Running Time
The proposed method				
0.55	1.25%	16.19%	8.96%	9.67s
0.60	0.70%	10.99%	7.93%	9.74s
0.65	0.18%	7.65%	5.64%	9.57s
0.70	0.10%	5.00%	4.61%	9.68s
0.75	0.43%	6.18%	3.51%	9.60s
Baseline: PCA-MDN method				
0.55	4.96%	11.74%	3.05%	7.24s
0.60	0.07%	2.69%	2.18%	7.26s
0.65	3.71%	8.79%	2.59%	7.40s
0.70	0.10%	3.41%	2.44%	7.15s
0.75	3.17%	6.27%	1.52%	7.26s
Baseline: MDN based deep learning inverse modeling				
0.55	2.85%	12.78%	3.89%	23.21s
0.60	7.87%	14.95%	3.56%	24.05s
0.65	11.00%	17.33%	2.63%	24.14s
0.70	3.03%	15.62%	4.09%	23.90s
0.75	8.44%	12.73%	3.20%	23.34s
Baseline: Optimization based inverse modeling				
0.55	15.51%	-	-	5.8h
0.60	-	-	-	12.1h
0.65	1.21%	-	-	4.2h
0.70	-	-	-	18.8h
0.75	-	-	-	3.2h



- The min REP and average REP for each target optical absorption property is extremely small, and the performance is comparable with that on Dataset No.1.
- It only takes around 10 seconds to produce designed microstructural images.

Acknowledge

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