MULTIGOAL-ORIENTED DUAL-WEIGHTED-RESIDUAL ERROR ESTIMATION USING DEEP NEURAL NETWORKS

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Ayan Chakraborty1, Thomas Wick2,6,*, Xiaoying Zhuang3,4,**, and Timon Rabczuk1,2

1Division of Computational Mechanics, Ton Duc Thang University, Ho Chi Minh City, 99423, Vietnam
2Faculty of Civil Engineering, Ton Duc Thang University, Ho Chi Minh City, 99423, Vietnam
3Department of Geotechnical Engineering, College of Civil Engineering, Tongji University, Shanghai, China
4Chair of Computational Science and Simulation Technology, Institute of Photonics, Faculty of Mathematics and Physics, Leibniz University, Hannover, 30163, Germany
5Institute of Applied Mathematics Welfengarten 1, AG Wissenschaftliches Rechnen, Leibniz University, Hannover, 30167, Germany
6Cluster of Excellence PhoenixD (Photonics, Optics, and Engineering - Innovation Across Disciplines), Leibniz University Hannover, Germany

*Corresponding author: thomas.wick@ifam.uni-hannover.de
**Corresponding author: zhuang@iop.uni-hannover.de

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ABSTRACT

Deep learning has shown successful application in visual recognition and certain artificial intelligence tasks. Deep learning is also considered as a powerful tool with high flexibility to approximate functions. In the present work, functions with desired properties are devised to approximate the solutions of PDEs. Our approach is based on a posteriori error estimation in which the adjoint problem is solved for the error localization to formulate an error estimator within the framework of neural network. An efficient and easy to implement algorithm is developed to obtain a posteriori error estimate for multiple goal functionals by employing the dual-weighted residual approach, which is followed by the computation of both primal and adjoint solutions using the neural network. The present study shows that such a data-driven model based learning has superior approximation of quantities of interest even with relatively less training data. The novel algorithmic developments are substantiated with numerical test examples. The advantages of using deep neural network over the shallow neural network are demonstrated and the convergence enhancing techniques are also presented.

Keywords Deep Learning · NURBS Geometry · Multi Objective Goal Functionals · A posteriori Error Estimation · Navier-Stokes Equations

1 Introduction

Differential equations are the cornerstone of a vast range of engineering fields and applied sciences. It is the most common class of simulation problem in science and engineering and is devised as a mathematical tool to study the physical world in a precise manner. So far a wide varieties of methods have been developed for solving differential equations, for instance see [1, 2, 3, 4] and the references therein. In most of the previous works, solving PDEs is restricted to solve a linear system of algebraic equations which result from the discretization of the computational domain. In particular approximating the solution is a crucial step and most of such contributions intend to explore variety of such possibilities.

In this paper, we view the problem from a different angle. We propose a promising method for solving PDEs that entirely relies on the function approximation capabilities of the feed forward neural networks that has achieved
immense success in approximation theory and set the foundations for a new paradigm in modelling as well as computations which also enriches deep learning with the longstanding developments and have made a transformative impact on modern technology. The recent breakthroughs in machine learning in the form of Deep Neural Network (DNN) have led to outstanding achievements in several areas and hence become extremely popular in computational sciences in recent years. Starting from visual recognition, image processing, natural language processing and in many other diversity, DNNs with the capability of holding large number of hidden layers has proven an extremely successful devise to approximate the target function. Thanks to the development of very powerful computational tools viz. Tensorflow [5], Pytorch [6] libraries that provide the building blocks to train the machine with respect to different problems and are currently ones main focus in the field of applied mathematics and computer science. Recent trends of applying DNN to approximate solutions are being increasingly used in the context of numerical computations of PDEs [7, 8, 9, 10]. With the explosive growth of computational resources, deep learning becomes rapidly evolving field. In the following, we will provide a brief overview. In [11, 12, 13] sequential threshold Ridge regression is proposed, i.e. Lasso regression to identify PDE from data. In [15], so called DL-PDE is proposed that combines neural network and data driven discovery via sparse regression. Long et al. [16] proposed PDE-Net to discovering PDE from complex data set, however their approach requires a large amount of data and is robust in some specific cases. Beck et al. [18] developed an algorithm for solving a class of quasilinear PDEs with high accuracy and speed. In addition, the authors in [19] have proposed a scheme to optimize deep neural networks using PDEs.

In this paper, we consider the strong form of PDEs, leading to a collocation based approach. Given the fact that the learning process of DNN can be considered as an iterative process of minimizing the loss function, therefore it seems natural to consider the residual of the system as an ideal candidate for this function. Our main aim is to develop goal-oriented a posteriori error estimation with two objectives in mind. At one hand, we focus on the dual-weighted residual method [20, 21, 22, 23, 38, 24, 25] and on the other hand, we consider multiple functionals of interest [28, 29, 32, 30, 31, 51, 32, 27]. These error estimators are formulated for nonlinear problems in which both the PDE and the functionals are nonlinear.

The main objective of this work is to study such multigoal-oriented error estimators in the framework of machine learning. We mainly focus on the Deep Collocation Method (DCM) and we have shown that our method is capable of achieving a good prediction accuracy given a sufficient number of collocation points on the domain with sufficiently expressive neural network architecture. Our network is fed with a relatively small number of training points (few hundred and up to few thousand at most) in all benchmark examples. The closest studies to ours are [14] and [34], where in the latter only the adjoint equation is approximated via a neural network. Using neural networks for both the primal and the adjoint equation is a difference to that prior works. Moreover, the extension to multiple goal functionals has not yet been treated in the state-of-the-art literature. By embedding deep learning modules we have build a novel and reliable framework that has been tested and validated for both linear and non linear PDEs in complex domain, with various boundary conditions and numerous goal functionals.

The paper is structured as follows: In Sect. 2 we introduce the model problem and discuss about the neural network features and implementation details for training purpose. Next in Sect. 3 the basic concept of goal functionals and the approach for dealing multiple goal functionals are presented. Sect. 4 briefly reviews the NURBS geometry and its application to represent complex geometry. In Sect. 5 several numerical tests substantiate our algorithm developments. Finally, in Sect. 6 conclusions are drawn and some ideas for are proposed future studies.

2 Problem setup & methodology

Let us consider a parameterized PDE in the following form:

\[ \mathcal{N}(u, \nabla u(x), \lambda) = f(x) \]

subjected to certain BCs (Dirichlet, Neumann or mixed) i.e., for \( x \in \partial \Omega \)

\[ B[u(x)] = g(x) \]

where \( \mathcal{N} : \mathcal{V} \rightarrow \mathbb{R} \) is any differential operator (linear or non linear), \( x \in \Omega \subset \mathbb{R}^n \) and define,

\[ \Gamma(x, u) := \mathcal{N}(u, \nabla u(x), \lambda) - f(x) \]

\( \lambda \) is real, for example in the Navier-Stokes problem it represents the viscosity of the fluid, Reynolds number etc.
Here $V$ is some suitably chosen function space containing the exact solution and the family of all neural network functions corresponding each set of deep collocation points covering the domain $\Omega$.

This version of the boundary value problem (BVP) is called strong form. We proceed by approximating $u$ and $\Gamma$ using Deep Neural Networks (DNNs) $U_\theta = U(x, \theta)$ and $\Gamma_\theta = \Gamma(x, U_\theta)$. Our approach adopts deep collocation method, which assumes a certain discretization of the domain $\Omega$ and its boundary $\partial \Omega$ into a collection of points $\pi_\Omega$ and $\pi_{\partial \Omega}$ respectively. The goal is to learn the parameters of NNs. These along with parameters of the operator $\mathcal{N}$ are learned by minimizing the error function under mean squared error (MSE) norm. For $x_i \in \pi_\Omega$ and $s_i \in \pi_{\partial \Omega}$ define:

$$
E[\theta] := \frac{1}{N_{\text{int}}} \sum_{i=1}^{N_{\text{int}}} |\Gamma_\theta(x_i)|^2 + \frac{1}{N_{\text{bnd}}} \sum_{i=1}^{N_{\text{bnd}}} |B[u(s_i)] - g(s_i)|^2
$$

$$
= ||\Gamma_\theta(x)||_{\pi_\Omega}^2 + ||B[u(s)] - g(s)||_{\pi_{\partial \Omega}}^2
$$

(1)

The points are uniformly sampled from the domain and its boundary. Basically this equation is a Monte Carlo approximation of

$$
E_{\text{err}}[\theta] := \mathbb{E}_{x \sim U(\Omega)} [ (\Gamma_\theta(x))^2 ] + \mathbb{E}_{s \sim \mathcal{U}(\partial \Omega)} [ (B[u(s)] - g(s))^2 ]
$$

where $U(\Omega)$ and $U(\partial \Omega)$ represent the uniform distribution on the domain and its boundary. This error function measures how well a neural network approximates the original solution and satisfies BVP w.r.t the defined norm. From an optimization point of view it could be more sophisticated to multiply the constraints with suitable penalty measures how well a neural network approximates the original solution and satisfies BVP w.r.t the defined norm. Moreover a prior knowledge of the exact solution is redundant here. Given any BVP the error loss can be computed directly up to a certain level of approximation of the solution. The main objective is to construct such a neural network function $U_\theta$ by fine tuning the parameters so that $E$ is as close to zero as possible.

2.1 Network architecture

An Artificial Neural Network (ANN) is a human brain inspired algorithm and is designed to approximate a continuous mapping based on the given input. The network chain categorized into three different classes of layers namely: input layer, hidden layers and output layer and each layer is made up of multiple neurons. The structure is shown in Fig. [1]. Again neurons in each layer is connected to every other neurons in the next layer. For example two adjacent layers are coupled as follows:

$$
y_\ell(x) := \sigma_\ell(W_\ell y_{\ell-1}(x) + \beta_\ell) \ ; \ \ell = 1, 2, 3 \ldots, L + 1
$$

where, $y_\ell$ is the output of layer $\ell$, $W_\ell$ are affine mappings and $\sigma_\ell$ is a fixed element wise activation function. The affine mappings are combinations of rectangular matrix whose elements are called weights, and $\beta_\ell$ is a bias vector. Consequently using the functional structure of DNN as a sequence of function composition or layers the relationship between an input vector $x_0$ and output prediction $y_{L+1}$ can be expressed in the form:

$$
y_{L+1} = \mathcal{N}(x_0; \theta) = W_L \sigma_L (\ldots \sigma_3(W_2 \sigma_2(W_1 x_0 + \beta_1) + \beta_2)\ldots) + \beta_L
$$

where, $\theta := \{W_1, \beta_1; W_2, \beta_2; \ldots; W_L, \beta_L\}$ is a set of all trainable parameters. Now suppose we have a sample of $T$ observation data $\{x_1, x_2, \ldots, x_T\}$ then training an ANN means to solve the optimization problem

$$
\theta_* := \arg \min_{\theta \in \Theta} \sum_{i=1}^{T} (u(x_i) - \mathcal{N}(x_i; \theta))^2
$$

where $\Theta$ is a collection of all admissible parameters.

The optimized numbers of required neurons and layers are the main hyper-parameters controlling the architecture of this black box model. There is no analytical way to calculate or easy rule of thumbs to follow. Depending on the nature of problems optimal values needed to be explore in order to avoid over-fitting and under-fitting inside the network. The signals are transmitted through this connection from one layer to another, while each input is multiplied by a set of weights and bias values associated with these, determines the parameter $\theta$. The whole signals are now summed together to feed the node’s activation function. The role of activation function is to introduce non linearity into the network. This is one of the crucial component in the network and if fits well it can reduce the computational cost while retaining the efficiency and accuracy of the model.
Once the architecture has been decided i.e. the number of layers, number of neurons on each layer, and the activation functions are frozen, the problem boils down to determine the parameter $\theta$. In our problem the process of obtaining these parameters through training the network or equivalently the problem of minimizing the loss function Eq 1. Here comes the importance of optimizers algorithm that are used to update those parameters in order to reduce the losses and provide the most accurate results as possible. As like activation functions numerous optimizers exist in the literature but the challenge is to segregate the useful one for gaining the optimal solution sacrificing nominal computational cost.

2.2 Implementation

The success of a neural network completely depends on its architecture. There is no rule of thumb for selecting, and therefore different problems ask for different architectures. Nevertheless a wise construction of an architecture can significantly improve the performances. Our novel architecture is build upon using Keras model [50] with Tensorflow backend. We don’t use original Keras instead build Keras model with tf.keras module. Even though standard gradient descent optimizers is dominating the training process of DNN model these days, however the estimation is cruder and therefore using a second order method for example L-BFGS attempts to compensate and results in better generalizations. The optimizers are imported from Tensorflow Probability [47] library to train tf.keras.model and its subclass. One of the main advantage of this workaround is this library is GPU-capable and hence it is possible to perform large-scale computations. Let us also briefly discuss about the activation function. As mentioned earlier it is the building blocks and requires to sort out between “useful” and “not so useful” from the plethora of information. Generally sigmoid or tanh are the most well known activation functions used in various deep learning models [36, 7] and we have also started with such functions but fail to obtain the optimum results. Therefore in our experiments we have proceeded via trial and error methods to make a better choices of an activation function for easy and fast convergence of the network. One thing to note that the final layer should always be the linear function of its preceding layers.

We now provide the implementation details of the algorithm and have highlighted some typical steps that one would have to follow for a Python based Tensorflow [5], an open source well documented and currently one of the most popular, fastest growing deep learning library. The idea is to demonstrate the general procedure. The full source code is available on Github and can be obtained by contacting the authors.

By using the Xavier Initialization technique [37] the weights and biases are initialized in the following manner:

```python
def initialize_NN(self,layers):
    weights = []
```
biases = []
num_layers = len(layers)
for l in range(0, num_layers - 1):
    W = self.xavier_init(size=[layers[l], layers[l + 1]])
    b = tf.Variable(tf.zeros([1, layers[l + 1]], dtype=tf.float64), dtype=tf.
    →
    float64)
    weights.append(W)
    biases.append(b)
return weights, biases

def xavier_init(self, size):
in_dim = size[0]
out_dim = size[1]
xavier_stddev = np.sqrt(2.0 / (in_dim + out_dim))
return tf.Variable(tf.truncated_normal([in_dim, out_dim], stddev=xavier_stddev),
    →
    dtype=tf.float64)

u(x) can be simply defined as follows:

def net_u(self,x,y):
    X = tf.concat([x,y],1)
    u = self.neural_net(X,self.weights,self.biases)

Finally, the neural network is defined using an activation function:

def neural_net(self,X,weights,biases):
    num_layers = len(weights) + 1
    H = 2.0*(X - self.lb)/(self.ub - self.lb) - 1.0
    for l in range(0,num_layers-2):
        W = weights[l]
        b = biases[l]
        H = tf.tanh(tf.add(tf.matmul(H, W), b))
    W = weights[-1]
    b = biases[-1]
    Y = tf.add(tf.matmul(H, W), b)
    return Y

3 Goal-oriented error estimation

In this section, the main objective is goal-oriented error estimation using adjoint sensitivity weights. This idea was originally proposed in [20, 21] and is the so-called dual-weighted residual (DWR) method.

3.1 Main concepts and goal functionals

In the following, we describe the DWR approach in more detail. Often, instead of an accurate approximation \( u_\theta \) everywhere in the computational domain, our focus of interest is a quantity of interest \( J(u_\theta) \), which should be computed to a certain accuracy. The objective is to measure the error \( e \) between the (often unknown) exact solution \( u \) and the (neural network) approximate solution \( u_\theta \) in terms of a goal functional \( J : V \rightarrow \mathbb{R} : \)

\[
e = J(u) - J(u_\theta).
\]

Examples for such goal functionals are the mean values, line integration or point value evaluations:

\[
J(u) = \int_\Omega u \, dx, \quad J(u) = \int_{\partial \Omega} \frac{\partial u}{\partial n} \, ds, \quad J(u) = u(x_0) \quad \text{for} \ x_0 \in \Omega.
\]
Moreover technical quantities such as stress evaluations, drag, lift, and vorticity evaluations can be represented with the help of \( J(\cdot) \).

The second goal functional can be computed using Green’s first identity. Following \( [21] \), the goal functional evaluation can be framed into an optimization problem in which the goal functional error (adjoint based) is minimized with respect to the governing partial differential equation. Hence

\[
\min (J(u) - J(u_\theta)) \quad \text{s.t.} \quad N(u) = f.
\]

The above goal functional error is computed with the numerical method leading to a discrete version \( u_\theta \). However the main objective is to control the error \( J(u) - J(u_\theta) \) in terms of the local residuals computed in each (collocation) point. To address this we assign an associated adjoint problem, for which we use the Lagrangian formalism. The Lagrangian \( L : \mathcal{V} \times \mathcal{V} \rightarrow \mathbb{R} \) is defined as

\[
L(u, z) = (J(u) - J(u_\theta)) - N(u)z + fz,
\]

with the adjoint variable \( z \in \mathcal{V} \). The corresponding optimality system is obtained by differentiation with respect to \( u \) and \( z \) resulting in the primal and adjoint equations:

Find \( u, z \in \mathcal{V} \) such that

\[
\begin{align*}
N'(u) - f &= 0 \\
N'(u)z - J'(u) &= 0
\end{align*}
\]

where \( N' \) and \( J' \) represent the Fréchet derivatives of the original operator \( N \) and goal functional \( J \), respectively.

**Remark 1.** For linear PDEs \( N(u) \) and linear goal functionals \( J(u) \), the above system reads

\[
\begin{align*}
N(u) - f &= 0 \\
N(z) - J(u_\theta) &= 0
\end{align*}
\]

In order to solve System \( [2] \), we approximate \( u \) and \( z \) by their neural network approximations \( u_\theta \) and \( z_\theta \), respectively. Find \( u_\theta \) and \( z_\theta \) such that

\[
\begin{align*}
N'(u_\theta) - f &= 0 \\
N'(u_\theta)z_\theta - J'(u_\theta) &= 0
\end{align*}
\]

We see that the adjoint problem yields as solution a sensitivity measure \( z_\theta \) of the primal solution \( u_\theta \) with respect to the given functional of interest \( J'(u_\theta) \).

Then, the main DWR theorem \( [21] \) yields the error identity

\[
e = J(u) - J(u_\theta) = \frac{1}{2} \rho(u_\theta)(z - z_\theta) + \frac{1}{2} \rho^*(u_\theta, z_\theta)(u - u_\theta) + R^{(3)}
\]

with the primal \( \rho \) and adjoint \( \rho^* \) error parts

\[
\begin{align*}
\rho(u_\theta)(\cdot) &:= -N'(u_\theta)(\cdot) + f(\cdot), \\
\rho^*(u_\theta, z_\theta)(\cdot) &:= J'(u_\theta)(\cdot) - N''(u_\theta)(\cdot, z_\theta) + f(\cdot).
\end{align*}
\]

For linear problems, we obtain immediately

\[
e = J(u) - J(u_\theta) = \rho(u_\theta)(z - z_\theta).
\]

For mildly nonlinear (i.e., known as semi-linear in PDE analysis; equations in which the highest derivative is still linear) problems as for instance Navier-Stokes, still the primal error part \( \rho(u_\theta)(z - z_\theta) \) is often used:

\[
e = J(u) - J(u_\theta) = \rho(u_\theta)(z - z_\theta) + R^{(2)}
\]

with a quadratic remainder term. By approximating the difference \( z - z_\theta =: \tilde{z}_\theta \) by a global higher order solution or local higher order interpolation and neglecting the remainder term, we obtain an approximation, which is used as computable error estimator \( \eta \):

\[
e = J(u) - J(u_\theta) \approx \eta := \eta(u_\theta, z_\theta) := \rho(u_\theta)(\tilde{z}_\theta)
\]
The approximation quality is measured with the help of the effectivity index

\[ I_{\text{eff}} := \frac{\eta}{e}. \]

Asymptotically, we aim for \( I_{\text{eff}} \to 1 \).

The approximations \( u_\theta \) and \( z_\theta \) are traditionally obtained with the help of finite elements [1, 39] or isogeometric analysis [40, 41]. In [34], \( u_\theta \) was computed with finite elements, and \( z_\theta \) was obtained by a neural network solution.

The main novelty in this paper is that we compute both \( u_\theta \) and \( z_\theta \) with the help of neural networks as explained in the previous section. Since in practice we are in general unaware about the exact adjoint solution \( z \) inside \( \tilde{z}_\theta \), we simply use in this work \( \tilde{z}_\theta := z_\theta \). To this end, we have

**Proposition 1.** Given the neural network approximated primal \( u_\theta \) and adjoint \( z_\theta \) solutions for the boundary value problem \( \mathcal{N}(u) = f \) and the goal functional \( J(u) \), we have an error estimator using the primal error part

\[ \eta = \rho(u_\theta)(z_\theta) = f(z_\theta) - \mathcal{N}(u_\theta)(z_\theta) \]

and as a posteriori error estimate

\[ |e| = |J(u) - J(u_\theta)| \leq |\eta| = |f(z_\theta) - \mathcal{N}(u_\theta)(z_\theta)|. \]

Both residual terms are assembled pointwise by summing up such that

\[ f(z_\theta) = \frac{1}{N} \sum_{i=1}^{N} f(z_\theta)_i, \]

\[ \mathcal{N}(u_\theta)(z_\theta) = \frac{1}{N} \sum_{i=1}^{N} \mathcal{N}(u_\theta)_i \cdot z_\theta_i \]

with \( f(z_\theta)_i := f_i \cdot z_\theta_i \) in each collocation point and for \( N = N_{\text{int}} + N_{\text{bnd}} \) and where \( z_\theta_i \) is the adjoint solution (obtained from the neural network) in each collocation point and summing over \( i \) means that we evaluate on each collocation point in the domain.

### 3.2 Multiple goal functionals

The main purpose of this section is to extend the previous approach from single to multiple goal functionals. In many applications (specifically multiphysics problems) several quantities of interest are simultaneously of importance. Given \( N \) target functionals say \( J_1, J_2, \ldots, J_N \) the standard procedure to compute the error estimators analogous to Eq. (2), i.e., for each individual \( J_n \), we introduce an adjoint problem: Find \( z_n \) such that

\[ \mathcal{N}'(u)(z_n) - J_n'(u) = 0, \quad n = 1, 2, \ldots, N. \]

Computing each adjoint problem separately involves the expensive cost of \( N \) computations. However this can be avoided following the techniques proposed [28, 29] with further improvements and extensions proposed in [30, 31] (see also [27, 32]) of combining the functionals. The core idea is to construct a linear combination to form a combined target functional

\[ J_c(\cdot) = \sum_{n=1}^{N} \omega_n J_n(\cdot) \]

where,

\[ \omega_n := \frac{\text{sign}(J_n(u) - J_n(u_\theta)) w_n}{|J_n(u_\theta)|} = \mu_n w_n \]

and \( w_n \) are self-chosen positive weights. Such choices lead to no error cancellation, however depending on the weights any particular functional may impact on \( J_c \). We may now proceed similarly as in single functionals to derive an error representation formula for the errors in \( J_c \):

**Proposition 2.** Given the neural network approximated primal \( u_\theta \) solution for the (discrete) boundary value problem \( \mathcal{N}(u_\theta) = f \) and adjoint solution \( z_\theta \) obtained by \( \mathcal{N}'(u_\theta)(z_\theta) = J'_n(u_\theta) \), with the combined goal functional \( J_c \), we have
as error estimator using the primal error part
\[ \eta = \rho(u_\theta)(z_\theta) = f(z_\theta) - \mathcal{N}(u_\theta)(z_\theta) \]
and as a posteriori error estimate
\[ |e| = |J_c(u) - J_c(u_\theta)| \leq |\eta| = |f(z_\theta) - \mathcal{N}(u_\theta)(z_\theta)|. \]

3.3 Algorithm

Our aim of the computation is to approximate the target quantity \( J(\cdot) \) so that it holds \( |J(u) - J(u_\theta)| < \text{TOL} \) with some user defined \( \text{Tol} > 0 \). In the case of multiple goal functionals, we aim for \( |J_c(u) - J_c(u_\theta)| < \text{TOL} \). The whole algorithm is tailored for an accurate and efficient approximation in order to obtain \( I_{eff} \approx 1 \). In practice the stopping criteria is enforced by a preassigned tolerance and if the condition is not satisfied then this can serve as an error indicator which is employed to guide the parameters in the neural network architecture. The weights and bias terms get updated accordingly and this process continues iteratively.

Summarizing all previous steps, we obtain as basic scheme:

**Algorithm 1:** Neural Network based goal oriented error approach

1. Initialize: Provide number of iteration steps, epochs and the neural network architecture.
2. Generate collocation points \((x_i, y_i)\) on \( \Omega \)
3. Initialize the neural network \( \mathcal{N}(\cdot, \cdot) \)
4. Initialize the weights of the network using Xavier initialization technique
5. Obtain the loss function \( E[\theta] \) for the current mini-batch points
6. Minimize the loss
7. If \( \text{Loss} < \text{TOL} \) then
   - STOP
8. Else
9.   repeat steps until the criteria is satisfied
10. Compute the adjoint solution \( z_\theta \)
11. Having just computed \( u_\theta \) and \( z_\theta \) construct error estimator \( \eta(u_\theta, z_\theta) \)
12. Evaluate \( \eta(u_\theta, z_\theta) \) and compare with true error \( e \)
13. Evaluate the quality of \( \eta \) by observing the effectivity index \( I_{eff} \)
14. If \( I_{eff} \approx 1 \) then
15.   - STOP
16. Else
17.   adjust \( Tol \) & repeat steps until the criteria is satisfied
18. Then, using finer neural networks (in order to obtain a higher approximation quality) for computing \( u_\theta \) and \( z_\theta \) and repeating all previous steps, we can compare the different \( I_{eff} \).

4 Modelling based on NURBS curves

Geometrical modelling of the computational domain is an essential tool for an accurate and computationally efficient approximation to the solutions of PDEs. Construction of a mesh based geometry is expensive and likely to creates inaccuracies for complex geometries. While this may be trivial for a regular shaped domain, but challenges arises when the domain is irregular for example “semi-annulus domain”. In this section we will briefly describe how NURBS based modelling are more effective and possesses the advantage of yielding highly accurate approximations. For a more detailed descriptions and applications see some classic literature [42, 40, 43, 41, 44, 45] and the references therein.

NURBS (Non Uniform Rational B-Splines) are built from B-Splines. The basic B-Splines are lack of ability to exactly represent some simple shapes (circles, ellipsoids etc) and thus NURBS are the generalizations of B-Splines through rational functions so as to remove this difficulty. The geometric modeling typically consist of two meshes physical mesh and control mesh. While the physical mesh is a representation of the original geometry, the control mesh
forms a scaffold of the geometry. NURBS shapes are defined by its degrees, knot vector and set of control points which are the inputs supposed to be provided by the users. A knot vector is an increasing set of coordinates in the parametric space generally denoted by $\Xi = \{\xi_k\}_{k=1}^{n+p+1}$ where $\xi_k$ is the $k$-th knot, $n$ is the number of basis functions and $p$ is the polynomial order. Depending on the degree of basis functions and the no of control points a knot can be repeated several times and it is even possible to insert a new knot without even changing the curve geometry and parameterization see Fig. (2). Analogously this is known as $h$-refinement. Knot refinement offers a wide range of tools to design and analyse the shape information. A univariate rational basis function is defined as:

$$R_{k,p}(\xi) := \frac{w_k N_{k,p}(\xi)}{\sum_{k=1}^{n} w_i N_{k,p}(\xi)} ; \quad k \in [1, p + 1]$$

Here, $\{N_{k,p}(\xi)\}_{k=1}^{n}$ is the set of basis functions of the B-Spline curves, $\{w_k : w_k > 0\}_{k=1}^{p}$ is the set of NURBS weight. Choosing appropriate weights permits the definition of varieties of curves and in particular if all the weights are equal its reduces to the B-Spline basis. These basis functions are multiplied with a set of weights and control points and summed up to generate a NURBS curve. Correct shape definition of a curve is strictly connected with the proper selection of control points, weights and knots. The implementation is done using NURBS-Python (geomdl) library. Following snippet of code is an illustration how to generate a 2D NURBS curve and visualizing it using NURBS-Python.

```python
from geomdl import NURBS

class Disc(NURBS):
    """
    Class for defining a circular domain
    Input: rad,center - radius and center of the circle
    """
    def __init__(self, rad, center):
        geomData = dict()

        # Users set degrees
        geomData['degree_u'] = x_1
        geomData['degree_v'] = x_2

        # Users set control points
        geomData['ctrlpts_size_u'] = y_1
        geomData['ctrlpts_size_v'] = y_2

        geomData['ctrlpts'] = [...,...,...,...,.....]

        geomData['weights'] = [...,...,...,...,.....]
```
# Users set knot vectors
```python
geomData['knotvector_u'] = [a_1, a_2, ..., ...]
geomData['knotvector_v'] = [b_1, b_2, ..., ...]
super().__init__(geomData)
```
# Plot the curve
```python
Disc.PlotSurf()
```

## 5 Numerical examples

In this section, we investigate adaptive refinement and error control using the DCM for different PDEs on complex domains. Specifically, we consider the regularized \( p \)-Laplacian, Poisson’s problem, and the stationary incompressible Navier-Stokes equations resulting in total in five numerical tests. The details of the network architecture such as relevant optimizers, activation functions, number of layers and neurons on each layers are provided in each example separately. To demonstrate the effectiveness of our method, we computed the reference solution, wherever mentioned on the same testing set and continued to investigate how well our error estimators perform in approximating the error by invoking the effectivity indices and also with various choices of weight parameters that lead to different levels of difficulties with respect to the problems. As mentioned earlier the implementation has been carried out in the TensorFlow framework. All of the following results obtained using Python version 3.8.5 and TensorFlow version 2.5.0. Unless mentioned otherwise the numerical examples reported were run on a 64-bit LinuxOS with Intel(R) Core(TM) i7-8850H CPU, 64GB memory. Nevertheless training on a CPU is significantly slower than training it on a GPU, which is why the training part was also performed on a GPU whenever required.

### 5.1 Example - 1: Regularized \( p \)-Laplacian

On a bounded Lipschitz domain \( \Omega \) in \( \mathbb{R}^2 \), and for \( p \geq 2 \) and \( \delta \geq 0 \), we define
\[
\mathcal{A}_{\delta,p}(u) \equiv \text{div}((\delta^2 + |\nabla u|^2)^{\frac{p-2}{2}} \nabla u)
\]
We consider the family: Find \( u \) such that,
\[
\begin{align*}
\mathcal{A}_{\delta,p}(u) &= f \quad \text{on } \Omega \\
\mathcal{B}[u] &= g \quad \text{on } \partial \Omega
\end{align*}
\]
The Fréchet derivative \( \mathcal{A}'_{\delta,p}(u) \) at the linearization point \( u \) of the non linear operator can be found in [31]. More specifically, we define as domain
\[
\Omega = \{(x, y) : 0 \leq x^2 + y^2 \leq 1 \text{ & } xy \leq 0\}
\]
This 2D shape has been constructed by repositioning control points, modifying knot vectors, adjusting weights and geometric degrees of a fitted NURBS disc.

We consider the following cases.

#### 5.1.1 Case - I \((p = 2, \delta = 0)\)

The first case considers the Poisson problem subjected to Dirichlet boundary conditions. Let,
\[
\begin{align*}
\mathcal{A}_{0,2}(u) &= 12xy \quad \text{on } \Omega \\
u &= 0 \quad \text{on } \partial \Omega
\end{align*}
\]
and the exact solution of (7) will be used as a reference solution which is given by \( U(x, y) = xy(1 - x^2 - y^2) \).

The geometrical set up and the arrangement of collocation points are demonstrated in Fig. (3). It clearly depicts the influence of the arrangement of points. The neural networks are trained to approximate the solution \( U_\theta \) which is obtained by the minimization of the loss function. The problem statement can be written as:
\[
\mathcal{E} := ||\mathcal{A}_{\delta,p}(U_\theta) - f(x, y)||_{L_2}^2 + ||U_\theta||_{L_2}^2
\]

The quantity of interest for this example is as follows:
Goal Functionals of Interest

We consider the following functionals:

\[ J_\partial(u) := \int_{\Gamma} \frac{\partial u}{\partial n} \, ds \]
\[ J_\Omega(u) := \int_{\Omega} u(x, y) \, d(x, y) \]
\[ J_\chi(u) := \int_{\Omega} \chi(x, y)u(x, y) \, d(x, y) \]

where, \( \chi(x, y) = \begin{cases} y - x & \text{if } x < y \\ 0 & \text{otherwise} \end{cases} \)

We are interested in the following goal functionals :

\[ J_1(u) := J_\partial(u)J_\chi(u) \quad J_2(u) := J_\Omega(u)J_\chi(u) \quad J_3(u) := J_\Omega(u)J_\partial(u) \]

\[ J_c(u) := 0.4\mu_1J_1(u) + 0.01\mu_2J_2(u) + \mu_3J_3(u) \]

We have used a 5 layers network (2-30-30-20-1) and swish activation function throughout the hidden layers to evaluate neural values in those layers. As an optimizer we used Adam with learning rate \( \alpha = 0.001 \) followed by BFGS. The entire domain is discretized with \( N_x \times N_y \) uniformly spaced training points where \( N_x = 35 \), \( N_y = 30 \). The training iterations has been stopped once the loss function reaches the tolerance \( Tol = 10^{-12} \). In order to quantify
the accuracy of our approach we compute the relative $L_2$ error as:

$$L_2 := \frac{\sqrt{\sum_{i=1}^{N_{\text{test}}} U_{\text{err}}^2(x_i,y_i)}}{\sqrt{\sum_{i=1}^{N_{\text{test}}} U^2(x_i,y_i)}}$$

where, $N_{\text{test}}$ is the no. of testing points and $U_{\text{err}}(x,y) = U(x,y) - U_\theta(x,y)$.

Let us now discuss on our findings. From the observation in Fig. (4) we deduce that “swish” activation function outperforming in deep neural networks in comparison to other mostly used activation functions in the literature. Considering accuracy in the approximation of adjoint solutions of

$$-A_{0,2}'(u) = J(u) \quad \text{on} \quad \Omega$$

we define reference solutions $U_{adj} = c_J(1 - x^2 - y^2)$ and compare relative errors with respect to proposed goal functionals $J$. Here $c_J \in \mathbb{R}$ and its value needed to be adjusted according to chosen $J$. We observe that initially relative error in $J_3$ badly approximates the functional with the largest error, however it is decreasing steeply w.r.t the collocation points, i.e., increasing collocation points deliver promising results. Similar behavior being also observed for $J_3$ because of the dominating weight $w_3$. Next we take a look at the effectivity indices for $J$, which are $I_{eff} \approx 1$. Therefore we conclude that we have almost approximate the true error with our error estimator. In particular the figure also shows that even with less amount of training points it is possible to obtain a reasonable approximations of the true error. Finally the error plots in general reveals a good agreement between DCM solution and the reference solution. However there has some relatively larger difference in the vicinity of boundaries and it is because less no of training points here in comparison to the interior which is again a trade-off.
In this particular example we have generated around 1500 training points \((N_x = 42, N_y = 35)\) over the entire domain as the feeding data to train our network. Tolerance used as \(10^{-12}\). A 6 layers neural network \((2-30-30-30-20-1)\) is constructed. Therein, we use 2 neurons in the input layer and 1 neuron in the output layer. In addition 3 hidden layers with 30 neurons and 1 hidden layer with 20 neurons are used to enforce the learning behavior. Fig. (7) perfectly depicts the benefits of using deep neural network instead of shallow wide neural network. We use “swish” activation in the first three hidden layers and “tanh” in the final hidden layer to evaluate neural values in those layers. The learning rate \(\alpha = 0.001\) is used in the BFGS optimizer following Adam.

5.1.2 Case - II \((p = 2.5, \delta = 0.05)\)

In the second example on the same domain we consider following problem with mixed boundary conditions: Find \(u\) such that,

\[
-\mathbf{A}_{\delta,p}(u) = \frac{4\delta^2 + 20(x^2 + y^2)}{[\delta^2 + 4(x^2 + y^2)]^{1/2}} \quad \text{on } \Omega
\]

\[
\begin{align*}
  u &= 0 \quad \text{whenever, } x^2 + y^2 = 1 \equiv \Gamma_1 \\
  \frac{\partial u}{\partial n} &= -2x \quad \text{at, } y = 0 \equiv \Gamma_2 \\
  \frac{\partial u}{\partial y} &= -2y \quad \text{at, } x = 0 \equiv \Gamma_3
\end{align*}
\]

\((x, y) \in \Gamma\)

The exact solution is given by: \(U(x, y) := 1 - x^2 - y^2\). Similar to earlier example we intend to minimize the loss function with respect to the training data.

\[
\mathcal{E} := ||\mathbf{A}_{\delta,p}(U_\theta) - f(x, y)||^2_{\Omega} + ||U_\theta||^2_{\Gamma_1} + \left|\left|\frac{\partial U_\theta}{\partial x} - U_x\right|\right|^2_{\Gamma_2} + \left|\left|\frac{\partial U_\theta}{\partial y} - U_y\right|\right|^2_{\Gamma_3}
\]

**Goal Functionals of Interest**

We are interested in the following functionals evaluation:

\[
J_1(u) := u(0.5, -0.5), \quad J_2(u) := \int_{\Omega} u(x, y) \, d(x, y), \quad J_3(u) := \int_{\Gamma} \frac{\partial u}{\partial n} \, ds
\]

and the combined functional

\[
J_c(u) := 0.5u_1J_1(u) + 0.25u_2J_2(u) + u_3J_3(u).
\]

In this particular example we have generated around 1500 training points \((N_x = 42, N_y = 35)\) over the entire domain as the feeding data to train our network. Tolerance used as \(10^{-12}\). A 6 layers neural network \((2-30-30-30-20-1)\) is constructed. Therein, we use 2 neurons in the input layer and 1 neuron in the output layer. In addition 3 hidden layers with 30 neurons and 1 hidden layer with 20 neurons are used to enforce the learning behavior. Fig. (7) perfectly depicts the benefits of using deep neural network instead of shallow wide neural network. We use “swish” activation in the first three hidden layers and “tanh” in the final hidden layer to evaluate neural values in those layers. The learning rate \(\alpha = 0.001\) is used in the BFGS optimizer following Adam.

We don’t know the exact solution for the adjoint problem in this case. Therefore in order to measure the accuracy we study the relative errors for the primal problem and residual errors for the adjoint problem. More hidden layers, with more neurons yield flattening of the errors. The residual error \(\mathcal{R}_{\text{err}}\) is computed using the formula :

\[
\mathcal{R}_{\text{err}} := ||\mathbf{A}_{\delta,p}'(u) - J(u)||^2_2
\]

Considering the accuracy of the functional evaluations above, we observe that the residual errors in the functionals \(J_1, J_2, J_3\) and \(J_c\) are less than \(10^{-10}\) cf Fig. (7). Furthermore, we observe that \(J_c\) is the dominating functional and \(J_1\) is the one with least error. We noticed that the error in \(J_2\) is similar to \(J_1\). This is because \(J_3\) is again the dominating part in the combination of \(J_c\). Hence \(J_1\) changes its behavior after the error of \(J_3\) starts to dominate. Therefore, we compute the effectivity index of this functional and obtain an excellent convergence towards 1 as the no of collocation points start to increases from 1000. As like before the interesting part is our methodology successfully approximate the true error with the error estimator.

As a part of the network architecture depicted in Fig. (6) we conclude that \((Adam, BFGS)\) performs better than \((RAdam, LBFGS)\) for the same network parameters. The convergence of the loss value is much slower requiring

13
Figure 5: Comparison of solutions for the primal problem

Figure 6: Comparisons in convergence

Figure 7: Residual errors and effectivity index.
almost 10 times more iteration. Therefore in all the cases we use Adam and BFGS to train the network and study the minimization problem.

5.1.3 Case - III \((2.5 \leq p \leq 5 \text{ and } 0 \leq \delta \leq 0.75)\)

In the final case we choose right hand side and the boundary conditions so that the exact solution remain same \(U(x, y) = 1 - x^2 - y^2\). We have also consider the same functionals of interest as in Case-II. In addition our neural network structures are also remain same.

As like preceding cases the interesting part is to observe the graph of effectivity index w.r.t increasing collocation points. As it can be seen in Fig. (9) how \(J_e\) changes its behavior depending on the parameters \((p, \delta)\). With regard to the error we observe that we hardly achieve any advantage at the beginning, \(J_e\) even deliver a worse result at a certain step, for relatively higher \(p\) and \(\delta\). However at one specific refinement step we start to obtain a better decrease. The poor convergence of \(J_e\) might result from the fact that \((p \geq 3, \delta \geq 0.25)\) requires much more refines on domain. Nevertheless in all the cases the convergence rate improves drastically and we obtain quite good effectivity index once we have \(>1000\) collocation points.

Define,

\[\Omega_{(a,b)} := \Omega \cap \{(x,y) \in \mathbb{R}^2 : ax > by\}\]

We consider the following functionals,
Figure 10: Approximated primal solution, \( I_{\text{eff}} \) plots and training loss history.

\[
J_1(u) := \int_{\Omega(0.75,0.5)} u(x,y) \, dx \, dy \approx 0.003513662 \pm 5 \cdot 10^{-9}
\]
\[
J_2(u) := \int_{\Omega(-0.75,0.5)} \Delta u(x,y) \, dx \, dy \approx 0.166887181 \pm 5 \cdot 10^{-9}
\]

Since the exact solution is unknown to us, we approximated the exact functionals by values that have been obtained by training over 10,000 collocation points and computed the integrals employing Gaussian quadrature over 7,500 points, in order to achieve higher order accuracy. Furthermore, we used three different configurations to formulate goal functionals:

- Configuration I : evaluating \( J_\alpha = 10^{-3} \mu_1 \cdot J_1(u) + 0.1 \mu_2 \cdot J_2(u) \)
- Configuration II : evaluating \( J_\beta = 0.01 \mu_1 \cdot J_1(u) + 0.25 \mu_2 \cdot J_2(u) \)
- Configuration III : evaluating \( J_\gamma = 0.09 \mu_1 \cdot J_1(u) + 0.5 \mu_2 \cdot J_2(u) \)

Even for a single goal functional the existing literature is rare. Therefore our results might serve a kind of benchmark for comparing algorithms related such problems. The effectivity index for all these configurations are depicted in Fig (10). Initially we observe that \( \eta \) was dominated by \( e \) and later we get some increases \( I_{\text{eff}} > 1 \) for all configurations even for larger amount of training data points, which shows that high inconsistency in the decrease of error and because of the loss of regularity in the domain it is not as close to 1 like earlier examples. However once the domain is refined with more data points, we obtain much better reduction for all configurations. An interesting aspects in this example is that for all the goal functionals we are obtaining almost similar order of reductions in the error. Consequently we notice that our refinement scheme also takes care of less regular problems while accurately approximating the error.
estimator as far as possible as displayed in the figures. In the final example, we consider the steady state Navier Stokes Equations.

The problem is motivated from [46]. The domain is given as

$$\Omega := \left\{ x : \frac{1}{2} < |x| < 1 \right\} \times [-1, 1] \cup [-1, 1] \times \left\{ y : \frac{1}{2} < |y| < 1 \right\}$$

5.2 Example-3: Stationary incompressible Navier-Stokes equations

In $\Omega$, the incompressible Navier-Stokes equations for a 2D velocity vector field $\mathbf{u}(x,y) = [u(x,y) \ v(x,y)]$ and a scalar pressure field $p(x,y)$ are given by

$$-\nu \Delta \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p = \mathbf{f} \quad \text{in} \; \Omega,$$

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in} \; \Omega,$$

$$\mathbf{u} = \psi \quad \text{on} \; \partial \Omega = \Gamma.$$

Here $\nu$ is constant dynamic viscosity of the fluid. We choose $\nu = 0.05$. As an exact solution to compare with, we use

$$u(x, y) = 1 - e^{-\frac{x}{\pi}} \sin 2\pi y$$

$$v(x, y) = \frac{1}{4\pi} e^{-\frac{x}{\pi}} \cos 2\pi y$$

$$p(x, y) = 1 - e^{-\frac{x+y}{\pi}}$$

and plug it into the original equation to compute $\mathbf{f}$ and $\psi$. The loss function is computed as

$$\mathcal{E} := \frac{1}{N_{\text{int}}} \sum_{i=1}^{N_{\text{int}}} \sum_{j=1}^{2} \left( \nu \Delta U_{\theta} - U_{\theta} \cdot \nabla U_{\theta} - \nabla P_{\theta} + f \right)^{2}(x_{i}) + \frac{1}{N_{\text{int}}} \sum_{i=1}^{N_{\text{int}}} (\nabla \cdot U_{\theta})^{2}(x_{i})$$

$$+ \frac{1}{N_{\text{bnd}}} \sum_{i=1}^{N_{\text{bnd}}} \sum_{j=1}^{2} (U_{\theta} - \psi)^{2}(s_{i})$$

We generate a dataset containing 5600 ($N_x = 80, N_y = 70$) samples of training data see Fig. (11). The network architecture used here consists of 6 layers ($2 - 80 - 80 - 80 - 80 - 3$), i.e, we have trained one neural network with 3 outputs. One can also train individually to approximate $u$ and $p$ but note that training different architecture is hard because obtaining optimal hyperparameters is itself a daunting task and also it requires lot of computation time. In addition former is relatively better in capturing the underlying equations. As mentioned earlier, the weights are initialized using a Xavier initialization while the biases are generated using a normal distribution with mean 0 and standard deviation 1. They are trained using an SGD optimizer with the fine tuned learning rate and momentum followed by BFGS. The first three hidden layers are connected with “swish” activation and the final layer is with “tanh” activation. The resulting prediction error is validated against the test data, Fig. (12-14) provides a comparison...
between exact solution and predicted outcome. It can be observed that predicted outputs and exact solutions are very close on the testing sets, which clearly shows that using only a handful amount of training data our model is capable to accurately capture the intricate non linear behavior of N-S equation. The tolerance value $Tol = 10^{-12}$ is adopted as a convergence criterion. In particular Fig. (15) summarizes the assessment of our architecture on this dataset.

**Functionals of Interest**

We consider the following quantities of interest simultaneously using the framework of multiple goal functionals

\[ \begin{align*}
J_1(\mathbf{u}) &:= c_{Re} \int_{\Gamma} \mathbf{n} \cdot \sigma \begin{bmatrix} 1 \\ 0 \end{bmatrix} \, ds \\
J_2(\mathbf{u}) &:= \pi \int_{\Omega} |1 - u(x,y)| \, d(x,y) \\
J_3(\mathbf{u}) &:= u(0.75, 0.25) + u(-0.75, -0.25) \\
J_4(\mathbf{u}) &:= c_{Re} \int_{\Gamma} \mathbf{n} \cdot \sigma \begin{bmatrix} 0 \\ 1 \end{bmatrix} \, ds \\
J_5(\mathbf{u}) &:= \pi^2 \int_{\Omega} |v(x,y)| \, d(x,y) \\
J_6(\mathbf{u}) &:= v(-0.75, 0.5)
\end{align*} \]

where, $\sigma = -pI_2 + \nu \nabla u + \nabla u^t$ is the Cauchy stress tensor for the Newtonian fluid, the constant $c_{Re} = \frac{1}{\nu Re}$ is depending upon Reynolds number $Re = 100$ and $n$ is the outer unit normal to $\Gamma$. In particular the scalar quantities $J_1$ and $J_4$ are known as drag and lift coefficients of some body immersed in the flow along the downwind and crosswind directions. We consider the goal functionals:

\[ \begin{align*}
J_\alpha(\mathbf{u}) &= 0.5 \mu_1 J_1(\mathbf{u}) + 0.75 \mu_2 J_2(\mathbf{u}) + \mu_3 J_3(\mathbf{u}) \\
J_\beta(\mathbf{u}) &= 0.1 \mu_4 J_4(\mathbf{u}) + 0.45 \mu_5 J_5(\mathbf{u}) + 0.6 \mu_6 J_6(\mathbf{u})
\end{align*} \]

The adjoint problem in strong form is given by

\[ -\nu \Delta \mathbf{z} - \mathbf{u} \cdot \nabla \mathbf{z} - (\nabla \cdot \mathbf{u}) \mathbf{z} + (\nabla \mathbf{u}) \mathbf{z} + \nabla \pi = J(\mathbf{u}) \]

For more detailed descriptions on this topic readers are referred to [48, 49, 23]. Other results for multigoal-oriented error estimation using the incompressible Navier-Stokes equations can be found in [26]. Next, we discuss our findings. A quantitative behavior of the error plots are displayed in Fig. (15). Here again we observe nearly perfect agreement of the estimator with true error yielding the effectivity indices closer to 1. Evidently our results indicate that the errors converge w.r.t a larger amount of training points.
6 Conclusions

In this work, we explored DNN to develop a posteriori error estimation using the dual weighted residual approach for multiple goal functionals. Our developments include both nonlinear PDEs and nonlinear goal functionals. In the error estimator, both the primal and adjoint solutions are approximated with the help of neural networks. This procedure is based on the deep collocation method. Moreover, we utilized NURBS for constructing the computational domain and Gaussian quadrature rules for an efficient approximation of numerical integration. We remain faithful to the philosophy of using gradient based optimization methods which also allows us to use standard libraries from the machine learning community. One of the principle advantage of our proposed approach is that a wealth of tools and concept developed by an active community used, that leads ease to implementation, trying different mathematical models and implementing them in straightforward and transparent manner. We have designed a well-tested framework for evaluating multiple goal functionals for the 2D $p$-Laplacian and stationary incompressible Navier-Stokes problem, however a more detailed study on the convergence of neural networks and investigating robust minimization procedures still remain open as possible research topics. In addition, the extension to evaluate the adjoint error part $\rho^*$ might be of future interest for highly nonlinear problems.

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