Abstract

We present an approach to designing neural network based models that will explicitly satisfy known linear constraints. To achieve this, the target function is modelled as a linear transformation of an underlying function. This transformation is chosen such that any prediction of the target function is guaranteed to satisfy the constraints and can be determined from known physics or, more generally, by following a constructive procedure that was previously presented for Gaussian processes. The approach is demonstrated on simulated and real-data examples.

1 Introduction

Improving the efficiency of neural networks is an intriguing research challenge. Developments during recent years have established deep learning as the perhaps most prominent member of the machine learning toolbox. Today neural networks are present in a broad range of applications and are used for both classification and regression problems. The popularity is to a large extent explained by the highly flexible nature that enables these models to encode a very large class of non-linear functions.

Nevertheless, the performance of the neural network is often dependent on a careful design and the amount of training data available. In particular, a larger network is more flexible but also requires more training data to reduce the risk of overfitting. Different types of regularisation techniques are sometimes used to facilitate this balance.

Instead of focusing on the network per se, it may be just as important to consider prior knowledge provided by the problem setting. For instance, the function of interest can represent a quantity subject to fundamental physical constraints. This includes many vector fields that are known to be either divergence- or curl-free. Examples of divergent-free vector fields (also known as solenoidal fields) are the magnetic field (Konopinski, 1978)—see Figure 1, the velocity of an anelastic flow (Durrant, 1989), the vorticity field (Kundu et al., 2015; Truesdell, 2018), and current density where the charge is constant over time as given by the continuity equation (Chow, 2006; Griffiths, 1962). Low-mach number flow is a simplification of the compressible Euler equations and describes flow with a prescribed divergence (Almgren et al., 2006) (i.e. it takes the form of an affine constraint). Moreover, Maxwell’s equations provide an example of fields with a prescribed curl and divergence corresponding to satisfying linear affine constraints (Fleisch, 2008). Within continuum mechanics the stress field and strain field within a solid object satisfy the equilibrium conditions and the strain field within a simply connected body satisfies the compatibility constraints (Sadd, 2009).

Figure 1: Magnetic field predictions (blue) using a constrained neural network trained on 500 observations (red) sampled from the trajectory indicated by the black curve. The magnetic field, \( \mathbf{B} \) is curl-free satisfying the constraint \( \nabla \mathbf{B} = 0 \), and the method proposed in this paper ensures that the predictions satisfy these constraints.

The list can be made longer, but the point is clear – by making sure that any constraints are fulfilled, we
(significantly) reduce the set of functions that could explain our measured data. This in turn implies that we can maintain a high performance without requiring the same amount of flexibility. Put simply: we can obtain the same results with a smaller network and less training data.

In this paper, an approach for designing neural network based models that satisfy linear operator constraints is presented. The approach models the target function as a linear transformation of an underlying function. The benefits of using this approach are two-fold:

1. Any predictions made using this approach will satisfy the constraints for the entire input space.
2. Incorporating the known constraints reduces the problem size. This reduces the amount of training data required and also allows a smaller neural network to be used while still achieving the same performance. Reducing the amount of data required can save time and money during the data collection phase.

As opposed to existing methods (see Section 6—Related Work), we present a general approach that can be used for any linear operator constraints and suggest two possible ways of determining an appropriate mapping.

2 Problem Formulation

Given a data set of $N$ observations $\{x_i, y_i\}_{i=1}^N$ where $x_i$ denotes the input and $y_i$ denotes the output. Both the input and output are potentially vector-valued with $x_i \in \mathbb{R}^D$ and $y_i \in \mathbb{R}^K$. Here we consider the regression problem where the data can be described by the non-linear function $y_i = f(x_i) + e_i$, where $e_i$ is zero-mean white noise representing the measurement uncertainty. In this work, a neural network is used to model $f$ and can be described by

$$f(x) = h_L(h_{L-1}(\cdots h_2(h_1(x)))))$$

where each $h_l(z)$ has the form

$$h_l(z) = \phi_l(W_lz + b_l),$$

Here, $L$ is the number of layers in the neural network, each $\phi_l$ is an element-wise non-linear function commonly referred to as an activation function and $\{W^l, b^l\}_{l=1}^L$ are the parameters of the neural network that are to be learned from the data.

In addition to the data, we know that the function $f$ should fulfill certain constraints

$$C_x[f] = 0,$$  \hspace{1cm} (3)

where $C_x$ is an operator mapping the function $f$ to another function $g$. That is $C_x[f] = g$. Further, we restrict $C_x$ to be a linear operator, meaning that $C_x[\lambda_1 f_1 + \lambda_2 f_2] = \lambda_1 C_x[f_1] + \lambda_2 C_x[f_2]$, where $\lambda_1, \lambda_2 \in \mathbb{R}$. A simple example is if the operator is a linear transformation $C_x[f] = Cf$ which together with the constraints (3) forces a certain linear combination of the outputs to be linearly dependent.

The operator $C_x$ could also include other linear operators on the function $f$. For example, we might know that the function $f : \mathbb{R}^2 \rightarrow \mathbb{R}^2$ should obey the partial differential equation $C_x[f] = \frac{\partial f_1}{\partial x_1} + \frac{\partial f_2}{\partial x_2} = 0$.

The constraints can come from either known physical laws or other prior knowledge about the data. Here, the objective is to determine an approach to derive models based on neural networks such that all predictions from these models will satisfy the constraints.

3 Building a Constrained Neural Network

In this section, an approach to learn a function using a neural network such that any resulting estimate satisfies the constraints (3) is proposed. First, the approach is presented and then a brief discussion of conditions that may be imposed on the neural network is given.

3.1 Our Approach

Instead of imposing constraints on the parameter values, our approach designs a neural network that satisfies these constraints for all possible values of its parameters. This is done by considering $f$ to be related to another function $g$ via some operator $G_x$:

$$f = G_x[g].$$  \hspace{1cm} (4)

The constraints (3) can then be written as

$$C_x[G_x[g]] = 0.$$  \hspace{1cm} (5)

We require that this relation holds true for any function $g$. To do this, we will interpret $C_x$ and $G_x$ as matrices and use a similar procedure to that of solving systems of linear equations. Since $C_x$ and $G_x$ are linear operators, we can think of $C_x[f]$ and $G_x[g]$ as
matrix-vector multiplications where \( C_x f = C_x f \), with 
\[
(C_x f)_i = \sum_{j=1}^{K} (C_x)_{ij} f_j
\]
where each element \((C_x)_{ij}\) in the operator matrix is a scalar operator. With this notation, (5) can be written as

\[
C_x G_x g = 0,
\]
where a solution is given by

\[
C_x G_x = 0.
\]

This reformulation imposes constraints on the operator \( G_x \) rather than on the neural network model of \( f \) directly. Given this reformulation, we can proceed by first modelling the function \( g \) as a neural network and then transform it using the mapping (4) to provide a neural network for \( f \) that explicitly satisfies the constraints:

\[
f = G_x g.
\]

An illustration of the constrained model is given in Figure 2. The procedure to design the neural network can now be divided into three steps:

1. Find an operator \( G_x \) that satisfies the condition (7).
2. Choose a neural network structure for \( g \).
3. Determine the neural network based model for \( f \) according to (8).

The choice of neural network structure in step 2 may have some conditions placed upon it by the transformation found in step 1 in order for the resulting model to be mathematically correct. For example, if the transformation contains partial derivatives then this may restrict the choice of activation function. A more detailed discussion is given in Section 3.2.

The parameters of the resulting model can be learned using existing methods such as stochastic gradient descent. It is worth noting that if the data requires scaling then care should be taken as this scaling can modify the form of the constraints.

In the case where the operator \( G_x \) contains partial derivatives, such as for curl-free and divergent-free fields, the implementation can be done using automatic differentiation such as the \texttt{grad} function in PyTorch (Paszke et al., 2017).

### 3.2 Conditions due to Derivative Transformations

When the transformation \( G_x \) contains partial derivatives the underlying neural network \( g \) must be chosen to satisfy some conditions. Intuitively, it is required that the partial derivative of the neural network must be a function of both the inputs and the network parameters. If this is not the case, then the model loses the ability to represent a spatially varying target function. Here, we provide a few examples of this.

If the transformation contains only first-order derivatives then this does not place any restrictive constraints. To see this consider a neural network with a single hidden layer and an identity activation function on its output layer, written along with its partial
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4.1 From Physics
system of linear equations.

could be found by proposing an ansatz and solving a
physics of a problem could inform the choice of oper-
ator
Here we have introduced the notation \( a_1 = W_1 x + b_1 \)
to simplify the description. Hence, it is required only
that the first derivative of the activation function with
respect to \( a_1 \) is not constant. However, for higher-
derivatives, there are requirements on the activa-
tion function needs to be non-zero in order for
To use this model it is required that the second deriva-
tive to be a function of the inputs.

This section presents two methods for determining
the derivative as
\[
g(x) = W_2 \phi_1(W_1 x + b_1) + b_2 = W_2 \phi_1(a_1) + b_2,
\]
\[
\frac{\partial g(x)}{\partial x_1} = W_2 \frac{\partial a_1 \phi_1(a_1)}{\partial a_1} = W_2 W_1 \frac{\partial \phi_1(a_1)}{\partial a_1}.
\]

Here we have introduced the notation \( a_1 = W_1 x + b_1 \)
to simplify the description. Hence, it is required only
that the first derivative of the activation function with
respect to \( a_1 \) is not constant. However, for higher-
derivatives, there are requirements on the activa-
tion function needs to be non-zero in order for

From this it is clear that the second derivative of the
activation function needs to be non-zero in order for
the derivative to be a function of the inputs.

4 Finding the Projection Operator

This section presents two methods for determining
a suitable operator \( G_x \). Prior knowledge about the
physics of a problem could inform the choice of oper-
ator. If this is not the case, then a suitable operator
could be found by proposing an ansatz and solving a
system of linear equations.

4.1 From Physics

From fundamental physics, it may be the case that
we know that the vector field of interest is related to
an underlying potential field. Common examples of
this are divergence-free (\( \nabla \cdot f = 0 \)) vector fields and
curl-free (\( \nabla \times f = 0 \)) vector fields. A curl-free vector
field can be written as a function of an underlying
scalar potential field \( g \):
\[
f = \nabla \cdot g,
\]

which gives \( G_x = \begin{bmatrix} \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \end{bmatrix}^T \). Whereas, diver-
geence free vector fields can be expressed as a function
of a vector potential field \( g \in \mathbb{R}^3 \):
\[
f = \nabla \times g,
\]

which gives
\[
G_x = \begin{bmatrix} 0 & -\frac{\partial}{\partial x} & -\frac{\partial}{\partial y} \\
\frac{\partial}{\partial x} & 0 & -\frac{\partial}{\partial z} \\
-\frac{\partial}{\partial y} & \frac{\partial}{\partial z} & 0 \end{bmatrix}
\]

Many natural phenomena can be modelled according
to these constraints, and several examples were given
in the Section 1.

4.2 Ansatz

In absence or ignorance of underlying mathematical
relations, the operator \( G_x \) can be constructed using
the pragmatic approach of which an exhaustive
version is described by Jidling et al. (2017); a brief out-
line is given below. A solid analysis of the mathe-
matical properties of this operator is provided by Lange-
Hegermann (2018).

The cornerstone of the approach is an ansatz on what
operators we assume that \( G_x \) contains; we formulate
it as
\[
G_x = \Gamma \xi,
\]

where \( \xi \) is a vector of operators, and \( \Gamma = [\gamma_{ij}] \)
is a real-valued matrix that we wish to determine. Here,
we have assumed for simplicity that \( G_x \) is a vector,
and so that \( g \) is a scalar function. We now use (15)
to rewrite (7) as
\[
C_x \Gamma \xi = 0.
\]

Expanding the product on the left hand side, we find
that it reduces to a linear combination of operators.
Requiring all coefficients to equal 0, we obtain a sys-
tem of equations from which we can determine \( \Gamma \),
and thus also \( G_x \).

\( \nabla^1 = \begin{bmatrix} \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \end{bmatrix}^T \).
For illustration, consider the toy example where

\[ C_x = \begin{bmatrix} \frac{\partial}{\partial x} & \frac{\partial}{\partial y} \end{bmatrix}. \] (17)

Assuming that \( G_x \) contains the same operators as \( C_x \), we let

\[ \xi = \begin{bmatrix} \frac{\partial}{\partial x} & \frac{\partial}{\partial y} \end{bmatrix}^T. \] (18)

We then expand

\[ C_x \Gamma \xi = \begin{bmatrix} \frac{\partial}{\partial x} & \frac{\partial}{\partial y} \end{bmatrix} \begin{bmatrix} \gamma_{11} & \gamma_{12} & \gamma_{21} & \gamma_{22} \end{bmatrix} \begin{bmatrix} \frac{\partial}{\partial x} & \frac{\partial}{\partial y} \end{bmatrix} \]

\[ = \gamma_{11} \frac{\partial^2}{\partial x^2} + (\gamma_{12} + \gamma_{21}) \frac{\partial^2}{\partial x \partial y} + \gamma_{22} \frac{\partial^2}{\partial y^2}. \] (19)

Requiring this expression to equal 0, we get the following system of equations

\[ \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \gamma_{11} \\ \gamma_{12} \\ \gamma_{21} \\ \gamma_{22} \end{bmatrix} = \mathbf{0}, \] (20)

which is solved by \( \gamma_{11} = \gamma_{22} = 0 \) and \( \gamma_{12} = -\gamma_{21} \). Letting \( \gamma_{21} = 1 \), we obtain

\[ G_x = \begin{bmatrix} -\frac{\partial}{\partial y} & \frac{\partial}{\partial x} \end{bmatrix}^T, \] (21)

which can easily be verified to satisfy (7).

In the general case, \( G_x \) may contain operators of higher order than those in \( C_x \). It is also possible that a suitable underlying function may have a vector rather than scalar output. The procedure should therefore be considered iterative. Additionally, within the supplementary material, we show that this approach can be extended to affine constraints.

### 5 Experimental Results

In this section we demonstrate the proposed approach on simulated data from a divergence-free field, simulated data of a strain field satisfying the equilibrium conditions, and real data of a magnetic field that satisfies the curl-free constraint. Additionally, an example on simulated data satisfying an affine constraint is provided in the supplementary material.

#### 5.1 Simulated Divergence-Free Function

Consider the problem of modelling a divergence-free vector field defined as

\[ f_1(x_1, x_2) = \exp(-ax_1 x_2)(x_1 \sin(x_1 x_2) - x_1 \cos(x_1 x_2)), \]

\[ f_2(x_1, x_2) = \exp(-ax_1 x_2)(x_2 \cos(x_1 x_2) - ax_2 \sin(x_1 x_2)), \] (22)

where \( a \) is a constant. This vector field satisfies the constraints \( \frac{\partial f_1}{\partial x_1} + \frac{\partial f_2}{\partial x_2} = 0 \). A neural network based model satisfying these constraints is given by

\[ f = \begin{bmatrix} \frac{\partial}{\partial x_2} \\ -\frac{\partial}{\partial x_1} \end{bmatrix} g. \] (23)

The regression of this problem using the proposed constrained neural network and an unconstrained (standard) neural network is compared. The networks root mean square error (RMSE) are compared in two studies:

1. Maintaining a constant network size of 2 hidden layers (100 neurons in the first and 50 in the second) and increasing the number of measurements. See Figure 3a.

2. Maintaining a constant number of measurements (4000) and increasing the network size. In this case the total number of neurons is reported with two thirds belonging to the first hidden layer and 1 third belonging to the second. See Figure 3b.

In both studies the measurements are randomly picked over the domain \( [0, 4] \times [0, 4] \), generated with zero-mean Gaussian noise of standard deviation \( \sigma = 0.1 \). For both networks, a tanh activation layer was placed on the output of the hidden layers. The networks were then trained using ADAM, with the learning rate reduced as the validation loss plateaued. A uniform grid of 20 × 20 points is chosen to predict the function values at. The root mean square error is calculated between the true vector field and the predictions at these locations. In order to focus this analysis on the impacts of the suggested approach, dropout, weight decay and other methods to reduce over-fitting have not been implemented.

In both these studies, the proposed approach yields a significantly lower RMSE than a standard neural network. To highlight a few points, the proposed approach with 500 measurements has the same RMSE as the standard neural network with 4000 measurements. Similarly, with 21 total neurons the proposed approach performs as well as the standard neural network with 150 neurons.
An example of the learned vector fields from 200 noisy observations is provided in Figure 4. For this comparison, both networks had two hidden layers with 100 neurons in the first and 50 in the second and a tanh activation function was placed on the outputs of both hidden layers.

These results indicate that the proposed approach can achieve equivalent performance with either less data or a smaller network size. Another property of our constrained neural network is that its predictions will automatically satisfy the constraints. This is true even in regions where no measurements have been made as illustrated in Figure 5. By comparison, the standard neural network gives estimates which violate the constraints.

### 5.2 Simulated Strain Field

An example of a more complex constraint can be given by considering the estimation of strain fields. Strain fields describe the relative deformation of points within a solid body and can be measured by neutron and X-ray diffraction (Noyan and Cohen, 1987) providing a means to study the stress—a quantity that cannot be directly measured. Maximum stresses are commonly accepted as a major contributing factor to component failure (Sadd, 2009) and hence studying stress is of interest for the design of engineering components.

Physical strain fields satisfy the equilibrium constraints and as such it is important to ensure that any estimates of these fields from measurements also satisfies these constraints (Sadd, 2009). Here, we consider a two-dimensional strain field with components described by \( \epsilon_{xx}(x, y) \), \( \epsilon_{yy}(x, y) \), and \( \epsilon_{xy}(x, y) \). Under the assumption of plane stress the equilibrium constraints are given by (Gregg et al., 2018)

\[
\begin{align*}
\frac{\partial}{\partial x}(\epsilon_{xx} + \nu \epsilon_{yy}) + \frac{\partial}{\partial y}((1-\nu) \epsilon_{xy}) &= 0, \\
\frac{\partial}{\partial y}(\epsilon_{yy} + \nu \epsilon_{xx}) + \frac{\partial}{\partial x}((1-\nu) \epsilon_{xy}) &= 0.
\end{align*}
\]  

(24)

A neural network based model satisfying these constraints can be derived from physics using the so-called Airy stress function (Sadd, 2009) and is given by

\[
\begin{bmatrix}
\epsilon_{xx} \\
\epsilon_{yy} \\
\epsilon_{xy}
\end{bmatrix} = \begin{bmatrix}
\frac{\partial^2}{\partial x^2} - \nu \frac{\partial^2}{\partial x \partial y} \\
\frac{\partial^2}{\partial y^2} - \nu \frac{\partial^2}{\partial y \partial x} \\
-(1+\nu) \frac{\partial^2}{\partial x \partial y}
\end{bmatrix} \mathbf{g}.
\]  

(25)

This model is used to learn the classical Saint-Venant cantilever beam strain field under an assumption of plane stress (Beer et al., 2010) from 200 noisy simulated measurements. Details of this strain field and the measurements is given in the supplementary material.

Predictions of this strain field using the proposed model and a standard neural network are shown in Figure 6. The proposed approach gives an RMSE of 5.52 \times 10^{-5} compared to 6.77 \times 10^{-4} for the standard neural network. Qualitatively, we can see that the proposed approach provides more accurate estimates of the strain field, particularly for the \( \epsilon_{xy} \) component.

### 5.3 Real Data

Magnetic fields can be mathematically described as a vector field mapping a 3D position to a 3D magnetic field vector, \( \mathbf{B} \). Based on the magnetostatic equations, this can be modelled as a curl-free vector field
Figure 4: Comparison of learning the divergence-free field from 200 noisy observations using an unconstrained neural network (NN) and our constrained approach. Left: the true field (grey) and observations (red). Center and right: learned fields subtracted from the true field. Done using 2 hidden layers, 100 neurons in first, 50 in second for both methods.

Figure 5: Comparison of learned fields constraint violations from 200 simulated noisy observations of a divergence-free field using an unconstrained neural network and our approach. Left: the true field (grey) and observations (red). Centre and right: the constraint violations. No measurements were made inside the dashed blue box. Center and right: Constraint violations for the learned fields calculated as $c = \frac{\partial f_1}{\partial x} + \frac{\partial f_2}{\partial x^2}$.

Figure 6: The theoretical Saint-Venant cantilever beam field and strain fields learned from 300 noisy measurements using the presented constrained approach and a standard neural network. Both networks have three hidden layers with 20, 10, and 5 neurons, respectively. Values are given in micro strain.

(Wahlström, 2015; Solin and Särkkä, 2014): As such, a neural network satisfying the curl-free constraint can be designed to model the magnetic field

$$\nabla \times \mathbf{B} = 0.$$  \hspace{1cm} (26)
according to
\[ \hat{B} = \begin{bmatrix} \frac{\partial}{\partial x_1} \\ \frac{\partial}{\partial x_2} \\ \frac{\partial}{\partial x_3} \end{bmatrix} g \]  
(27)

With a magnetic field sensor and an optical positioning system, both position and magnetic field data have been collected in a magnetically distorted indoor environment — with a total of 16,782 data points collected. Details of the data acquisition can be found in the supplementary materials of Jidling et al. (2017), where this data was previously published. Figure 1 illustrates magnetic field predictions using a constrained neural network trained on 500 measurements sampled from the trajectory shown in black. The constrained neural network had two hidden layers of 150 and 75 neurons, with \text{Tanh} activation layers. Using the remaining data points for validation, our constrained model has a RMSE validation loss of 0.048 compared to 0.053 for a standard unconstrained neural network of the same size and structure.

Two studies were run comparing the proposed approach and a standard neural network for a range of training data sizes and neural network sizes. The networks RMSE when validated against 8,000 reserved validation data points

1. Maintaining a constant network size of 2 hidden layers (150 neurons in the first and 75 in the second) and increasing the number of measurements. See Figure 7a.

2. Maintaining a constant number of measurements (6000) and increasing the network size. In this case the total number of neurons is reported with two thirds belonging to the first hidden layer and one third belonging to the second. See Figure 7b.

For both studies 100 random trials are run and the average result is reported.

The studies show that the proposed approach performs better than the standard neural network for a smaller number of measurements or a smaller network size. As the number of measurements or neurons is increased, the performance of both networks converges. This is expected as given enough measurements and a large enough network size, both methods should converge to the true field and hence a minimum validation RMSE.

6 Related work

Focusing on neural networks, related work falls into two broad categorises: incorporating known physics relations as prior knowledge, and solving constrained optimisation problems using neural networks. Here, we discuss some of these methods that are closely related or of particular interest.

The idea of modelling potential functions using neural networks as a means to include prior knowledge about the problem is not new and has been used to learn models of dynamic systems and vector fields.

There are a number of examples of using neural networks to learn the Hamiltonian or Lagrangian of a dynamic system and training this model using the derivatives of the neural network (Greydanus et al., 2019; Lutter et al., 2019; Zhong et al., 2019; Gupta et al., 2019). These methods ensure that the learned dynamics are conservative, i.e. the total energy in the system is constant. Another approach to learning dynamic systems is presented by Chen et al. (2018) in which neural networks are used to model solutions to ODEs and Massaroli et al. (2019) proposes a Port-Hamiltonian based approach to training these models.

A method for simultaneous fitting of magnetic potential fields and force fields using neural networks is studied by Pukrittayakamee et al. (2009). This method uses a neural network to model the potential field and the force field is then the partial derivatives of the neural network. In their work, measurements of both the potential field and the force field are used to train the model. A similar approach is taken by Handley and Popelier (2010) where it is used for modelling molecular dynamics and Monte Carlo studies on gas-phase chemical reactions.

Although it was not the motivation for the method, the model for the force field given in Pukrittayakamee et al. (2009) will obey the curl-free constraint and is equivalent to that presented in Section 5.3. In our work, we extend the idea of representing the target function by a transformation of a potential function modelled by a neural network to a broader range of problems that obey a variety of constraints. Additionally, we focus only on the transformed target function and do not require measurements of the potential function.

In Tompson et al. (2017), convolutional networks are used to simulate Eulerian fluid flows. Although fluid flow can be expressed as partial derivatives of vector quantities, this work does not incorporate this as prior knowledge.

Another interesting idea is presented by Schmidt and Lipson (2009) in which a method for distilling natural laws from data is presented. In this work, symbolic terms including partial derivatives are used as build-
Figure 7: Two studies comparing the performance of the proposed constrained neural network based model with a standard unconstrained neural network using data collected of a magnetic field. The RMSE is compared as (a) the number of measurements is increased and (b) as the size of the neural network is increased.

7 Conclusion

An approach for designing neural network based models for regression problems in which the target function is known to obey linear operator constraints has been proposed. It has been demonstrated on simulated data and real data that this approach provides benefits by reducing the size of the problem. This reduces the required number of data points and the size of the neural network — potentially providing savings in terms of time and cost required to collect the data set. By construction, this approach also guarantees that any prediction made by the model will obey the constraints for any point in the input space.

The proposed approach constructs the model by a transformation of an underlying potential function, where the construction is chosen such that the constraints will always be satisfied. It is suggested that this transformation may be known from physics or in the absence of such knowledge using a method of ansatz. Additionally, we provide an example of extending this approach to affine constraints (constraints with a non-zero right hand side) in the supplementary materials.

An interesting area for future research would be to determine if it is possible to learn the transformation as a combination of symbolic elements using tools similar to those presented in (Schmidt and Lipson, 2009).

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A Simulated Affine Example

It is also possible to design a model to satisfy an affine constraint $C_x f = b$. This type of constraint arises for vector fields that have a prescribed divergence of curl. For example, Maxwell’s equations (Fleisch, 2008) and low-mach number flow (Almgren et al., 2006).

To illustrate the approach, we design a neural network that will satisfy constant divergence, i.e. $\nabla f = b$, and demonstrate the method in simulation. The model satisfying this constraint can be built by starting from the model used in the previous section that satisfies $\nabla f = 0$. From this starting model, we need to add an
additional component that when mapped through the constraints results in a constant term. This is easily achieved using a 2 input 1 output linear layer with no bias term, giving the final model as

$$\hat{f} = \left[ \frac{\partial}{\partial x^2} c_0 \right] \mathbf{g} + c_0 x_1 + c_1 x_2, \quad (28)$$

where the weights $c_0$ and $c_1$ will be learned along with the rest of the neural network parameters.

Figure 8 shows the results of learning a field satisfying these constraints using our approach and a standard neural network. Measurement locations are randomly picked over the domain $[0, 4] \times [0, 4]$, with 200 measurements simulated from the field given by

$$f_1(x_1, x_2) = \exp(-ax_1 x_2) ax_1 \sin(x_1 x_2) - \exp(-ax_1 x_2) x_1 \cos(x_1 x_2) + 1.1 x_1,$$

$$f_2(x_1, x_2) = \exp(-ax_1 x_2) x_2 \cos(x_1 x_2) - \exp(-ax_1 x_2) ax_2 \sin(x_1 x_2) - 0.3 x_2, \quad (29)$$

and zero-mean Gaussian noise of standard deviation $\sigma = 0.1$ added. For both networks, two hidden layers are used with 100 and 50 neurons respectively and Tanh activation layers. The field is then predicted at a grid of 20 $\times$ 20 points with the proposed approach achieving an rms error of 0.21 compared to 0.48 for the standard neural network.

## B Strain Field and Measurement Details

This section provides details of the strain field equations and the simulated measurements used for the simulated strain field example in the main paper. The simulation uses the classical Saint-Venant cantilever beam strain field equations under an assumption of plane stress (Beer et al., 2010);

$$\epsilon_{xx}(x, y) = \frac{P}{EI}(l - x)y,$$

$$\epsilon_{yy}(x, y) = -\frac{\nu P}{EI}(l - x)y,$$

$$\epsilon_{xy}(x, y) = -\frac{(1 + \nu) P}{2EI} \left( \frac{h}{2} \right)^2 - y^2, \quad (30)$$

where $P = 2$ kN is the applied load, $E = 200$ GPa is the elastic modulus, $\nu = 0.28$ is Poisson’s ratio, $l = 20$ mm is the beam length, $h = 10$ mm is the beam height, $t = 5$ mm is the beam width, and $I = \frac{th^3}{12}$ is the second moment of inertia.

Simulated measurements of this strain field were made at random locations within the beam and were corrupted by zero-mean Gaussian noise with standard deviation $2.5 \times 10^{-4}$. In practice, such measurements can be made by X-ray or neutron diffraction and correspond to the average strain within a small volume of material inside the sample, known as a gauge volume (Noyan and Cohen, 1987). Gauge volumes can be made small enough that it is practical to treat these measurements as corresponding to points in the sample, and noise levels as low as $1 \times 10^{-4}$ or better can be achieved.

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Figure 8: Comparison of learning the affine constrained field from 200 noisy observations using an unconstrained neural network and our approach. Left: the true field (grey) and observations (red). Center and right: learned fields subtracted from the true field. Done using 2 hidden layers, 100 neurons in first, 50 in second for both methods.

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