

On the use of Generative adversarial neural networks for computing photonic crystal fiber optical properties

Aimen Zelaci, Ahmet Yaşı, Cem Kalyoncu, and Hüseyin Ademgil

Abstract—Photonic crystal fibers (PCF) for specific applications are designed and optimized by both industry experts and researches. However, the potential number of combinations possible for a single application is very large. This issue combined by the speed of the commonly used Full Vectorial Finite Element Method (FV-FEM) causes the task to take significant amount of time. As stated in the previous works, artificial neural networks (ANN) can predict the result of numerical simulations much faster. However, there are two issues with the methods proposed previously. Namely, the required number of samples for training and the overall accuracy of these methods. In this paper, we propose the use of generative adversarial networks (GAN) to augment the real data set to train an ANN model. Experimental analysis suggest that the proposed combination not only accurately predicts the confinement loss even with limited amount of data but also GAN can be used to improve existing methods in the literature. Finally, it is shown that this system can predict the confinement loss over a range of analytes and wavelengths in a completely new set of geometric configuration.

I. INTRODUCTION

Importance of PCF and SPR, written by AY or HA

Machine Learning (ML) techniques are coming to the forefront of many fields, surpassing human performance in many tasks, namely automatic speech recognition, image recognition, natural language processing, drug

discovery and toxicology. Additionally, ANN can approximate any function proven by Universality theorem [1]. This fact propelled researchers to widen the applications of ANN even further, including the study of nanophotonic structures [2], optimization of photonic crystal nanocavities [3], and more recently, computing optical properties of a photonic crystal fiber [4].

One of the most difficult challenges that deep learning models face is that they benefit from large amounts of data to train, which may be costly to acquire. One of the solutions to overcome this issue is to artificially expand the original training dataset by the means of generative networks. Introduced by Goodfellow et al., Generative Adversarial Networks (GAN) [5], proved to be successful in data generation [6]–[10].

In this paper, we focus on estimating confinement loss, one of the propagation features of multi-channel Photonic Crystal Fiber (PCF) sensors, using artificial neural networks. Specifically, we have based our system on Surface Plasmon Resonance (SPR). However, in the experiments section we have demonstrated that the designed system is generic enough to apply to multiple PCF designs. The most important contribution of this research is the use of GAN phase, where the available data is expanded to be used in the training phase.

!! Literature survey !!

Use of ANN in PCF

SPR in PCF

This paper is organized as follows. Section II details the use of GAN to generate additional training samples for ANN as well as the proposed neural network architecture. Photonic crystal fiber design that is used for testing is described in details in section III. Detailed analysis of the experimental results are discussed in section IV. Finally, concluding remarks are made in section V.

II. PROPOSED METHOD

In this section details of the proposed method is discussed. Training of the system contains two phases: a GAN phase and regression training phase. At the start of the training, a GAN is trained to generate additional data by using training samples. These generated samples are filtered to ensure they fall within the applicable range. Original training samples and remaining samples are joined to train a fully-connected feed-forward multi layer perceptron neural network. At the end of the training, the ANN that is trained for the regression task will be used to decide the output of a particular input parameters. This architecture is illustrated in Figure 1. The details of the proposed ANN architecture and the GAN is discussed in the following subsections.

A. Generative adversarial network design

Generative adversarial networks are introduced in [5]. We have employed GAN to augment the number of samples that are used in training. A GAN is composed of two neural networks: generator and discriminator. The aim of the generator is to transform fully randomized data into data that follows the distribution of the original dataset. Discriminator assesses the performance of the generator and provides feedback for training. Instead of directly training generator, it is trained through this

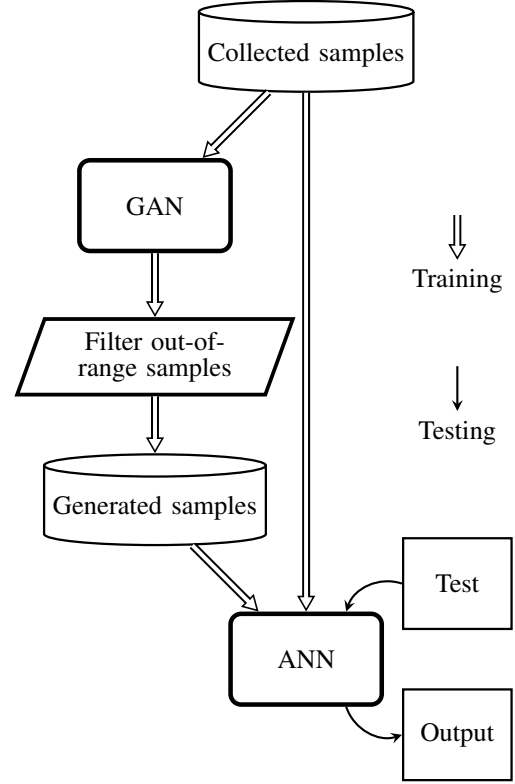


Figure 1: System architecture

feedback. This paradigm avoids over-fitting the data in the generator side.

It is possible to use different metrics for training in GAN [references here], for this project we have selected WGAN Wasserstein distance metric. This variant has been proposed by Arjovsky et al in [16]. In this system, discriminator is named as critic and it measures the distance between the generated data and the real data. The reason behind choosing WGAN over other methods is to be able to determine a stopping criteria. In a regular GAN system, training is stopped when the generated data is deemed viable by an observer. Since GAN is often used in generation of image, video or audio, using a human in the loop is effective. However, in our problem, it is not viable for a human to judge the generated data. Automating this procedure to remove the human in-the-loop can lead to over or under-fitting, which in

turn degrades the performance. WGAN uses an adaptive stopping criteria that does not have the issue mentioned above. Additionally, we have selected to incorporate Gradient penalty to improve WGAN proposed in [17]. This improved WGAN system converges in a stable manner without having to fine tune hyper-parameters of the system. The flowchart of this system is given in Figure 2.

In this work, both the Critic and the generator are fully connected feed forward MLP models. The details of the networks are given in Table I. The output from this system should be input and output pairs that will be used to train ANN part of the system. In our PCF system we have 6 input parameters and a single output parameter making a total of 7 parameters that will be used in the GAN phase. In Section IV, we have experimented using a different PCF system with different inputs, resulting a different number of parameters for the system. The generator is supplied with the same number of parameters as its expected output, that is 7 for our PCF system. These parameters are generated using Gaussian noise and is called latent variable. Once the training phase is complete, the generator and the filter is used to augment the number of training samples that are available for ANN.

Previous works [11], [12], demonstrated that it is possible for random data augmentation to weaken the performance of the model. Hence, it is important to sample the generated data in way to prevent performance degradation [13]. In the proposed system, we have included a filtering step for the generated data. This step uses a simple condition to discard the values that fall out of the desired range, for both the independent variables ($n_{analyte}, \lambda, \Lambda, d1, d2, d3$), and the confinement loss.

CK: continue here.

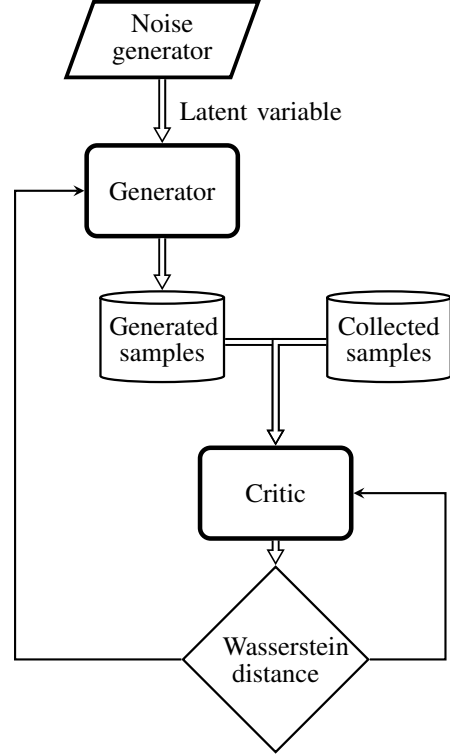


Figure 2: WGAN training

Parameter	Generator	Critic
Hidden layers	5	5
Neurons	2^2 batchsize	$2^{\text{layers}} \text{ batchsize}$
Activation	ReLU	Leaky ReLU
Optimizer	Adam [ref]	Adam [ref]
Normalization	-	Batch [15]

Table I: Details of WGAN model

B. Artificial neural network design

Adam [14] as the optimizer and the mean squared error as the loss/cost function. To reduce overfitting we use the Early stopping method, that is by saving checkpoints where the best validation mean squared error occurred as we iterate. To accelerate training and mitigate the problem of internal covariate shift Batch Normalization algorithm was used [15].

We will first train ANN model to predict the confinement loss of a SPR based PCF using the original data

set collected. Then we will augment the original training data set with generated samples by the GAN, to improve the performance of the ANN model. Previous works [11], [12], demonstrated that random data augmentation actually had weakened the performance of the model. Hence, active researches are ongoing to find ways to optimally sample the generated data [13], in other words to filter out the "good" generated data after training the GAN. In this paper, we will use a simple if-statement to discard values that fall out of our desired ranges for both the independent variables, and the confinement loss. In the following sub-sections we discuss the networks architectures. Before we proceed, it is worth mentioning that the choices made for the parameters of the networks are by no means a robust set of rules, rather, they are rules of thumb and heuristics, as no such rules have been yet developed for ANN models.

C. Artificial neural network design

The ANN model employed in this research is a fully-connected feed-forward MLP (Multi Layer Perceptron) consisting of an input layer, an output layer, and 5 hidden layers. Each hidden layer consists of 50 neurons and uses Rectified Linear Unit (ReLU) activation function. Table II summarizes the details of the model. Due to the nature of the problem, over-fitting is an important issue. We have used early stopping method [ref] to reduce over-fitting. This method works by saving checkpoints where the best validation mean squared error occurred as it iterates before the model starts to over-fit. To accelerate training and mitigate the problem of internal covariate shift Batch Normalization algorithm [15] was used.

III. PHOTONIC CRYSTAL FIBER DESIGN

We will fix the pattern and geometrical shape of the cladding air holes, and vary the wavelength λ , index of refraction $n_{analyte}$, air-hole to air-hole distance Λ , and

Number of hidden layers	6
Number of neurons per hidden layers	50
Activation function	Rectified Linear Unit (ReLU)
Optimizer	Adam [14]
Loss function	Mean Squared Error (MSE)

Table II: Details of the ANN model

the air holes radii per ring $d1$, $d2$ and $d3$. Then the results of this study can be carried to different types of SPR-based PCF sensors, using other suitable deep learning approaches such as Recurrent and Convolutional neural networks.

PCF design details, written by AY

IV. EXPERIMENTS

A. Experimental setup

A labelled data set of only 432 samples was collected in this work, through simulations using FV-FEM. This length of the data set made the task of building ANN model look quiet impossible, however the results were satisfying to some extent. This data set consists of the wavelength λ , index of refraction $n_{analyte}$, air-hole to air-hole distance Λ , and the air holes radii per ring $d1$, $d2$ and $d3$, taken as our independent variables. The labels are the confinement loss of the PCF. The set consists of nine different configurations of the geometric properties (Λ , $d1$, $d2$, $d3$), for each configuration the confinement loss was calculated for three different analytes (Water ($n=1.33$), Ethanol ($n=1.35$) and several commercial hydrocarbon mixtures ($n=1.36$)). Seven configurations were randomly selected for training both the WGAN-GP and the ANN, one configuration was held out for validation, and the last configuration for testing. By slicing the data set this way we are guiding the network to learn an entirely new set of geometric properties, and this is the reason what made the task impossible, since we only have nine configurations, as we discussed at

the beginning of this subsection. In contrast, randomly shuffling the data set as a whole is an easy task in this situation, and the ANN model would make great predictions on the test set, however a sense of generality towards new geometric sets will be lost.

This data was preprocessed before fed in the networks. The indices of refraction are very close, which made it quiet difficult for the neural networks to differentiate between them, after many trials, the best choice was to take only the tens digit of 134,135,136, giving 4, 5, 6. Finally, we transform the confinement loss to the log scale, for the purpose of shortening the distances between the confinement loss points.

Metrics used in the comparisons

B. Performance of ANN

We train the ANN model for more than 2000 epochs, starting from the original data set. Then we augment the latter set by 1000 generated samples by our WGAN-GP, which will be demonstrated in the next subsection, and train again with the new augmented data set. The following table summarizes the hyper-parameters chosen for the ANN model:

Length of the training data-set	Learning rate	Mini batch size	β_1	β_2
336	1×10^{-04}	8	0.9	0.999
336 + 1000	1×10^{-04}	8	0.9	0.999
336 + 2000	2×10^{-04}	16	0.9	0.999
336 + 3000	2.5×10^{-04}	20	0.9	0.999

Table III: Hyper-parameters chosen for the ANN model, where β_1 and β_2 are a part of Adam parameters

The MSE on the training sets ranged from 0.0030 to 0.0050. For all training data sets the MSE decreased in an acceptable manner. Next, we plot the predictions the ANN model made on the test set, after training using only the original set. As shown in the following figure.

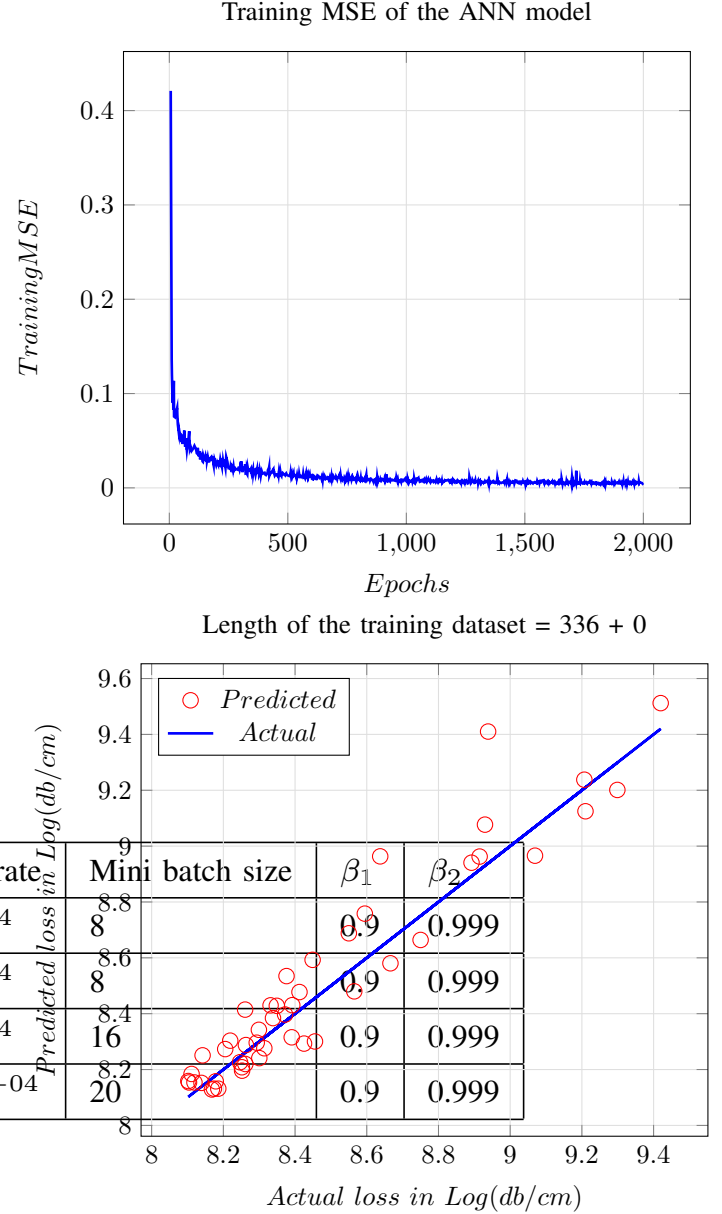


Figure 3

C. Performance boost of GAN

During training, the metric used to monitor the WGAN-GP is the loss function of the Critic network. Its convergence signals the ending of the training phase, shown in Figure(4). In this subsection we discuss the results of augmenting the real data set with generated samples. Figure(4) demonstrates the predictions made by the ANN model after training with different sizes of the data set. This might look paradoxical to what we mentioned earlier, that ANN model benefit from large amounts of data. There are several reasons for why our ANN model is driven in the wrong direction. Even though our WGAN-GP seemed well trained, there still a domain gap between the real data and the generated data, or the expansion of data is growing in the wrong direction to that of entirely containing the real data. Furthermore, the generated data might lack realism. Or the sampling strategy adopted is poor. But the most convincing reason is the limited original training data set size of 336 samples, used to train the WGAN model in the first place. After all, with 1000 generated data samples the ANN model made quiet accurate predictions with which we are satisfied, that is we have achieved what we set out to accomplish at the beginning, to improve the accuracy of the ANN model by artificially expanding the original set.

It can readily be seen that by augmenting with 1000 samples the ANN model made the best predictions, which then can be better viewed when we plot the confinement loss of the PCF versus the wavelength(λ) in Figure(5). The most important result in these experiments is that the ANN model predicted the correct location of the peak value of the confinement loss distributions for the three different analytes used.

D. Computational performance

Training and execution time of ANN versus simulation method

This work had been conduct on a laptop:

- Intel(R) Core(TM) i7-5600 CPU @2.60GHz (4 CPUs)
- 8GB RAM
- No GPU on board

For comparasion purposes we ran the expirements on a machine with GPU on board:

CEM PC SPECS

Epirements conducted on the latter machine will be labeled as GPU based, whereas on the former as CPU based.

By taking advantage of Cloud Computing technology, one does not have to spend large amounts of money to obtain high-specs machine, rather, rent readily available deep learning instances in the cloud for pennies on the dollar.

The code for this work is available at: https://github.com/Aimen-Zelaci/SPRPCF_ANN/.

The elapsed training time of an ANN model depends on the parameters of the model, for example, the number of hidden layers and hidden neurons, mini batch size, data set size, number of epochs, the framework used to code the model, and of course the specifications of the machine. In this work we fixed the number of epochs to 2000 and executed training using Tensorflow(Keras) and Pytorch frameworks. As demonstrated in Tables(5,6). It is worth mentioning the differences between training with full batch or mini batches. In full batch training, the whole data set is passed to the model for each iteration. In contrast, mini-batch-training, the data set is split into small mini batches of equal sizes, then passed to the model seperately, thus for each epoch there will be exactly length of the data set devided by the mini

batch size steps, and hence slowing down the training process. Previous works [18], [19] have firmly proved the advantages of using the correct mini batch size as oppose to large batch sizes. Mini batches allow for more frequent gradient calculations, that results in more stable and reliable training. Perhaps one of the main downsides of using large batch size is the poor generalization resulting in a phenomena know as the "generalization gap". Active research [20] is on going to actually use large batch sizes while mainting the performance of the model and shortning the training runtime. A closely related recent work [4], conducted their expirements using full batch to train the model. In this work we will use the latter paper availabe code on Github for Pytorch expirements, with slight modifications to fit our purposes. Finally, we compare the performance of the WGAN model, using Tensorflow(Keras) framework, of CPU based to that of GPU based.

	data set size	mini batch size	Time elapsed (sec)
Mini batches	336 + 0	8	214
	336 + 1000	8	744
	336 + 2000	16	685
	336 + 3000	20	861
	data set size	Time elapsed (sec)	
Full batch	336 + 0	23	
	336 + 1000	34	
	336 + 2000	45	
	336 + 3000	57	

Table IV: Training performance using Tensorflow(Keras). CPU based training.

WGAN EXCUTION WITH GPU VS CPU BY CEM

Next, we compare the testing runtime of the ANN model to that of simulation methods used to compute the confinement loss for 3 different analytes and 16 wavelenghts, i.e a total of 48 values of the confinement loss, demonstrated in Table(7). This result is absolutely staggering. The ANN model calculated 48 confinement

	data set size	mini batch size	Time elapsed (sec)
Mini batches	336 + 0	8	1315
	336 + 1000	8	6453
	336 + 2000	16	4751
	336 + 3000	20	5132
	data set size	Time elapsed (sec)	
Full batch	336 + 0	36	
	336 + 1000	98	
	336 + 2000	195	
	336 + 3000	336	

Table V: Training performance using Pytorch. CPU based training.

losses in just 0.17 seconds, while simulations took about 2 hours. Therefore, a well trained ANN model can be used to accurately find the best PCF geometric properties set that maximise the distance between the confinement loss distributions of each analyte in a matter of seconds to minutes. Hence, accelerate the search for the best PCF sensor.

	Time elapsed
ANN	0.17 sec
Simulation	7872 sec = 2.18 hours

Table VI: ANN vs Simulation test runtime performance

V. CONCLUSION

about the improved speed

reduced amount of training samples

increased generality of the system

This Idea is very important

In this work we built a feed forward ANN model that learned the confinement loss given the geometric properties of a SPR-based PCF sensor with fixed pattern and geometrical shape of the cladding air holes. For different types of sensors, Convolutional and Recurrent neural networks can be of great advantage, to discover the spatial insights of variety of patterns and geometrical shape of the cladding air holes. The latter will be conducted in future work.

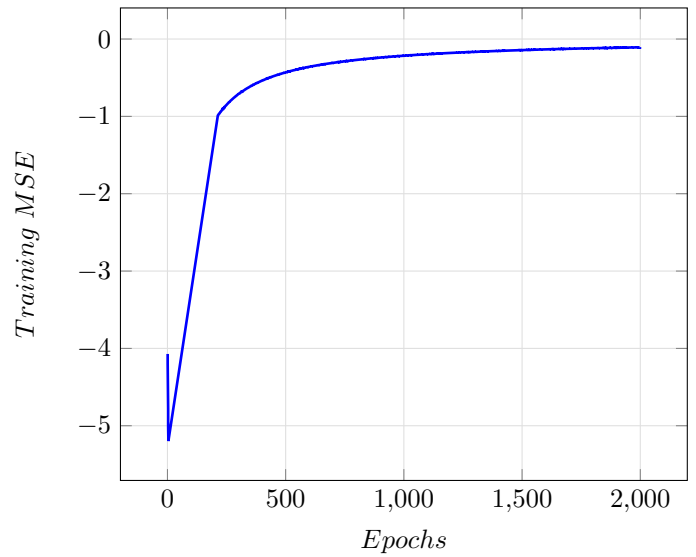
Machine learning approaches has an inherit strength on top of classical simulation methods: they could model hidden parameters in a system which we have no knowledge about. Therefore, not only ANN can improve the speed of PCF simulation, but also accuracy of the simulations. However, this final claim requires further analysis and experimentation.

REFERENCES

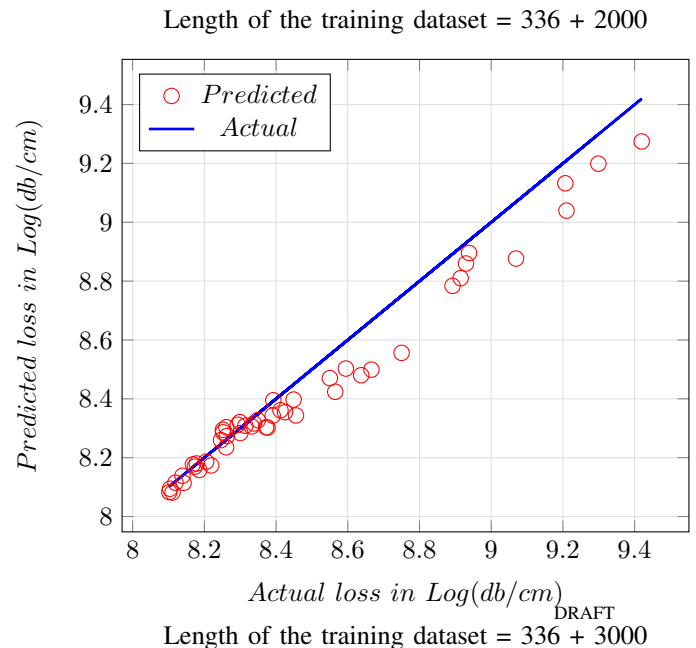
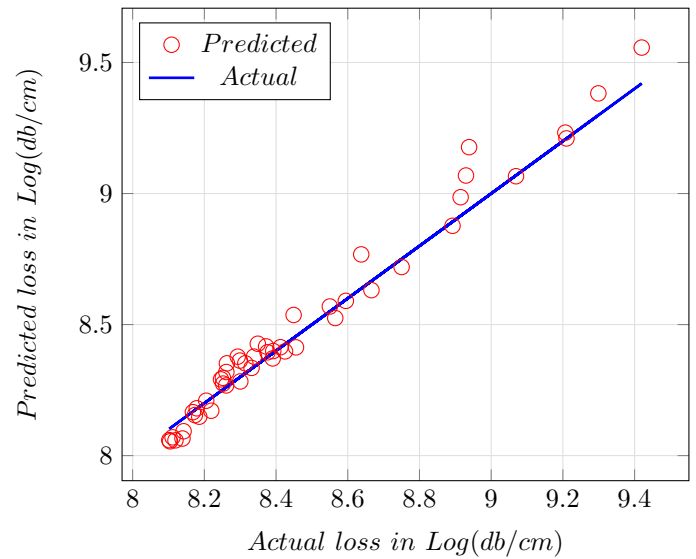
- [1] K. Hornik, "Approximation capabilities of multilayer feedforward networks," *Neural Networks*, vol. 4, no. 2, pp. 251 – 257, 1991. [Online]. Available: <http://www.sciencedirect.com/science/article/pii/089360809190009T>
- [2] Y. Kiarashinejad, M. Zandeshshavar, S. Abdollahramezani, O. Hemmatyar, R. Pourabolghasem, and A. Adibi, "Knowledge discovery in nanophotonics using geometric deep learning," *Advanced Intelligent Systems*, vol. 2, no. 2, p. 1900132, 2020.
- [3] T. Asano and S. Noda, "Optimization of photonic crystal nanocavities based on deep learning," *Optics express*, vol. 26, no. 25, pp. 32 704–32 717, 2018.
- [4] S. Chugh, A. Gulistan, S. Ghosh, and B. Rahman, "Machine learning approach for computing optical properties of a photonic crystal fiber," *Optics Express*, vol. 27, no. 25, pp. 36 414–36 425, 2019.
- [5] I. Goodfellow, J. Pouget-Abadie, M. Mirza, B. Xu, D. Warde-Farley, S. Ozair, A. Courville, and Y. Bengio, "Generative adversarial nets," in *Advances in neural information processing systems*, 2014, pp. 2672–2680.

- [6] T. Schlegl, P. Seeböck, S. M. Waldstein, U. Schmidt-Erfurth, and G. Langs, "Unsupervised anomaly detection with generative adversarial networks to guide marker discovery," in *International conference on information processing in medical imaging*. Springer, 2017, pp. 146–157.
- [7] Z. Zheng, L. Zheng, and Y. Yang, "Unlabeled samples generated by gan improve the person re-identification baseline in vitro," in *Proceedings of the IEEE International Conference on Computer Vision*, 2017, pp. 3754–3762.
- [8] M. Frid-Adar, E. Klang, M. Amitai, J. Goldberger, and H. Greenspan, "Synthetic data augmentation using gan for improved liver lesion classification," in *2018 IEEE 15th international symposium on biomedical imaging (ISBI 2018)*. IEEE, 2018, pp. 289–293.
- [9] F. H. K. d. S. Tanaka and C. Aranha, "Data augmentation using gans," *arXiv preprint arXiv:1904.09135*, 2019.
- [10] L. Perez and J. Wang, "The effectiveness of data augmentation in image classification using deep learning," *arXiv preprint arXiv:1712.04621*, 2017.
- [11] S. Ravuri and O. Vinyals, "Seeing is not necessarily believing: Limitations of biggans for data augmentation," 2019.
- [12] K. Shmelkov, C. Schmid, and K. Alahari, "How good is my gan?" in *Proceedings of the European Conference on Computer Vision (ECCV)*, 2018, pp. 213–229.
- [13] B. Bhattarai, S. Baek, R. Bodur, and T.-K. Kim, "Sampling strategies for gan synthetic data," *arXiv preprint arXiv:1909.04689*, 2019.
- [14] D. P. Kingma and J. Ba, "Adam: A method for stochastic optimization," *arXiv preprint arXiv:1412.6980*, 2014.
- [15] S. Ioffe and C. Szegedy, "Batch normalization: Accelerating deep network training by reducing internal covariate shift," *arXiv preprint arXiv:1502.03167*, 2015.
- [16] M. Arjovsky, S. Chintala, and L. Bottou, "Wasserstein gan," *arXiv preprint arXiv:1701.07875*, 2017.
- [17] I. Gulrajani, F. Ahmed, M. Arjovsky, V. Dumoulin, and A. C. Courville, "Improved training of wasserstein gans," in *Advances in neural information processing systems*, 2017, pp. 5767–5777.
- [18] D. Masters and C. Luschi, "Revisiting small batch training for deep neural networks," *arXiv preprint arXiv:1804.07612*, 2018.
- [19] N. S. Keskar, D. Mudigere, J. Nocedal, M. Smelyanskiy, and P. T. P. Tang, "On large-batch training for deep learning: Generalization gap and sharp minima," *arXiv preprint arXiv:1609.04836*, 2016.
- [20] E. Hoffer, I. Hubara, and D. Soudry, "Train longer, generalize better: closing the generalization gap in large batch training of neural networks," in *Advances in Neural Information Processing Systems*, 2017, pp. 1731–1741.

Training loss function of the Critic network



Length of the training dataset = 336 + 1000



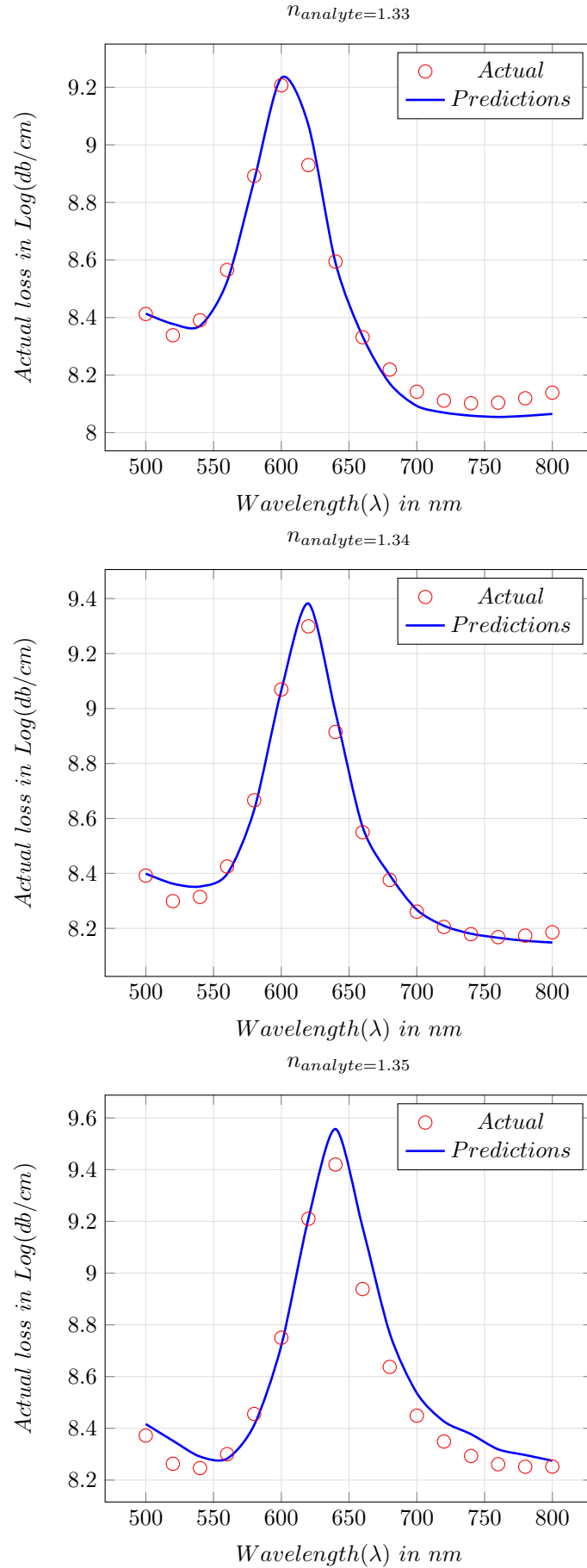


Figure 5