Deep Learning and Inverse Design in Plasmonics

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***Abstract*— Laser pulses can colour noble metals by inducing nanoparticles on their surface. The colours are linked to laser parameters and nanoparticles geometry. We apply deep learning to the direct prediction of colours from a laser parameter set or a nanoparticle particle distribution. A new method for inverse design via deep learning is also proposed to retrieve the appropriate laser parameters or nanoparticle distribution given the desired colour.**

Keywords—Deep Learning, Inverse Design, FDTD, Plasmonic Colours

I. Introduction

Deep learning (DL) is a sub-field of artificial intelligence where multi-layered artificial neural networks, or deep neural networks (DNNs), are used for accurate prediction and classification [1]. Recently, we have seen a growing interest in applying DL to nanophotonic problems [2] because this approach holds the promise for reducing costs associated with laboratory experiments and simulations. If data from previous experiments is available, further experiments or simulations can be replaced by a DNN.

The interest is even higher for inverse design in nanophotonics, where we are seeing the use of DL to search for non-intuitive and optimized designs to produce a desired outcome [2]. If data is available, these DL based methods are an improvement on traditional gradient-based or genetic-based algorithms commonly used in nanophotonics [3]. These traditional methods require the use of multiple simulations which, in the case of large-scale calculations common in plasmonics, can be very time consuming.

Here we discuss how to take advantage of large datasets produced in previous research for prediction and inverse design using DL. In [4], [5], picosecond laser pulses were used to create colours on noble metal surfaces. These colours are due to the plasmonic effects arising from the nanoparticle distributions generated from ablation and redeposition. Large-scale finite difference time-domain (FDTD) simulations were conducted to calculate the colour from a wide range of nanoparticle distributions to explain the colour transition reported in experiments. In this work, we use the experimental (colours vs. laser parameters) and simulation (colours vs. nanoparticle distribution) data sets compiled from [4] to train DNNs for the direct prediction of colours from laser settings or nanoparticle distributions. We also introduce a simple method for the inverse predicition of the laser/nanoparticle parameters for a desired colour which can easily be implemented for a number of applications.

II. Direct Prediction

We apply DL to the direct prediction of the (R, G, B) colour values from new laser parameters where the DNN is trained using the experimental data set linking four laser parameters (fluence, scanning speed, hatch spacing, and number of bursts per pulse) to perceived colours. We also predict colours from new nanoparticle distributions, where the DNN is trained using the simulated data set linking three nanoparticle distribution parameters (particle radius, inter-particle spacing, and amount of the particle radius embedded into the surface) to the computed colours.

Cross-validation was used to find DNN architectures that provide minimum error and minimize the size of the DNN. A three hidden layer DNN with sixty nodes per hidden layer was used for the laser parameter data set, and a four hidden layer DNN with twelve nodes per hidden layer was chosen to model the simulation data set. The two DNNs are trained using 90% of the available data. The other 10% is used for testing. The DNNs were created using TensorFlow [6] and were trained on the SOSCIP GPU cluster [7].

Some of the colours from the testing set are displayed for the laser set in Fig. 1(a) and the simulation set in Fig. 1(b). We see excellent agreement between the measured/simulated colours and those predicted by the DNN. To differentiate between the real and predicted colours, we use ΔE [8], a quantitative measure that describes the similarity of colours. A ΔE of 7 or lower is usually used as a benchmark for if the colour is close enough to the desired colour for industrial use. The mean ΔE is 5.3 for the laser parameter test set and 2.67 for the FDTD test set.

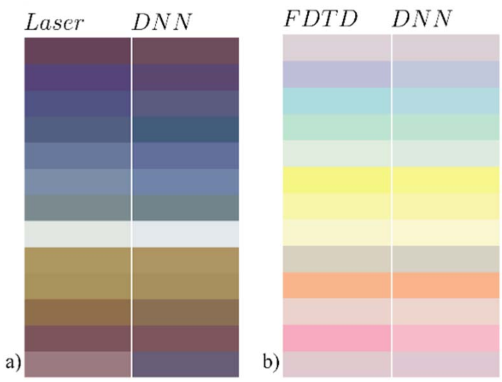

Fig. 1: (a) Comparison between the measured laser colours (left) and DNN predicted colours (right) on the laser test set. (b) Comparison between the FDTD calculated colours (left) and the DNN predicted colour (right).

The accuracy of these methods demonstrates the ability to replace experiments and simulations with DL when enough data exists. These methods can even be used for small extrapolations, thus expanding the dataset further without the need for further experiment or simulation.

III. Inverse Design

The prediction of laser/nanoparticle parameters from a desired colour can't be done directly through training an inverse DNN because of non-uniqueness. Multiple laser parameters or nanoparticle geometries can result in the same colour. Training a single inverse DNN using the data would confuse the DNN resulting in inaccurate predictions.

There are several published suggestions to get around this problem [9]–[11] however these methods would be complicated to implement for a novice. A simpler method is to train N DNNs, where N is the number of input parameters (4 for the laser set and 3 for the simulation dataset). Each DNN is used to predict a single parameter from the desired colours and the other parameters.

As an example, suppose we want to know what nanoparticle geometry will give us a specific colour. For this situation, $N=3$ DNNs are trained, one predicting the particle spacing (from the colour, radius, and embedding), another predicting the embedding (from the colour, radius, and spacing), and the last predicting the radius (from the colour, embedding, and spacing).

Once these are trained, we can then use them iteratively to predict geometric parameters required for that colour. We initialize the particle radius and embedding with random values (or the mean value of the data set). We then use the first DNN to calculate the particle spacing. Using this and the random radius, we can use the second DNN to calculate the new embedding. We then use the embedding and spacing to calculate the radius with the last DNN. This iterative procedure is run until the parameters relax to their final values which will give the desired colour (if the colour is feasible through the laser/nanoparticle technology). This process is called the *iterative multivariable inverse design method* and is shown in Fig. 2. This method is also used for the laser parameter set where $N=4$ DNNs are trained and used.

We again use 90% of the data for training and the other 10% for testing. After we receive the output laser (or nanoparticle distribution) parameters, we compare the input colour to the actual colour generated by the output parameters. A render of some colours from the test set is shown in Fig. 3(a) for the laser set and Fig. 3(b) for the FDTD set. The input colours are shown on the left, and the colour from the output parameters are shown on the right. The mean ΔE is 6.31 for the laser test set and 2.83 for the FDTD test set.

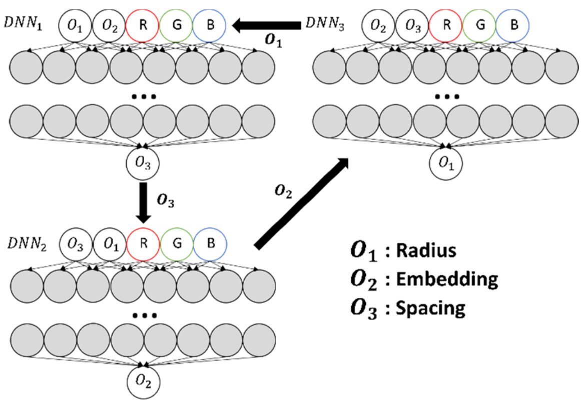

Fig. 2: Iterative multivariable inverse design method. Initial values are assumed for the radius and embedding are assumed. Then DNNs are used to iteratively find the proper radius, embedding, and spacing for a given colour.

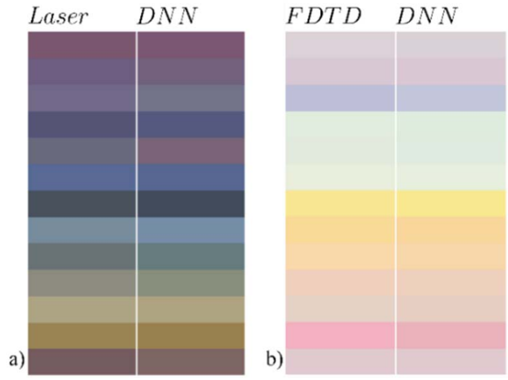

Fig. 3: (a) Comparison between the input laser colours (left) and colours resulting from DNN predicted laser parameters (right) on the test set. (b) Comparison between the input colours (left) and colours resulting from DNN predicted geometric parameters (right) on the test set.

This method is simple in implementation and accurate in prediction. This can be applied for industry. For example, in [4] plasmonic artwork was created on silver surfaces at the Royal Canadian Mint by handpicking colours from a database, which limited the artistic ability of the designers. Instead of designing plasmonic artwork by manually searching for colours that are achievable, the inverse design algorithm can be used to find the laser parameters best suited for the wanted design even if they are not exactly contained in the data set.

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