A novel method to produce nonlinear empirical physical formulas for experimental nonlinear electro-optical responses of doped nematic liquid crystals: Feedforward neural network approach

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ABSTRACT

Among other significant obstacles, inherent nonlinearity in experimental physical response data poses severe difficulty in empirical physical formula (EPF) construction. In this paper, we applied a novel method (namely layered feedforward neural network (LFNN) approach) to produce explicit nonlinear EPFs for experimental nonlinear electro-optical responses of doped nematic liquid crystals (NLCs). Our motivation was that, as we showed in a previous theoretical work, an appropriate LFNN, due to its exceptional nonlinear function approximation capabilities, is highly relevant to EPF construction. Therefore, in this paper, we obtained excellently produced LFNN approximation functions as our desired EPFs for above-mentioned highly nonlinear response data of NLCs. In other words, by using suitable LFNNs, we successfully fitted the experimentally measured response and predicted the new (yet-to-be measured) response data. The experimental data (response versus input) were diffraction and dielectric properties versus bias voltage; and they were all taken from our previous experimental work. We conclude that in general, LFNN can be applied to construct various types of EPFs for the corresponding various nonlinear physical perturbation (thermal, electronic, molecular, electric, optical, etc.) data of doped NLCs.

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1. Introduction

The ultimate purpose of scientific pursuit is to provide the essential means for the unity of humanity. These, among other things, include instantaneous and universal accessibility of information (data, voice, and video) in general. In this respect, we now witness a highly accelerated research into developing holographic and diffractive optical devices for integrated optics, displays and optical data storage. Holographic (three-dimensional) data storage is a potential candidate to replace the currently dominating magnetic and optical recording on the surface of medium. Additionally, holographic storing and retrieving are much faster. In holographic storage, at the point where the reference and the data carrying laser signal beams interfere, the hologram is recorded in the photorefractive storage medium as diffraction pattern of dark and light pixels. Because both recording and retrieving the data are of volumetric character, only the specifically addressed pixel must significantly interact with the addressing laser beam. This process inevitably necessitates a highly nonlinear optical interaction of laser and the storing medium. As a result of this interaction, a large index of refraction alteration (birefringence) in the storing medium is created. In this respect, liquid crystals (LCs) have now become of great interest because they are highly nonlinear optical materials. That is, their physical parameters (thermal, electronic, molecular, optical, etc.) can easily be perturbed by an applied optical field [1, p. 190ff]. Actually, LCs are also extremely sensitive to other weak external fields, for example temperature, pressure, electric, and magnetic. Hence, in addition to large birefringence property, LCs consume only low power. For these reasons, as mentioned above, LCs are under very active research. Some examples of recent studies into nonlinear opto/electro optical properties of LCs are as follows: optical amplification [2], photorefractivity [3,4], holography [5,6], and director reorientation effects [7,8].

Because nonlinearity is the key issue in this paper, it is useful to mention more on the nonlinear optical properties of LCs. Among thermotropic LCs, nematic liquid crystals (NLCs) are the simplest and the most widely used. In NLCs, the liquid molecules have no positional order, but they are directionally correlated, aligned in a general direction of unit vector \( \hat{n} \), the so-called director. Most nematics are uniaxial with the optical axis along \( \hat{n} \).
The measured refractive indices with polarizations parallel or normal to director \( \hat{n} \) show quite large difference. There is a complete rotational symmetry around the director. It is an apolar vector, that is, \( \hat{n} \) and \(-\hat{n}\) are physically equivalent. If the individual molecules have permanent electric dipoles, the medium is still apolar since all molecules orient in such a way that there is no net polarization in the medium. Also, contrary to solid crystal, the orientational polarization in LCs can contribute significantly to the dielectric constant \( \varepsilon \). Due to apolar character of \( \hat{n} \), an external electric field couples to the medium through its dielectric anisotropy \( \Delta \varepsilon = \varepsilon_0 - \varepsilon_\perp \), where \( \varepsilon_0 \) and \( \varepsilon_\perp \) are, respectively, dielectric constants measured with electric field parallel and perpendicular to the director \( \hat{n} \). The corresponding refractive indices are (Eq. (1))

\[
n_l \sim \sqrt{\varepsilon_0}, \quad n_\perp \sim \sqrt{\varepsilon_\perp}
\]

(1)

giving index change \( \Delta n = n_\perp - n_l \). Again, the large birefringence (\( \Delta n \approx 0.2 \)), observed throughout the whole optical region, is an interesting property of NLCs. So, a small director axis reorientation by the light produces different refractive index changes. These changes are enough to generate observable optical effects, such as modifying the propagation, intensity, and polarization states, etc. of the light itself. All these are nonlinear optical processes, as already mentioned above, in which the properties of the medium are modified by the light. Therefore, they have great potential for developing optical information technology devices of exceptional optical quality, low cost and easy of fabrication. In addition to pure NLCs, doping NLCs with dye or nanoparticles further enhance the nonlinear optical properties. For a recent and comprehensive review of nonlinear optics of LCs, see Ref. [9]. Due to extreme importance of director reorientation for LCs, before closing this short passage on NLCs, we must state that realization of reorientation requires application of certain critical external field. More clearly, when an external field (electric or magnetic) is applied to the nematics sample, the orienting effect of the boundaries (elastic forces) conflicts with the orienting effect of the applied field; as a result, a reorientation of director \( \hat{n} \) occurs. However, this reorientation occurs only if the applied field exceeds a well defined threshold value \( V_F \) (Freedericksz transition). \( V_F \) (independent of the sample thickness \( d \)) is inversely proportional to dielectric anisotropy \( \Delta \varepsilon \) (Eq. (2)).

\[
V_F \sim \left( \frac{K_{11}}{\Delta \varepsilon} \right)^{1/2}
\]

(2)

where \( K_{11} \) is the splay elastic constant, relevant to the initial distortion of the director. For photorefractive studies \( V_F \approx 1 \text{ V} \) (for ac applied field), for dc \( \approx 2 - 3 \text{ V} \). Indeed, such a low critical voltage is natural, because among all known materials, NLCs have the smallest elastic constants and the largest birefringence \( \Delta n \) (or equivalently dielectric anisotropy \( \Delta \varepsilon \)).

We see that nonlinear optical properties of NLCs are very important for both theoretical and experimental studies. We concentrate only to experimental side. As in any general physical experimental study, the physical studies in NLCs also pose several significant practical difficulties. One of these is, as we showed in Ref. [10], the inherent nonlinearity in EPF construction. This fact also applies to experimental data for nonlinear, among other physical parameters, electro-optical responses of NLCs.

In this paper we applied a novel method (namely layered feedforward neural network (LFNN) approach) to produce explicit nonlinear empirical physical formulas (EPFs) for experimentally measured nonlinear electro-optical responses of carbon nanoparticles doped NLCs. However, the choice of carbon nanoparticles (as we also mention in Section 3) is accidental, because the aim here is simply to illustrate the LFNN relevance to doped NLC EPF construction. So, the LFNN EPFs construction can also be equally applied to other kind of nanoparticles dispersed or dye dissolved and the like NLCs. Our motivation was that, as we showed in a previous theoretical work [10], an appropriate LFNN, due to its exceptional nonlinear function approximation capabilities [11], is highly relevant to EPF construction. The novelty of the method in this paper is simply the following: although neural networks have been successfully applied to various physical problems (see for instance [10], and references therein), in this paper explicit EPFs constructions for highly nonlinear electro-optical responses for doped NLCs have been first realized by using appropriate LFNNs. Some potential applications are that first, the LFNN EPFs obtained here can be applied to predict the yet-to-be-measured responses, second, new response EPFs can be derived from these LFNN EPFs for doped NLCs. More generally, this novel approach is of the advantage that regardless of the embedded nonlinearity in the empirical (deterministic or random) data, one can always construct suitable nonlinear LFNN approximations in a fast (measured by the relatively low number of iterations) and consistent (excellent ability to generalize over test data sets) manner (see, Sections 4.1–4.3).

As we mention more in Section 2, a LFNN (alternatively multilayer perceptron) is a one input–many intermediate–one output layer device. All layers consist of artificial neurons which are totally connected to each other via adaptable weights. The ultimate aim in LFNN training is to obtain the optimal weights to estimate the functional relationship between input and output [12, p. 156ff]. In this paper, we obtained excellently produced LFNN approximation functions as our desired EPFs for above-mentioned highly nonlinear response data of NLCs. In other words, by using suitable LFNNs, we successfully fitted the experimentally measured response and predicted the new (yet-to-be measured) response data (Sections 3 and 4). The experimental data (response versus input) were diffraction and dielectric properties versus bias voltage; and they were all taken from our previous experimental work [13]. We conclude the paper in Section 5.

2. A brief theory

2.1. The LFNN

In this paper, our specific problem is to find a suitable EPF to fit and predict experimental data for nonlinear electro-optical responses of carbon nanoparticles doped NLCs. The EPF construction is difficult for several reasons, including severe nonlinearity in the experimentally measured response data, (for more, see Ref. [10]). In this context, as a universal nonlinear input–output function approximation device, a suitable LFNN [11], is highly relevant to EPF (input–output relationship) construction [10]. Therefore, a LFNN must also be relevant for our specific EPF construction for doped NLCs. But, to see this, although given in depth in Ref. [10], here again we give the minimum basics of a LFNN and its relevance to EPF construction.

An artificial neural network (ANN), resembling the brain functionality, consists of artificial neurons which interconnect with each other by adaptive weights. Through a learning process, the ANN adapts itself (by modifying weights) to a new environment. That is, it learns how to deal with a set of new initial conditions. As a particular type of ANN, LFNN is a one input–many intermediate (hidden)-one output layer device, with all layers being interconnected through weights (Fig. 1).

As rigorously proved in Ref. [11], a single hidden layer LFNN with enough number of hidden neurons is sufficient for an arbitrarily accurate approximation. For this reason, in this paper,
we only used single hidden layer LFNNs. But, if it is desired, higher number of hidden layers can equally be used. The reason is that the single hidden layer sufficiency in Ref. [11] is only an existence theorem, and does not say that a single hidden layer is optimum for ease of implementation or generalization (see, for more Ref. [12, p. 209ff]). But, our practice with LFNNs show that a single hidden layer is mostly suitable provided enough number of hidden units is used, although a second hidden layer can be added for complex situations [12, p. 212ff]. Now, given an input vector \( x_i \), to compute the output of LFNN, for simplicity we first consider a single hidden layer with only one output component \( r = 1 \) in Fig. 1. In truth, in this paper, we used multi component output LFNNs \( r > 1 \), and we later consider it in Eq. (6). For \( r = 1 \) in Fig. 1, the network output, in line with the rigorous definitions in Ref. [11], is given by Eq. (3)

\[
(f : \mathbb{R}^p \to \mathbb{R} : f(x) = \sum_{j=1}^{b_j} \beta_j G(A_j(x)), x \in \mathbb{R}^p, \beta_j \in \mathbb{R}, A_j \in \mathbb{A})
\]

where \( \mathbb{A} \) is the set of all functions from \( \mathbb{R}^p \) to \( \mathbb{R} \) which are defined by \( A(x) = w^T x + b \). Here, “.” is usual scalar product, \( w \) is a weight vector from input to hidden layer (column vector of matrix \( w^1 \) in Fig. 1), \( x \) is the network input vector in Fig. 1, and \( b \) is the bias (not shown in Fig. 1). Also, in Eq. (3), the hidden neuron activation function \( G : \mathbb{R} \to \mathbb{R} \) is any well-behaved nonlinear function. Because of this universal property of function \( G \), a LFNN is a universal nonlinear function approximator. In most LFNN applications, the activation function \( G \) is a kind of nonlinear sigmoid defined by Eq. (4).

\[
G : \mathbb{R} \to [-1, 1], \text{non-decreasing, } \lim_{\lambda \to -\infty} G(\lambda) = 1, \text{ and } \lim_{\lambda \to +\infty} G(\lambda) = 0 \text{ or } 1
\]

Moreover, for a single hidden layer and one component output layer LFNN, the columns of the weight matrices \( w^1 \) and \( w^2 \) in Fig. 1 correspond to weight vectors defined in \( A(x) \) and \( \beta \) in Eq. (3). Now, given the LFNN defined in Eqs. (3) and (4), the sample data from the material to be learned are simultaneously presented to both input and output layers. The network, by appropriately modifying its weights, iterates to fit the sample training data until a predetermined error level between predicted and desired outputs is attained (for more see Section 4.1 and Fig. 2). The final weights are stored at this stage without further weight modification. Then, by using the final weights, the performance of the network is tested over a test data set which has not been used during training stage. If these test data values are successfully predicted by the LFNN, then the task is complete. That is, the LFNN has learned (generalized) the inherent functional relationship between input and output data.

2.2. Relevance of LFNN to EPF construction

Now, one might naturally wonder why particularly LFNN (not any other ANN) is relevant to EPF construction. It is simple. Because an EPF (either deterministic or random) is generally expressed as a mathematical function between the physical variables considered, the LFNN in Eq. (3) (as a general input–output mathematical function estimator) is particularly suitable in this context. Sample data for independent and dependent physical variables are presented to the input and output layers, respectively. Then the network iterates to discover the unknown generally nonlinear EPF based on the experimental data. We must state very clearly that depending on structure of the LFNN chosen (number of hidden layer, hidden units, activation functions, etc.), we can obtain infinitely many final approximation functions. But, as shown in Ref. [10], within experimental tolerance, any of the final approximation function in Eq. (3) can be used as the desired EPF. As mentioned above, in this paper, the structure of our LFNN is a single hidden layer with multi component output. Consequently, the EPFs we obtained are based on this particular structure (Sections 3 and 4). Also note that the arguments in this Section 2.2 are quite general and abstract. Therefore, for more specific and concrete physical examples for which the LFNNs were actually used to obtain suitable EPFs, see Sections 4.2 and 4.3.

3. The NLC data and the structure of the LFNN used

In order to test and demonstrate the EPF construction capability of the LFNN, in this paper, we used nonlinear electro-optical response of carbon nanoparticles doped NLC literature data. However, the choice of carbon nanoparticles (as already mentioned above) is accidental; therefore, the LFNN EPFs construction can also be equally applied to other kind of nanoparticles dispersed or dye dissolved and the like NLCs. Briefly, as the general considerations in Section 4.2 below (Eq. (6) and the rest) will reveal, due to general nonlinear approximation capability, the LFNN is relevant to EPF of doped NLCs, regardless of the kind of the doping material. The data were taken from our previous experimental work by San et al. [13]. There were two main experiments to obtain this literature data in Ref. [13]: First (Figs. 3a and b) is for grating diffraction measurements (dc bias voltage aided laser induced two-wave mixing diffraction). This experiment is a basis for holography. Second (for Figs. 4a–6b) is for dielectric measurements (real and imaginary parts of permittivity) versus dc bias voltage. Electrical measurements were taken an impedance analyzer HP41994A, under dark. All the measurements were made at room temperature and at 100 kHz spot frequency.

Here, for all LFNN (as depicted in all Figs. 3a–6b), the input value for LFNN was the bias voltage. That is, from Fig. 1, here we take \( p = 1 \), only one input component, namely \( x = dc \) bias voltage. The output components (six in total) of the LFNN (in Fig. 3) were
diffraction signals for both pure and NLC specimen. That is, for Figs. 3a and b, from Fig. 1, \( y_i = \) diffraction signals, for \( i = 1 \) to \( i = r = 6 \). The output components for Figs. 4a–6b, from Fig. 1 were \( y_i = \) real and imaginary parts of permittivity, for \( i = 1 \) to \( i = r \). Here \( r = 6 \) (for Figs. 4a–5b) or \( r = 4 \) for Figs. 6a and b. Note that although in the literature data real and imaginary parts of permittivity were separately treated, in this paper we treated them together for comparison purposes. Since a single hidden layer with enough hidden neurons is sufficient for arbitrary nonlinear approximation [11], we used one hidden layer (with 4–6 hidden neurons) LFNN. There was no bias weight. Also we used both input and output values without normalizing them before train and test phases. Note that it is a commonly employed practice that the original train and test data are normalized into unit interval. That is, the data finally fit in a multi-dimensional region \( \Gamma = \prod_{i=1}^{R} R_i \), where each \( R_i \) is the [0,1] real interval. But, here we intended to show decisively that the LFNN also performs extraordinarily well in much larger multidimensional intervals than \( \Gamma \) above. The activation functions \( g \) in Eq. (3) were, respectively, hyperbolic tangent (a kind of nonlinear sigmoid) \( \tanh (e^{x} - e^{-x}) / (e^{x} + e^{-x}) \) for hidden and linear for output layer. The LFNN weight adapting (learning) was back-propagation with momentum algorithm. The final weight components, depending on the complexity of the nonlinear data, varied between 6.9 and \(-3.15\). The error function between desired and actual neural network outputs was the most commonly used mean square error (MSE). MSE is computed, depending on the task, either for training or test set. MSE is defined as (Eq. (5))

\[
\text{MSE} = \frac{1}{N} \sum_{i=1}^{N} (d_i - o_i)^2
\]

where \( d \), \( o \) and \( N \) are, respectively, desired output, predicted output and the number of training (or test) samples. In Section 4, in each figure NLC data were uniformly partitioned into two separate sets as training and test sets. The test sets were used for prediction (generalization) while training sets were used for fittings. In all cases, each test set was about 20% of its corresponding train set.

4. LFNN simulation results and discussion

4.1. Error function and its minimization

We must first point out that in this paper we do not, in any physical context, re-interpret and re-analyze the experimental literature data in Ref. [13]. Here, we primarily use this data solely to demonstrate the relevance of the LFNN to EPF of NLCs construction. The error function used was MSE of Eq. (5). Here desired \( d \) values were diffraction signals for Fig. 3, and permittivity (real or imaginary) for Figs. 4–6. The \( o \) values were network’s output for estimating the \( d \) values. \( N \) was the number of train (or test) samples. The neural network software used was NeuroSolutions V5.06. The LFNN training was stopped when the pre-assigned epoch (one complete presentation of input-desired data to the network being trained) number (=1000) was attained. The choice of this number is quite arbitrary, which is seemingly set by the LFNN software as a kind of default average. Actually epoch numbers much < 1000 (such as 200) or much greater (such as 10,000) can also be easily pre-assigned by the user. However, significant number of trial trainings in this paper suggested that few hundreds epochs were sufficient in this paper (see Fig. 2), while much higher epochs more than 1000 contributed only little to approximation improvements. Therefore, the epoch number set (=1000) was a compromise. However, these are only observational remarks. Regarding general robustness (stability) and convergence rate problem of back-propagation LFNN, some brief further general remarks can be made. As detailed in Ref. [12, p. 230 ff], back-propagation (BP) algorithm is locally \( H^\ast \)-optimal filter. This means that for the small input–desired output disturbances, the new the initial weight vector is sufficiently close to the undisturbed LFNN optimal final weight vector to ensure the BP training not to end in undesired local minima. In this sense, the back-propagation algorithm is robust. On the other hand, the rate of convergence of BP algorithm is in general relatively slow. Still, some improvements into the accelerated learning rates are also in existence [12, p. 233ff].

For all Figs. 3–6, the train data MSE in Fig. 2 declined to very low levels considerably quickly. The final error levels were nearly \(10^{-5}\), and were achieved in about \( \log_{10}(\text{epoch}) = 1–2\), which corresponds to 100–200 epochs. Note that in Fig. 2, the horizontal axis is plotted in logarithm to obtain a better picture resolution. For each figure NLC train data, the corresponding best MSE curve in Fig. 2 was selected after 5–10 trial LFNN trainings for this particular figure. In summary, the MSE for NLC data reaches to very low values considerably quickly.

4.2. The LFNN construction of EPF for doped NLC data

Let the function \( g: \mathbb{R} \rightarrow \mathbb{R} \) be the desired EPF corresponding to any of the experimentally plotted graph in Figs. 3a–6b. Here, \( p = 1 \) (dc bias voltage) and \( r = 1 \) (either diffraction signal or dielectric permittivity (real or imaginary)). Because the outcome on any given graph (Figs. 3a–6b) is not linear, producing a suitable EPF may be difficult for several probable general reasons, including severe nonlinearity in physical response data [10]. So, in most cases, producing an EPF can be totally ignored. Instead, some physical remarks are made in line with the tendencies involved in the graph. A satisfying explicit formula can appear only much later. Therefore, it would be highly desirable if we had an explicit EPF just after the physical experiment was performed. The LFNN can be used for this purpose. First note that a typical EPF is a relationship between only one output (dependent variable) and probably more than one input (independent) variables. For example, in kinetic energy there are one dependent \( K \) and two independent variables, \( m \) (mass) and \( v \) (velocity). But, in this paper we used a multi-output \( (r = 4 \text{ or } 6) \) LFNN, depending on the number of doped nanoparticles used in the literature experiments in Ref. [13]. Also note that, because different types of carbon nanoparticles were used for each separate figure (Figs. 3–6), we used separate multi-output LFNNs for each of them. Therefore, we obtained separate multi-output final weight LFNNs for each figure. For a concrete consideration, for instance let us choose the final LFNN for Fig. 3. Each component of the LFNN output vector corresponds to a nonlinear electro-optical response (diffraction signal in Fig. 3) of the corresponding doped or pure NLC. We had two reasons in mind when using multi-output (instead of one) LFNN. First, we wanted to deal with only one LFNN error function rather than dealing with several separate error functions for each doped or pure NLC. Second, it would be awkward to present too many (22 in total) LFNN visual data (instead of one) LFNN. First, we wanted to deal with only one LFNN error function rather than dealing with several separate error functions for each doped or pure NLC. Second, it would be awkward to present too many (22 in total) LFNN visual data (instead of one) LFNN. First, we wanted to deal with only one LFNN error function rather than dealing with several separate error functions for each doped or pure NLC. Second, it would be awkward to present too many (22 in total) LFNN visual data (instead of one) LFNN.
The LFNN output function $f$ in Eq. (6), is a nonlinear approximation to the desired nonlinear EPF $g: R^n \rightarrow R'$. Note that $f$ in Eq. (6) is obtained through a weight adaptive error minimization algorithm given the train sample of the input vectors $x$ (dc bias voltage in this paper) and desired vector $y$ (diffraction signal or permittivity). Although desired vector $y$ does not explicitly appear in Eq. (6), it is implicitly involved in minimization process leading to the final LFNN output function $f$. The final weight components are embedded in $A(x)$ and $\beta (w^1$ and $w^2$ in this paper in Fig. 1). With these optimal final weight vectors, because we know the explicit forms of $G$ and $A$ functions in Eq. (6) in advance, we can completely determine the multi-dimensional approximation function $f$ in Eq. (6). $f$ can be used as the desired EPF for experimentally measured nonlinear electro-optical responses of carbon nanoparticles doped NLCs. It is always possible (theorem 2.5 of Ref.[11]) to fit the experimental data with zero error by a sufficient size of single hidden layer. But, in practice, this is not aimed because the LFNN must also perform acceptably well on previously unseen new data. Therefore, as detailed in Ref.[10], with a reasonable number of hidden layer neurons ($n_h$), a sufficiently low final non-zero error level (say $10^{-5}$) is accepted.
In summary, appropriate LFNN output functions \( f \) (defined in Eqs. (3) or (6)) of final weights (embedded in \( A(x) \) and \( b \) of Eq. (6)) can be taken as the nonlinear EPFs (desired functions) of NLCs in this paper. More concretely, by “appropriateness” we have in mind the LFNN with the following properties: (1) sufficient number of hidden neurons (generally determined by a number of trial simulations), (2) a kind of sigmoid activation function in the hidden layer (for instance hyperbolic tangent in this paper), and (3) linear activation function in the output layer.

4.3. LFNN fittings and predictions

In all figures (Figs. 3a–6b), the abbreviation exp is used for experimental results, while nno is for neural network output. In Figs. 3a and b, laser induced and dc voltage aided grating diffraction signals for pure (E7) and carbon doped NLCs were compared with LFNN findings. Fig. 3a (for train data) shows that the LFNN fits the experimental nonlinear response values (diffraction signal) very well. Notice that there is no particular range of data in Fig. 3a where the LFNN performs (fits) relatively poorly. In other words, LFNN fits well for peak, tail and threshold values of diffraction signal data. One might argue that because the LFNN simply memorizes the train data (the problem of overfitting), it will certainly fail to predict previously unseen test data response values. However, as we see from Fig. 3b, contrary to the argument, the LFNN predicts (generalizes) successfully the previously unseen test data as well. Again note that in Fig. 3b, the striking prediction ability of the LFNN is evenly distributed over all the test data. In other words, for test data also, LFNN predicts well for peak, tail and threshold values of diffraction signal data.

(Figs. 4a–6b), nonlinear permittivity (real and imaginary) electro-optical response data (in Ref. [13]) values of carbon nanoparticle doped were compared with LFNN fittings and predictions. As mentioned in Section 3, spot frequency was 100 kHz. The literature data for Figs. 4a (for fitting) and 4b (prediction) were for fullerenes in C\(_{60}\) and C\(_{70}\) forms. In Figs. 4a and b, the striking performance of the LFNN is again evenly distributed over all data values. In other words, the experimental values for the threshold, rise and saturation of the nonlinear permittivity (Re or Im) against dc bias voltage have been successfully fitted and predicted by the LFNN.

Nonlinear permittivity (real and imaginary) electro-optical response data values (in Ref. [13]) of carbon nanotube (CNT) doped NLCs were compared with LFNN fittings (in Fig. 5a) and predictions (in Fig. 5b). The striking LFNN performance is evenly distributed over all data values of nonlinear permittivity responses of CNT doped NLCs against dc bias voltage. Briefly, the experimental nonlinear response trend has been successfully fitted and predicted by the LFNN.

Finally, nonlinear permittivity response data (in Ref. [13]) of graphene doped NLCs were compared with LFNN fittings (in Fig. 6a) and predictions (in Fig. 6b). The striking uniform performance of the LFNN over all data values is again obvious. In other words, the experimental values for the threshold, rise and saturation of the nonlinear response have been again successfully fitted and predicted by the LFNN. One final note can be that in Fig. 3, the experimental laser induced grating diffraction measurements naturally include the significant amount of inherent light scattering and re-absorption losses. Therefore, the LFNN fittings and predictions also inherently include these losses as they are already embedded in the measured data. If the measurement techniques were improved to avoid (at least to some extent) the losses, the LFNN EPFs would accordingly change to comply with these new improved experimental data.
5. Conclusions and some future remarks

In this paper, we have, for the first time, introduced a novel LFNN approach to construct explicit EPFs for nonlinear electro-optical response functions of carbon nanoparticles NLCs. This approach is of the advantage that regardless of the embedded nonlinearity in the empirical (deterministic or random) data, one can always construct suitable nonlinear LFNN approximations in a fast (measured by the relatively low number of epochs) and consistent (ability to generalize over test sets) manner.

5.1. Conclusions

(1) Appropriate LFNNs can successfully estimate the nonlinear physical responses embedded in the experimental literature data of carbon nanoparticle doped NLCs.

(2) The obtained LFNN EPFs also successfully predict the yet-to-be measured experimental literature data mentioned above.

(3) By combining the conclusions 1 and 2, we have produced nonlinear EPFs for experimental nonlinear electro-optical responses of carbon nanoparticle doped nematic liquid crystals.

(4) Since nonlinear LFNN approximation capability is valid for any well-behaved nonlinear multi-dimensional function, although not attempted in this paper, these LFNN EPFs of NLCs, by such mathematical operations as derivation, integration, minimization, etc. can be used to obtain further diffraction signal or permittivity related physical quantities.

5.2. Some future remarks

As already mentioned in the Introduction above, LCs have interesting and promising nonlinear optical properties. Indeed, nearly all conceivable nonlinear optical effects have been observed in LCs, with varying time scales (picoseconds to hours) and powers (nano-watts to megawatts) [9]. Among all these, some brief special further remarks may be given to the nonlinear optical properties of chiral soft materials, including chiral NLCs. We believe that, with extraordinary nonlinear approximation capabilities, the LFNN relevance to nonlinear optics (NLO) of these special soft materials (which are of interest for producing complex photonic devices [14]) might be an exciting future pursuit.

(1) Chiroptical and polarization effects in NLO: Recall that, in the field of linear optics (LO) the material polarization vector $\mathbf{P}$ is related to applied electric field vector $\mathbf{E}$ through a second order dielectric susceptibility tensor $\chi^{(2)}$ by the relation $P_i^{(2)} = \chi_{ijkl}^{(2)} E_k E_l$, where $i,j = 1, 2, 3$. In LO, chiral molecules (that is, molecules lacking a center of inversion symmetry, non-centrosymmetric) possess a special linear property known as optical activity, that is the rotation of the direction of linear polarization of light as it propagates through the material. For NLO domain, the second-order $P_i^{(2)} = \chi_{ijkl}^{(2)} E_k E_l$, and third-order polarizations $P_i^{(3)} = \chi_{ijklm}^{(3)} E_k E_l E_m$, ($i,j,k,l = 1, 2, 3$, etc.) are given by, respectively, $\chi^{(2)}$ (third-order tensor), $\chi^{(3)}$ (fourth-order tensor). Although NLCs have no second-order NLO responses because they are centrosymmetric, chiral NLCs (cholesterics) do have second-order sum or difference frequency (SFG or DFG) NLO responses if only two input fields are orthogonally polarized and non-collinear. The third-order NLO responses give rise to NLO circular dichroism and NLO optical rotation and make it possible to observe dynamic chiral processes at ultrafast time spans [15]. Also, it would have great technological importance if a linear electro-optic effect could exist in an isotropic aggregation of chiral molecules. Investigation of such an effect would require either laboratory measurements or detailed quantum mechanical calculation of optical responses [16]. This may require the involvement of $\chi^{(2)}$, which belongs to NLO domain. In this respect, for calculation purposes, suitable LFNN can still offer some help.

(2) In general, LFNN can be applied to construct various types of EPFs for the corresponding various nonlinear physical perturbation (thermal, electronic, molecular, electric, optical, etc.) data of doped NLCs.

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