Neural network approach for faster optical properties predictions for different PCF designs

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Abstract. Photonic Crystal Fibres (PCFs) are emerging as an alternative to standard fibres for applications in many disciplines like fibre lasers & amplifiers, imaging, spectroscopy and telecommunications. They have superior light guiding properties compared to ordinary Optical Fibres (OFs). This paper illustrates the potential of neural networks to efficiently and accurately compute the optical properties of PCFs including solid-core, hollow-core and multi-core designs. The proposed method takes a range of design parameters and wavelengths as input to predict PCF optical properties like effective index, effective mode area, confinement loss and dispersion desired for optimal specifications. The neural network approach is significantly better in terms of the low computational runtimes (~5 milli-sec) required for predicting the properties against the longer runtimes (~18 sec) required for similar calculations by traditional numerical methods.

Keywords: Photonic Crystal Fibres, Optical Properties, Artificial Neural Network, Numerical Simulation, Computation Time

1. Introduction
Photonic Crystal Fibres (PCFs) are a special class of optical fibres that are characterized by a periodic arrangement of microcapillaries that form the fibre's cladding around a solid or hollow defect core [1]. They have the advantage of being low loss and endlessly single mode along with a high birefringence and low confinement loss [2]. This paper extends the past approach of using Machine Learning (ML) technique to predict the optical properties of a solid core photonic crystal fibre design based on variation in input design parameters like no. of rings, pitch length, diameter of holes and wavelength of light [3]. A simple yet effective neural network model is trained for three different design types of PCFs namely, solid core, hollow core and a six core multi-core PCF to predict their important optical properties. This is a robust model which has the capacity to generalise the results while maintaining high accuracy and negligible compute times.

The designing of photonic crystal fibres can be an exacting task because of the many time and resource draining computations that are required to be done for arriving at the optimum combination of PCF design attributes. The effective mode index, effective area, confinement loss and dispersion values at different combinations of these input parameters like hole diameter and pitch length vary greatly in magnitude with slight changes in dimensions. The combinations with high loss and high dispersion values are sub-optimal and need to be improved. The best possible optimal combination of PCF parameters where light propagates in the fundamental mode with the least loss is obtained by iterative analysis. The numerical methods generally used for this process are Finite Element Method, Finite Difference Time Domain method, Coupled Mode Model (CMM), and Plane-Wave Admittance Transfer (PWAT) [4]. All of these methods have high compute times in the range of tens of hours and also use heavy computer resources [5].

Recently, Machine Learning and Deep Learning techniques are finding applications in solving complex mathematical problems in the field of optics and photonics including plasmonics [6], nano-photonic structures [7], neuromorphic photonics [8], bio-printing [9], metamaterials [10] and optical communications and networks [11].
The deep learning neural network approach is based on identifying complex patterns in the training dataset which are then used to make connections between the given and desired attributes. The bigger and wider the provided training dataset will be, the more efficient and reliable will be the learning pattern and predictions of the model. This way a neural network can make predictions about the new data without being explicitly programmed. This saves precious time that would be otherwise wasted if using traditional algorithms. This paper serves the purpose to highlight the usefulness of deep learning predictions in the designing of photonic crystal fibres.

A brief about different PCF designs and considered optical properties are explained in Section 2. The detailed proposed approach and neural network architecture used for modelling is explained in section 3. Prediction results are explained for different types of PCF Design in Section 4. The conclusion of this paper is discussed in the last section, i.e., Section 5.

2. Designs Considered and Optical Properties
For our study we have considered simple Solid Core, Hollow Core and Multi Core PCF designs. The main variation amongst the designs is in the arrangements of air holes around the silica core which results in the wave-guiding structure. A solid core PCF has a solid silica core in the centre of fibre with air holes surrounding it. A hollow core PCF differs from Solid core PCF by having a hole filled with air or a different material in the centre instead of solid silica. A multicore PCF has multiple cores of solid silica. The PCFs have a core of pure silica as in case of solid and multicore PCFs or air as in the case of hollow core with a cladding made up of air-holes separated by pitch length Λ and of diameter d arranged in a hexagonal lattice. We have taken four and five concentric rings designs into consideration. The thickness of fibre is 12 µm and thickness of PML is taken as 4 µm.

2.1 Solid Core PCF:
A Solid Core PCF is a type of photonic crystal fibre which gets its wave guiding characteristics from an order of very small and closely spaced air holes that run through whole length of fibre as shown in Figure 1(i) [12]. The light propagation mechanism in a solid core PCF can be explained via Modified Total Internal Reflection theory [13]. A solid core PCF with a large enough core has a capability of being single mode for a large range of wavelength[2] [14]. It finds its application in the field of telecommunications. If the solid core is big enough then light can be guided through the fibre with high power without the power density causing non-linear effects [15]. This allows distance between repeaters to be greatly increased.

![Figure 1. Concentric hexagonal ring designs with 4 rings: (i) Solid core, (ii) Hollow Core and (iii) Multi-core designs taken into consideration.](image)

2.2 Hollow Core PCF:
A hollow-core fibre is an optical fibre in which the light propagates inside a hollow zone of the PCF, such that just a small fraction of the light is guided inside solid fibre(generally made of silica) [16]. Here hollow core PCF design is achieved by having a hollow hole in the centre of the fibre instead of a solid core as seen in Figure 1 (ii). The hollow hole may contain air or some other gaseous material [17]. We have considered a hollow core fibre which have air holes to train our model. Light propagation in hollow core PCFs can be explained only by
using photonic band gap effect [18]. The wavelength range for confinement of these fibres is very small, of the order of few nanometres in the visible or infrared spectrum.

2.3 Multi Core PCF:
Most optical fibres have a single fibre core, which is usually located on the fibre axis. However, there are also specialty fibres containing multiple cores, which may be arranged on a ring around the fibre axis or on some 2D arrangement [19]. Multi-core PCFs guidance principle is that of modified total internal reflection just like solid core PCFs and are designed for high power supercontinuum generation due to their high beam quality output good thermal dissipation properties and large effective mode area [20]. We have taken a design with 6 cores for light guiding into consideration as shown in Figure 1 (iii).

2.4 Desired Optical Properties
For our study we have considered the following optical properties of PCF to compare their values with variation in design parameters.

2.4.1 Effective Refractive Index. It is a figure calculated using the band structure of the surrounding arrangement of holes. It refers to an “effective index” associated with the largest value possible for the propagation constant $\beta$ for the frequency in the microstructure. Which means at a particular frequency, light with a component $\beta$ of the wave vector along the axis of the holes greater than a specific $\beta_{\text{MAX}}$ value cannot propagate in the micro-structured part of the fibre [15].

2.4.2 Effective Mode Area. It a measure of the area effectively swept by a waveguide in the transverse dimensions [21]. The effective area is a very crucial quantity. It was put in place to evaluate non-linearities: lesser effective area leads to a higher density of power required for non-linear influences to be noteworthy [22], [23]. The spot-size radius $w$ for a gaussian beam is related to the effective area through the following equation [24]:

$$A_{\text{eff}} = \pi w^2$$  \hspace{1cm} (1)

Thus, it is crucial in the context of micro-bending loss, confinement loss [25], splicing loss [26], macro-bending loss [23] and numerical aperture [24]. We used the below formula to calculate the effective mode area:

$$A_{\text{eff}} = \frac{\iint_{\Omega} |H_t|^2 \, dx \, dy}{\iint_{\Omega} |H_t|^4 \, dx \, dy}$$  \hspace{1cm} (2)

Where $\Omega$ denotes area enclosed within the computational domain and $H_t$ denotes transverse magnetic field vector.

2.4.3 Dispersion. Dispersion represents all occurrences causing light pulses to broaden while propagating. Dispersion is essentially caused by 4 basic causes [27], [28]: Material dispersion, Inter-modal dispersion, Polarization mode dispersion, and Waveguide dispersion. In optical telecommunications, to keep the bandwidth as large as possible, the optic pulses keep their starting widths. That is because if optic pulses spread, they will overlap further down the path and cannot be differentiated by the receiver. Chromatic dispersion ($D$) is the dispersion which is the consequence of combined effects of waveguide dispersion and material dispersion. When chromatic dispersion has value greater than zero (the dispersion regime is said to be anomalous), shorter wavelengths are propagated at higher pace than longer wavelengths. In the opposite case, when $D$ is less than zero, the dispersion regime is said to be normal [29]. The following equation has been used to calculate dispersion [30]:

$$D = -\frac{\lambda}{c} \frac{d^2 \text{Re}(neff)}{d\lambda^2} \text{ (ps/km.nm)}$$  \hspace{1cm} (3)

Where $\text{Re}$ stands for the real part of the effective refractive index and $c$ denotes the free-space speed of light.
2.4.4 Confinement loss. Light propagation because of modified total internal reflection between core and micro structured cladding which consist inclusions in a matrix. Irrespective of the approach used to substantiate propagation in PCFs, if guidance is due to a fixed number of holes layer, leakage from the core to the outer matrix of material is unavoidable. These are losses due to the finite extent of the cladding as Confinement losses [31]. The following equation has been used to calculate confinement loss [32]:

$$\alpha_c = 86.86 \left( \frac{2n}{\lambda} \right) \text{Im}(n_{eff}) \text{dB/m} \quad (4)$$

Where \text{Im} stands for the imaginary part of effective index $n_{eff}$.

3. Proposed Approach

This section discusses our proposed approach which includes major modules as: Dataset Generation, Pre-processing, Modelling Neural Network. An overview of the approach is presented in the Figure 2.

![Figure 2. Proposed approach for our task.](image)

3.1 Dataset Generation

The dataset is prepared by running simulations in COMSOL Multiphysics 5.4. For computation of Effective mode index ($n_{eff}$), Dispersion, Effective mode area ($A_{eff}$) and Confinement Loss, the input design parameters are varied as follow:

- Pitch [um]: Range (0.8-2.0) with step of 0.2
- Diameter of Holes [um]: Range (0.6-0.9) with step of 0.1
- Wavelength [um]: Range (0.5-1.8) with values divided into 20 steps
- Number of Rings: 4 and 5
- Types of PCF: Solid Core, Multi Core and Hollow Core
- Mesh Size: Finer

The total computed values i.e. around 3359 data instances are combined together for further processing.

3.2 Pre-processing

The various feature values in the dataset have non-uniform ranges of values which is not an ideal condition for neural network modelling. We have used MinMax normalization which rescales the data into [0,1] range values. It improves the robustness of the model accuracy and also reduces the model training time [33]. Categorical features like type of PCF which contain string values are mapped to integers by label encoding.

The dataset is then shuffled to eliminate the bias towards any particular set of values and keep similar distribution in all sets. The data was split into three sets namely, training, validation and test sets in the aspect ratios of 80%, 10% and 10% respectively.
3.3 Modelling Neural Network

In supervised machine learning, Artificial Neural Network (ANN) is considered one of the best techniques because of its ability to learn highly non-linear complicated patterns and features [34]. Neural network architecture consists of a number of layers and each layer can have multiple nodes (or Neurons). Here we have considered a regression problem to predict PCF optical properties as output.

The architecture as shown in Figure 3. contains one input layer, two hidden layers and an output layer all connected to each other via nodes. The nodes in input and output layers contain the vectored data. The nodes in hidden layers are basically responsible to convert the input data into corresponding output data by learning the underlying complex rules or patterns.

For training of our neural network, we used Rectified Linear Unit (ReLU) as activation function which is responsible for approximating the non-linear learning function [35]. To optimise the weights of nodes during the training process Adam optimizer was selected as it performs well on big datasets as compared to other optimizers [36]. We set the learning rate parameter to 0.001. Our second and third hidden layers contain 70 and 60 nodes, respectively. Generally, it's a good idea to keep relatively more nodes in early layers as they learn the more complex patterns. In vanilla feed forward neural networks, every node of each layer is interconnected to one another [37]. However, it has been observed often that when training with such architecture, the model suffers overfitting i.e., it predicts well on the training data but suffers relatively more loss on test data. To overcome this a dropout technique is used which basically cuts-off a few connections between nodes randomly [38]. We used dropout in our third layer with value set to 10%. For back-propagation phenomenon [39], mean squared error is calculated between the predicted and actual values and then used iteratively to update the weights of hidden layer nodes [40].

For our experiment we have chosen 2000 epochs because that gives an acceptable stable MSE on both training and validation data. Once these hyperparameters were finalised and the model was trained, we generated the predicted output values for the unseen data of the test set.

4. Results and Discussion

This section presents the performance of our neural network model on validation set and on the unseen test set. The difference between the true and predicted values of target variables are evaluated on the basis of some error metrics used in regression tasks.

Mean squared error (MSE) is one of the metrics to gauge model performance in regression task [40]. For N observation it is defined as the averaged squared difference between the predicted and true values (5), where \( y_i \) and \( \hat{y}_i \) are the predicted and true value of data points, respectively. Smaller the value of MSE, smaller the difference between predicted values and actual values and hence model can be considered well trained. Another
metric used here is R Squared (R2), it is a statistical measure of fit which indicates how much variation of a dependent (or target) variable is explained by independent variable(s) in a regression problem [41]. Its value ranges between [0,1], where 1 indicates that the predicted values perfectly fit the data (6).

\[ MSE = \frac{1}{N} \sum_{i=1}^{N} (\hat{y}_i - y_i)^2 \]  

\[ R^2 = 1 - \frac{\text{Unexplained Variation}}{\text{Total Variation}} \]  

The validation set is available to the model in training process to evaluate the loss on every epoch and update it accordingly. The Figure 4 shows the plot of MSE for both training and validation set for different number of epochs. The negligible difference can be observed between the two and how quickly they converge to a stable low MSE loss.

![Figure 4. Mean Squared Error Vs No of Epochs](image)

The plot of Actual and Predicted Optical Properties values of Solid Core PCF against different wavelengths is shown in Figure 5.

![Figure 5. Plot of Actual and Predicted Optical Properties values of Solid Core PCF against different wavelengths](image)
The variation in predicted and actual values of properties of a solid core PCF design is plotted in Figure 5. Generally, with increase in wavelength the effective index value of fundamental mode decreases, the same can be observed in Fig 5(i). The predicted $n_{eff}$ values deviates a bit in the range of 1.3-1.5 um wavelength. Confinement loss values are plotted in Fig 5(ii), Logarithmic conversion is used to obtain a linear relation against wavelength as real values were mostly confined to a particular range value. Dispersion predicted values suffer from a relatively significant error as compared to real values which can be observed in Fig 5(iii). Effective mode area values also follow the same pattern as other predictions, the difference between actual and predicted values are almost negligible.

Following tables show the performance of the Neural Network in prediction across the three chosen PCF designs:

**Table 1. Performance indices for output optical properties of Solid Core PCF**

|                        | Validation Set | Test Set |
|------------------------|----------------|----------|
| Effective Index (neff) | 0.001 0.99     | 0.001 0.99 |
| Confinement Loss       | 0.001 0.98     | 0.002 0.99 |
| Dispersion              | 0.009 0.81     | 0.016 0.83 |
| Effective Mode Area (Aeff) | 0.001 0.99     | 0.002 0.98 |
| Combined Data           | **0.003**      | **0.004** |

**Table 2. Performance indices for output optical properties of Multi Core PCF**

|                        | Validation Set | Test Set |
|------------------------|----------------|----------|
| Effective Index (neff) | 0.001 0.99     | 0.001 0.99 |
| Confinement Loss       | 0.003 0.98     | 0.004 0.97 |
| Dispersion              | 0.019 0.90     | 0.036 0.86 |
| Effective Mode Area (Aeff) | 0.001 0.99     | 0.002 0.93 |
| Combined Data           | **0.005**      | **0.009** |

**Table 3. Performance indices for output optical properties of Hollow Core PCF**

|                        | Validation Set | Test Set |
|------------------------|----------------|----------|
| Effective Index (neff) | 0.001 0.99     | 0.001 0.99 |
| Confinement Loss       | 0.009 0.82     | 0.013 0.89 |
| Dispersion              | 0.001 0.99     | 0.001 0.99 |
| Effective Mode Area (Aeff) | 0.001 0.98     | 0.002 0.98 |
| Combined Data           | **0.003**      | **0.005** |

Table 1 show the prediction errors of various optical properties of Solid Core Design. It can be observed that the MSE of $n_{eff}$, confinement loss and $A_{eff}$ are negligibly small and R2 value is close to 1 in both validation and test set. There is relatively more error in dispersion as compared to other values but overall, the MSE on combined data is consistent and very small. The same trend continues on the Hollow Core design as well. From Table 3, a consistent error of both validation set and test can be observed on combined data. However, in Table 3 of Multi-Core PCF design, the error in Dispersion value is relatively more. The reason for this could be the uneven distribution of values in dataset. However, the significance of 0.036 MSE is still very small. The high R2 value across all the predictions showed that model performs consistently well with negligible loss. R2 is generally not used to evaluate multi-output predictions as every variable can have different data distribution and a combined good fit may not be achieved.

**Computation Time**

The main motivation of this work was to leverage the advantage of machine learning techniques in terms of faster and accurate prediction of values given the training parameters. For our experiments we used a workstation with Intel i5 dual core processor, 8GB RAM running window 10 operating system.
5. Conclusions
This paper presents that a simple neural network can be successfully used as a generalised model to predict the optical properties of the various diverse PCFs efficiently. The compute times and computer resources required by the model are significantly lower than used by tradition numerical method techniques. The trained neural network requires only 5 milli seconds to predict optical properties for a new set of PCF design parameters. The same single calculation would take 18 seconds using COMSOL Multiphysics. The overall MSE error of predicted optical properties observed in different PCF design are in range of 0.004-0.009 which is highly insignificant. Such a neural network approach carries the potential to be exploited more in fields where numerical methods are heavily used for computation and simulation.

Disclosures
The authors declare no conflicts of interest.

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