We develop an error estimator for neural network approximations of PDEs. The proposed approach is based on dual weighted residual estimator (DWR). It is destined to serve as a stopping criterion that guarantees the accuracy of the solution independently of the design of the neural network training. The result is equipped with computational examples for Laplace and Stokes problems.

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*Otto-von-Guericke Universität Magdeburg, Magdeburg, Germany, piotr.minakowski@ovgu.de
†Otto-von-Guericke Universität Magdeburg, Magdeburg, Germany, thomas.richter@ovgu.de
1 Introduction

In recent years, the emerging field of (deep) neural networks has reached the numerical approximation of partial differential equations (PDE). Several approaches have been proposed that aim at directly representing the solution to the PDE by a deep neural network. For this purpose the network is considered as (differentiable) function $N : \Omega \to \mathbb{R}^c$, where $\Omega \subset \mathbb{R}^d$ is the computational domain of dimension $d \in \mathbb{N}$ and $c \in \mathbb{N}$ is the size of the differential system.

The network is trained by integrating the differential equation (and the boundary conditions) into the loss function. Several different approaches based on different realizations have been presented:

The Deep Ritz method by E and Yu [8] aims at minimizing the energy functional and it can be applied to symmetric problems. For the Laplace equation, $-\Delta u = f$ in $\Omega$ with $u = g$ on $\partial \Omega$, this means to minimize

$$E(N) = \frac{1}{2} \int_{\Omega} |\nabla N(x)|^2 \, dx - \int_{\Omega} N(x) \cdot f(x) \, dx + \lambda \int_{\partial \Omega} |N(x) - g(x)|^2 \, dx,$$

with a parameter $\lambda > 0$, where the integrals are approximated by Monte-Carlo integration. Training data is generated by picking random integration points. See [20] for an overview and further examples.

Another approach, denoted as DeepXDE (Lu, Meng, Mao and Karniadakis [13]), Unified Deep Artificial Network [6] or Deep Galerkin Method (DGM) [23], see also [1], minimizes the strong residual of the equation, either as collocation method in randomly picked points within the domain and on the boundary, formulated once more for the Laplace problem,

$$E(N) = \frac{1}{N_1} \sum_{i=1}^{N_1} |f(x_i) + \Delta N(x_i)|^2 + \frac{\lambda}{N_2} \sum_{j=1}^{N_2} |N(x_j) - g(x_j)|^2,$$

or by Monte-Carlo integration of the (strong) residual

$$E(N) = \|f + \Delta N\|_{L^2(\Omega)}^2 + \lambda \|g - N\|_{L^2(\partial \Omega)}^2.$$

This second approach naturally extends to non-symmetric and nonlinear problems and we refer to the above mentioned literature for examples.

Finally, a third variant, variational physics-informed neural network VPINN (Kharazmi, Zhang Karniadakis) [11] approach is based on the variational formulation

$$E(N) = \left| \int_{\Omega} \nabla N(x) \cdot \nabla \phi_k(x) \, dx - \int_{\Omega} f(x) \cdot \nabla \phi_k(x) \, dx \right|^2$$

and training data is generated by choosing specific test functions $\phi_k$.

Training points can be chosen in several ways: fix points before training, e.g. grid points on a lattice or random points, in each training epoch. One could select different training points, or points can be chosen adaptively during training.
In [13] the authors propose Residual-Based Adaptive Refinement, in order to improve the distribution of residual points during the training process. After training for a fixed number of epochs on the initial set of residual points, the mean PDE residual is estimated by Monte Carlo integration, i.e., by the average of values at a set of randomly sampled dense locations. Then the training set is extended by new points with the largest residuals until the specified threshold for the mean is reached. Similar strategy called adaptive collocation has been proposed in [1]. Starting from the coarse set of points, the additional points are added to the training set based on the evaluation of the residual.

Evaluating the model at a larger number of points is quite inexpensive computationally, while the number of training points impacts the performance significantly. These adaptivity techniques are based on strong formulation.

The common rationale for the three different approaches discussed above is the excellent approximation property of neural networks, in particular Pinkus [18] proved the capability of deep neural networks to uniformly and simultaneously approximate differential functions and their derivatives. In the context of PDEs Ghring and coworkers [9] showed approximation results in Sobolev spaces and also gave convergence rates in the number of layers, neurons and weights. In particular for high dimensional differential equations, deep neural network based approaches promise to be superior [13,23]. On the other hand, it must be noted that the previous approaches, applied to common, low-dimensional (d = 1, 2, 3) problems, cannot compete with established methods in terms of efficiency. While algorithms of O(N) complexity exist for finite element or finite difference approximations of elliptic problems, the training of the deep neural network is a by far more challenging task.

Deep learning techniques can be applied in the context of numerical simulation, as an extension of existing CFD codes to increase their efficiency. One can generalize existing numerical methods as artificial neural networks with a set of trainable parameters. In [14] the authors recast finite volume schemes as neural networks and train the underlying parameters to improve accuracy on coarse grids, for the solution of time-dependent ODEs and PDEs. This approach was extended to finite element methods in [7].

The stopping criteria of the training process have not been studied. Commonly fixed number of epochs is performed, see e.g. [8] or train until mean residual reaches specific threshold [13]. According to the authors knowledge this result is the first that introduces error estimation based stopping criterion.

In this contribution we tackle the question of reliability of deep neural network approaches, i.e. we derive a posteriori error bounds for a trained network. This aspect is approached within the concept of the dual weighted residual estimator (DWR) that has been introduced by Becker and Rannacher [3]. We will handle the error between real solution $u(x)$ and neural network solution $N(x)$ as a mixture of Galerkin error and consistency error. What we derive is not a rigorous bound, but an efficient computational tool that can be used to validate neural network solutions and serve as an estimate in stopping criteria during the network training.

The course of this article is the following. After a brief introduction in Section 1 Section 2 discusses finite element and neural network approximations. In Section 3 we
quickly recapitulate the DWR method in its easiest form and extend it to estimate the network error. Later we briefly present network architecture in Section 4. Section 5 demonstrates the accuracy of the estimator for different applications and shows how the estimator can be integrated as a stopping criterion in training. After presenting different numerical examples we conclude in Section 6.

2 Finite element and neural network approximations

To keep the notation simple we focus on Laplace problem. Let \( \Omega \subset \mathbb{R}^d \) be a \( d \)-dimensional domain. We find the weak solution \( u \in V := H_0^1(\Omega) \) to

\[
- \Delta u = f \quad \text{in } \Omega, \quad u = 0 \quad \text{on } \partial \Omega,
\]

where \( f \in L^2(\Omega) \) is the right hand side. By \( V = H_0^1(\Omega) \) we denote the space of \( L^2 \)-functions with first weak derivative in \( L^2 \) with vanishing trace on \( \partial \Omega \). The solution \( u \in V \) is characterized by the variational problem

\[
(\nabla u, \nabla v) = (f, \phi) \quad \forall \phi \in V,
\]

where we denote by \( (\cdot, \cdot) \) the \( L^2 \)-inner product on \( \Omega \). Further, the solution is also equivalently characterized as minimizer of the functional

\[
E(u) \leq E(v) := \frac{1}{2} \|\nabla v \|^2 - (f, v) \quad \forall v \in V,
\]

where \( \| \cdot \| \) is the \( L^2 \)-norm.

2.1 Finite element approximation

Now, let \( \Omega_h \) be a triangulation of \( \Omega \) into open triangular or quadrilateral (in 2d) elements satisfying usual regularity requirements on the structure and the form of the elements. For an element \( T \in \Omega_h \) we denote by \( h_T = \text{diam}(T) \) the element size and by

\[
h = \max_{T \in \Omega_h} h_T
\]

the maximum mesh size of the discretization which serves as a parameter for measuring the fineness.

**Finite element error analysis** By \( V_h \subset V \) we denote the finite dimensional (finite element) subspace of \( H_0^1(\Omega) \). Then, let \( u_h \in V_h \) be the approximation to \( u \in V \) given by

\[
(\nabla u_h, \nabla v_h) = (f, v_h) \quad \forall v_h \in V_h.
\]

It holds

\[
\|\nabla(u - u_h)\| \leq \|\nabla(u - \phi_h)\| \quad \forall \phi_h \in V_h,
\]
such that the finite element error $u - u_h$ is bound by the interpolation error yielding the standard estimate

$$\|\nabla (u - u_h)\| \leq c h^r \| f \|_{H^{r-1}(\Omega)},$$

where $r$ is the polynomial degree of the finite element space and using the notation $H^0(\Omega) := L^2(\Omega)$ in the case of linear finite elements, $r = 1$. Naturally, this estimate requires sufficient regularity of the right hand side $f \in H^{r-1}(\Omega)$ and also of the domain boundary, i.e. $\partial \Omega$ must be convex polygonal for $r = 1$ or locally parameterizable by a $C^{r+1}$-function for $r \geq 1$.

### 2.2 Deep Ritz approximation of the Laplace problem

In principle, the Deep Ritz method as proposed by E and Yu [8] is based on minimizing the energy functional (3) by representing the unknown solution $u_N, u : \mathbb{R}^d \to \mathbb{R}$ by a neural network instead of a finite element function. Here, we denote by $N$ the topology of the neural network and by $u \in \mathbb{R}^N$ the parameters of the network, where $N = \#\mathcal{N}$ is the total number of free parameters. Finally, $u_{\mathcal{N},u}$ is the function that is realized by this specific combination of network topology and parameter choice. Mostly, we will simply use the notation $u_N$ and skip the indication of the parameter vector $u$ unless it is of relevance in the given context.

E and Yu [8] considered a network layout $\mathcal{N}$ with residual connection and differentiable activation functions, but we could also use different layouts. The framework of the Deep Ritz method requires differentiability of the network, i.e. differentiable activation functions. Fig. 1 shows the layout of the deep neural network as chosen by E and Yu, but also a simpler feedforward network that can be used.

Having a certain network topology $\mathcal{N}$ in mind, the neural network approximation space $W_{\mathcal{N}}$ used in the Deep Ritz method is then given by

$$W_{\mathcal{N}} := \{u_{\mathcal{N},w} : \mathbb{R}^d \to \mathbb{R}, \mid w \in \mathbb{R}^N\}.$$

(5)

If $N$ is finite and if the activation functions are differentiable it holds $V_{\mathcal{N}} \subset H^1(\Omega)$. We can however not expect $u_{\mathcal{N}} = 0$ on $\partial \Omega$ for $u_{\mathcal{N}} \in V_{\mathcal{N}}$, hence $V_{\mathcal{N}} \not\subset V = H^1_0(\Omega)$. In [6], the authors discussed a modified setup of the neural network that strongly satisfies the homogeneous Dirichlet condition.

Here we consider the penalized energy functional, compare [8],

$$E_\lambda(v) := \frac{1}{2} \|\nabla v\|^2 - (f, v) + \frac{\lambda}{2} \|v\|_{\partial \Omega}^2,$$

(6)

where $\lambda \in \mathbb{R}_+$ is a parameter and $\|\cdot\|_{\partial \Omega}$ is the $L^2$-norm on the boundary of the domain. The additional penalty term forces $v$ to be close to zero along the boundary. The minimizer of (6) in $u_\lambda \in H^1(\Omega)$ is characterized by the variational problem

$$(\nabla u_\lambda, \nabla v) + \lambda (u_\lambda, v) = (f, v) \quad \forall v \in H^1(\Omega),$$

(7)

where $(\cdot, \cdot)$ denote the $L^2$-inner product on the boundary $\partial \Omega$. The weak solution $u_\lambda \in H^1(\Omega)$ solves the Laplace problem with a disturbed Robin boundary condition, i.e.

$$-\Delta u_\lambda = f \text{ in } \Omega, \quad u_\lambda + \lambda^{-1} \partial_n u_\lambda = 0 \text{ on } \partial \Omega.$$
The penalized energy functional does hence introduce an additional modeling error term $\|u - u_\lambda\|$ that will depend on the parameter $\lambda$ and that will converge to zero for $\lambda \to \infty$.

Training of the neural network minimizes the modified energy functional (6) expressed in terms of Monte Carlo integration. To be precise: $N^i \in \mathbb{N}$ inner quadrature points $x^i \in \Omega$ and $N^b \in \mathbb{N}$ boundary quadrature points $x^b \in \partial \Omega$ are chosen, either randomly or based on a mesh of the domain. The loss function is given by

$$l(u_N; x^i, x^b) := \frac{|\Omega|}{N^i} \sum_{h=1}^{N^i} \left( \frac{1}{2} |\nabla u_N(x^i_j)|^2 - f(x^i_j) \right) + \frac{|\partial \Omega|}{N^b} \sum_{j=1}^{N^b} \frac{\lambda}{2} |u_N(x^b_j)|^2.$$ (9)

Details on this training process and also a study on the convergence of the neural network Deep Ritz approximation is presented in Section 4.1.

Minimizing (9) will identify the weights $u \in \mathbb{R}^N$ and result in an approximation $u_N, u$ to the optimal network realization $u_N, u$.

**Error analysis** An error analysis of the Deep Ritz approach is more delicate as compared to the case of finite elements. First, a modeling error is introduced as the energy functional (6) is distorted by the boundary penalty term and the minimizer $u_\lambda \in H^1(\Omega)$ does not exactly satisfy Dirichlet conditions, i.e. there is the error $u - u_\lambda$. Next, the approximation error $u_\lambda - u_N$ of the neural network space $W_N$ enters considering exact integration of the energy functional. This is followed by the error introduced by Monte Carlo integration $u_N - u_N, \hat{u}$ considering that $\hat{u} \in \mathbb{R}^N$ represents an exact minimum and finally, $u_N, \hat{u} - u_N, u$ is the training error. All together, four distinct contributions can be identified

$$\|u - u_N, u\| \leq \|u - u_\lambda\| + \|u_\lambda - u_N\| + \|u_N - u_N, \hat{u}\| + \|u_N, \hat{u} - u_N, u\|.$$

The first we call model error, the second is the network approximation error, the third the quadrature error or generalization error and finally, the fourth is the optimization or training error.

**Lemma 1** (Model error). Let $f \in L^2(\Omega)$, $\lambda \in \mathbb{R}$ with $\lambda > 0$ and $\Omega$ be such that the solutions $u \in H^1(\Omega)$ and $u_\lambda \in H^1(\Omega)$ to

$$(\nabla u, \nabla \phi) = (f, \phi) \quad \forall \phi \in H^1_0(\Omega), \quad (\nabla u_\lambda, \nabla \phi_\lambda) + \lambda (u_\lambda, \phi_\lambda)_{\partial \Omega} = (f, \phi_\lambda) \quad \forall \phi_\lambda \in H^1(\Omega)$$

satisfy $\|u\|_{H^2(\Omega)} \leq c_1 \|f\|$ and $\|u_\lambda\|_{H^2(\Omega)} \leq c_2 \|f\|$. It holds

$$\|\nabla (u - u_\lambda)\| \leq \frac{c}{\lambda} \|f\|,$$

where $c > 0$ depends on the domain $\Omega$ only.

**Proof.** Let $z \in H^1_0(\Omega)$ be the solution to the adjoint problem

$$- \Delta z = \frac{\nabla(u - u_\lambda)}{\|\nabla(u - u_\lambda)\|} \quad \text{in } \Omega, \quad z = 0 \text{ on } \partial \Omega.$$ (10)
Since the right hand side of this problem is in $L^2(\Omega)$, $z \in H^2(\Omega)$ and $\|z\|_{H^2(\Omega)} \leq c$ holds for sufficiently smooth (or convex polygonal) domain $\Omega$.

Multiplication of (10) with the error $u - u_\lambda$ and integration over the domain gives the error identity

$$\|\nabla (u - u_\lambda)\| = (\nabla z, \nabla (u - u_\lambda)) - \langle \partial_n z, u - u_\lambda \rangle_{\partial \Omega}.$$ 

As $u = 0$ and $z = 0$ on $\partial \Omega$ this gives

$$\|\nabla (u - u_\lambda)\| = (\nabla (u - u_\lambda), \nabla z) + \lambda (u - u_\lambda, z)_{\partial \Omega} + \langle \partial_n z, u - u_\lambda \rangle_{\partial \Omega}.$$ 

Finally, with (8) using the trace inequality and the regularity of both adjoint and primal solution we obtain

$$\|\nabla (u - u_\lambda)\| \leq |\partial_n z|_{L^2(\partial \Omega)} |u_\lambda|_{L^2(\partial \Omega)} \leq \frac{c}{\lambda} \|z\|_{H^2} \|u_\lambda\|_{H^2(\Omega)} \leq \frac{c}{\lambda} \|f\|.$$ 

The approximation properties of neural networks are already extensively studied in literature [2, 9] and they show convergence $\|u_\lambda - u_N\| \to 0$ for an increasing size of the neural networks. For example, [9, Theorem 4.1] states that for all $\epsilon > 0$ the bound

$$\|\nabla (u_\lambda - u_N)\| = O(\epsilon)$$

is obtainable, given $u_\lambda \in H^2(\Omega)$, with a neural network consisting of $L = \log_2(\epsilon^{-2})$ layers and $N = L \cdot 2^L$ weights and neurons. This approximately corresponds to

$$\|\nabla (u_\lambda - u_N)\| \approx O\left(\frac{\log(N)}{\sqrt{N}}\right)$$

which, in terms of the number of unknowns $N$, is comparable to the linear finite element approximation.

The choice of the numerical quadrature points gives rise to the generalization error of the neural network representation. Does the training based on a certain set of quadrature points also gives an approximation on the complete domain? There are no a priori bounds for such kind of errors but it has been shown [16, 21] that such generalization bounds are equivalent to the stability of the training under perturbation of the training data, e.g. in the context of Deep Ritz, by perturbing or leaving out single quadrature point. In the context of PINNs [22] shows the convergence of neural network solution, to solutions of linear elliptic and parabolic PDEs as the number of training samples is increased. Moreover [15] provides rigorous upper bounds on the generalization error. Under stability assumptions of the PDEs, the authors show that the generalization error is bounded by the training error and the quadrature error. Finally, the optimization error remains for which there is also no a priori error bound. Further, there usually is no guarantee that we obtain a global minimum.

In the following sections we present an a posteriori error estimator that is be able to give predictions on the complete error $u - u_{N,u}$ in goal functionals. While all error contributions are included we are however not able to distinguish between the different sources.
2.3 Deep Ritz approximation of the Stokes equations

As a second example we consider the Stokes equation on a two dimensional domain \( \Omega \subset \mathbb{R}^2 \), i.e. we find the velocity \( v \in V^2 := H^1_0(\Omega)^2 \) and the pressure \( p \in L := L^2(\Omega) \) such that

\[
\text{div } v = 0, \quad -\Delta v + \nabla p = f \text{ in } \Omega, \quad v = 0 \text{ on } \partial \Omega,
\]

where we denote by \( f \in L^2(\Omega)^2 \) a given right hand side. Considering a discrete pair of subspaces \( V_h \times L_h \subset V \times L \), the finite element solution is defined by

\[
(\text{div } v_h, \xi_h) + (\nabla v_h, \nabla \phi_h) - (p_h, \nabla \cdot \phi_h) = (f_h, \phi_h) \quad \forall (\phi_h, \xi_h) \in V_h \times L_h.
\]

Assuming inf-sup stability of the discrete finite element pair the solution exists uniquely and standard best approximation results hold, e.g. for the \( P^2 - P^1 \) Taylor-Hood element it holds

\[
\|\nabla (v - v_h)\| + \|p - p_h\| \leq c h^2 \|f\|_{H^1(\Omega)},
\]

or, for equal-order linear finite elements for the pressure and the velocity, the solution to the stabilized formulation

\[
(\text{div } v_h, \xi_h) + (\nabla v_h, \nabla \phi_h) - (p_h, \nabla \cdot \phi_h) + h^2 (\nabla p_h, \nabla \xi_h) = (f_h, \phi_h) \quad \forall (\phi_h, \xi_h) \in V_h \times L_h
\]

satisfies the estimate

\[
\|\nabla (v - v_h)\| + \|p - p_h\| \leq ch\|f\|.
\]

We refer to the literature, e.g. the monography of John [10] for these and further aspects on the finite element approximations to the Stokes equations.

Having a saddle-point structure the Stokes system is not directly associated to an energy form. Instead we realize the Deep Ritz method by introducing a penalty term to enforce the divergence condition, i.e.

\[
E_{\lambda,\alpha}(v) := \frac{1}{2}\|\nabla v\|^2 - (f, v) + \frac{\alpha}{2}\|\text{div } v\|^2 + \frac{\lambda}{2}\|v\|_{\partial \Omega}^2,
\]

where \( \alpha, \lambda > 0 \) are two parameters controlling the balance between minimizing the energy and satisfying the divergence constraint and the boundary values. The solution is characterized by the variational problem \( v_{\lambda,\alpha} \in H^1(\Omega)^2 \)

\[
(\nabla v_{\lambda,\alpha}, \nabla \phi) + \alpha (\text{div } v_{\lambda,\alpha}, \text{div } \phi) + \lambda (v_{\lambda,\alpha}, \phi)_{\partial \Omega} = (f, \phi) \quad \forall \phi \in H^1(\Omega).
\]

This variational problem corresponds to the following classical formulation which also reveals the disturbed boundary condition

\[
-\Delta v_{\lambda,\alpha} - \alpha \text{div } v_{\lambda,\alpha} = f \text{ in } \Omega, \quad \lambda v_{\lambda,\alpha} + \alpha \vec{n} \cdot \text{div } v_{\lambda,\alpha} - \partial_n v_{\lambda,\alpha} = 0 \text{ on } \partial \Omega.
\]

Hereby, similar to Lemma 1 we get
**Lemma 2** (Stokes model error). Let \( f \in L^2(\Omega)^2 \), \( \lambda, \alpha \in \mathbb{R} \) with \( \lambda, \alpha > 0 \) and \( \Omega \) be such that the solutions \((v, p) \in V \times \mathcal{L}\) and \( v_{\lambda, \alpha} \in H^1(\Omega)^2 \) to (11) and (17), respectively, satisfy \( \|v\|_{H^2(\Omega)} + \|p\|_{H^1(\Omega)} \leq c_s\|f\| \) and \( \|u_{\lambda, \alpha}\|_{H^2(\Omega)} \leq c_s\|f\| \). It holds

\[
\|\nabla (v - v_{\lambda, \alpha})\| \leq c\left(\frac{1}{\sqrt{\lambda}} + \frac{1}{\sqrt{\alpha}}\right)\|f\|,
\]

where \( c > 0 \) depends on the domain \( \Omega \) only.

**Proof.** Due to similarity to Lemma 1 we just give a sketch, considering the adjoint \((z, p) \in V \times \mathcal{L}\)

\[
\nabla (v - v_{\lambda, \alpha}) = -\Delta z - \nabla q, \quad \text{div } z = 0,
\]

which gives the error identity

\[
\|\nabla (v - v_{\lambda, \alpha})\| = (\nabla z, \nabla (v - v_{\lambda, \alpha})) + (q, \text{div} (v - v_{\lambda, \alpha})) + (\partial_n z + q\vec{n}, v_{\lambda, \alpha})_{\partial \Omega}
\]

\[
-\alpha(\text{div} v_{\lambda, \alpha}, \text{div} z) - \lambda(v_{\lambda, \alpha}, z)_{\partial \Omega} - (p, \text{div} z)
\]

\[
= 0 = \frac{1}{\lambda}(\partial_n z + q\vec{n}, v_{\lambda, \alpha})_{\partial \Omega} - (\text{div} v_{\lambda, \alpha}, q), \quad (19)
\]

to be estimated as

\[
\|\nabla (v - v_{\lambda, \alpha})\| \leq c\left(\|z\|_{H^2(\Omega)} + \|q\|_{H^1(\Omega)}\right)\|f\|\left(\|\text{div} v_{\lambda, \alpha}\| + \|v_{\lambda, \alpha}|_{\partial \Omega}\right).
\]

Diagonal testing of (17) then gives the claimed estimate

\[
\|\nabla (v - v_{\lambda, \alpha})\| \leq c\left(\frac{1}{\sqrt{\lambda}} + \frac{1}{\sqrt{\alpha}}\right)\|f\|.
\]

For optimal scaling the two parameters \( \alpha \) and \( \lambda \) should be chosen similarly. This penalized energy minimization formulation does not produce an approximation to the pressure.

### 3 A posteriori error estimation for neural network solutions

#### 3.1 The dual weighted residual method

We start by giving a very short description of the dual weighted residual method such as presented in [3, 4] for the most simple case of the Laplace problem \(-\Delta u = f\) with homogeneous Dirichlet data \( u = 0 \). As introduced above, \( V = H^1_0(\Omega) \) and \( V_h \subset V \) is a discrete subspace.
Now, let $J : \mathcal{V} \to \mathbb{R}$ be a linear functional and let $z \in \mathcal{V}$ be the solution to the adjoint problem
\[ -\Delta z = J \text{ in } \Omega, \quad z = 0 \text{ on } \partial\Omega, \tag{20} \]
in variational formulation given as
\[ (\nabla v, \nabla z) = J(v) \quad \forall v \in \mathcal{V}. \tag{21} \]
This already gives the **primal error identity**
\[ J(u - u_h) = (\nabla (u - u_h), \nabla z) = (f, z) - (\nabla u_h, \nabla z). \tag{22} \]
By Galerkin orthogonality $(\nabla (u - u_h), \nabla v_h) = 0$ for all $v_h \in V_h$ the corresponding **dual error identity** reads
\[ J(u - u_h) = (\nabla (u - u_h), \nabla (z - z_h)) = (\nabla u, \nabla (z - z_h)) = J(u) - (\nabla u, \nabla z_h), \tag{23} \]
where $z_h \in V_h \subset \mathcal{V}$ is the discrete solution to the adjoint problem.

Both simple error identities, (22) and (23), cannot be used in practice since the adjoint solution $z \in \mathcal{V}$ and the primal solution $u \in \mathcal{V}$ are not known. Applying the DWR method calls for an approximation of the primal or adjoint solutions in a subspace $V_{hh} \subset \mathcal{V}$ which is not a subspace of the discrete space, e.g. $V_{hh} \not\subset V_h$ and to replace the error identities by
\[ J(u - u_h) \approx (f, z_{hh}) - (\nabla u_h, \nabla z_{hh}) \approx J(u_{hh}) - (\nabla u_{hh}, \nabla z_h). \tag{24} \]
Various approaches are discussed in [3, Sec. 5] or [19, Sec. 3]. In general, they are based on the higher-order postprocessing of same-space approximations $u_h, v_h \in V_h$, e.g. polynomial of double degree on a coarser mesh has been proven to be both reliable and efficient. However, this reconstruction of higher order information is an approximation only such that the DWR method usually does not give a rigorous error bound but only an estimate to the error. This approximation is usually highly accurate.

The accuracy of the error estimator can be numerically validated by considering the **effectivity index**, e.g. the quotient of estimator value by real error, which in the case of the primal formulation reads
\[ \text{eff}_h := \frac{(F, z_{hh}) - (\nabla u_h, \nabla z_{hh})}{J(u - u_h)}, \tag{25} \]
what of course requires a guess of the **true error** $J(u - u_h)$. For linear elliptic problems one usually observes effectiveness going to 1, as $h \to 0$.

The DWR method is easily extended to nonlinear problems, to systems of differential equations and to time dependent problems. All these further extensions and various applications have been demonstrated by Becker and Rannacher [3]. The fundamental problem that is still open is a reliable and efficient procedure for approximating the weights and, in the case of nonlinear problems, bounds on a higher order remainder that must usually be dropped.
3.2 Estimating the network error for the Laplace equation

Within this framework we now aim at estimating the functional error of the neural network solution \( u_N \in V_N \) obtained with the Deep Ritz approach. Since the network minimizer \( u_N \notin V \) does not satisfy the Dirichlet condition \( u = 0 \), a consistency term remains when multiplying the error \( u - u_N \) with the adjoint problem

\[
J(u - u_N) = (\nabla (u - u_N), \nabla v) + \langle \partial_n z, u_N \rangle.
\]

The remaining steps are as in (22) and we derive the error identity

\[
J(u - u_N) = (f, z) - (\nabla u_N, \nabla z) + \langle \partial_n z, u_N \rangle.
\]

Again, we must approximate \( z \in V \) by a discrete solution which is accurate, efficiently achievable and which does not fall into the vicinity of Galerkin orthogonality, which, in the case of the neural network error \( u - u_N \) imposes the condition \( z_h \notin V_N \). The neural network spaces introduced in Section 4 have no similarity to local finite element spaces. Hence, we will approximate the adjoint solution in as coarse as possible finite element space \( z_h \in V_h \subset V \) and approximate

\[
\eta(u_N, z_h) = (f, z_h)_\Omega - (\nabla u_N, \nabla z_h) + \langle \partial_n z_h, u_N \rangle.
\]

This error estimator is efficiently evaluated on the finite element mesh using a numerical quadrature rule within the domain and along the boundaries. The effectivity of the estimate is measured by means of the effectivity index (25). We finally note that the error estimator (28) is not specific to the Deep Ritz method, instead it could also be used in the context of DeepXDE, see [13], or for any other approximation technique that yields a \( H^1 \)-conforming solution.

3.3 Estimating the network error for the Stokes equations

The estimate can directly be transferred to the Stokes equations, where we approximate the solution based on the penalized energy form (16) such as described in Section 2.3. For a goal functional \( J : H^1_0(\Omega)^2 \to \mathbb{R} \) we introduce the adjoint solution

\[
\text{div } z = 0, \quad -\Delta z - \nabla q = J \text{ in } \Omega, \quad z = 0 \text{ on } \partial \Omega.
\]

The error identity for the network solution \( v_N \) minimizing (16) is then derived as

\[
J(v - v_N) = (\nabla v, \nabla (v - v_N)) + (q, \text{div } (v - v_N)) - \langle \partial_n z + q\vec{n}, v - v_N \rangle_{\partial \Omega}
= (f, z) - (\nabla v_N, \nabla z) - (\text{div } v_N, q) + \langle v_N, \partial_n z + q\vec{n} \rangle_{\partial \Omega}.
\]

To evaluate and approximate this error identity we compute a coarse finite element approximation \((z_h, q_h) \in V_h \times L_h\)

\[
-(\text{div } z_h, \phi_h) + (\nabla z_h, \nabla \phi_h) + (q_h, \text{div } \phi_h) = J(\phi_h) \quad \forall (\phi_h, \xi_h) \in V_h \times L_h,
\]

and define the Stokes error estimate as

\[
\eta(v_N, z_h, q_h) := (f, z_h) - (\nabla v_N, \nabla z_h) - (\text{div } v_N, q_h) + \langle \partial_n z_h + q_h \vec{n}, v_N \rangle_{\partial \Omega}.
\]
4 Network architecture and training

Let us recall from the introduction that the network is considered as function $N : \Omega \to \mathbb{R}^c$. More precisely, $N$ is a $L$-layer neural network with $N_l$ neurons in the $l$-th layer. We denote the weight matrix and bias vector in $l$-th layer by $W^l \in \mathbb{R}^{N_{l} \times N_{l-1}}$ and $b^l \in \mathbb{R}^{N_l}$, respectively. An activation function $\sigma$ is applied elementwise.

We consider two different architectures: feed forward neural network (FFNet)

\[
\begin{align*}
N^0(x) &= x \in \Omega, \\
N^l(x) &= \sigma(W^lN^{l-1}(x) + b^l) \in \mathbb{R}^{N_l}, \text{ for } 1 \leq l \leq L \\
N^{L+1}(x) &= W^L N^{L-1}(x) + b^L \in \mathbb{R}^c,
\end{align*}
\]

and residual neural network (ResNet)

\[
\begin{align*}
N^0(x) &= x \in \Omega, \\
N^k(x) &= \sigma \left(W^l \left(\sigma(W^{l-1}N^{l-2}(x) + b^{l-1}) + b^l \right) + N^{k-2}(x) \right) \in \mathbb{R}^{N_l}, \text{ for } 1 \leq l \leq L/2 \\
N^{L+1}(x) &= W^l N^{L-1}(x) + b^l \in \mathbb{R}^c, \\
N^{L+1}(x) &= W^L N^{L-1}(x) + b^L \in \mathbb{R}^c.
\end{align*}
\]

With the employed notation $N^0$ is an input layer with $l_0 = d$ and $N^{L+1}$ is an output layer with $N_{l+1} = c$. All hidden layers are of the same size $H$, i.e. $l = H$ for $1 \leq l \leq L$

Remark 3. In [5] the authors used a ResNet architecture, however we observed that in practise even simpler neural networks give good results.
In this section we present some insights into the training process for the Deep Ritz method applied to Laplace problem on a L-shaped domain. We refer to Section 5.1 for a precise definition of the test case. Here, we study the effect of the network architecture, i.e. a Feed Forward Neural Network (FFNet) and a Residual Neural Network (ResNet) on the training. To train the neural network, we use the Adam optimizer \[12\].

In Figure 2 we present training progress for residual networks of various size. In the left sketch we show the loss function, i.e. the value of the penalized and approximated energy functional \[9\] and on the right, we show the \[L_2\] error of the resulting approximations \[\|u - u_Nu\|\] during training. In general, the bigger the network the fewer epochs are needed to reach a certain error. However, this is not always the case. We observe a certain threshold for the number of network parameters above which increasing the size of the network does not improve the solution. In general, the slope of the loss function is similar to the progress of the \[L_2\]-error. Naturally, once low loss levels are reached, larger networks are able to yield better approximations.

In Figure 3 we present the training and approximation progress of networks with Feed Forward and Residual architectures and same sizes. To be precise, for each architecture we consider a small network with 481 parameters and a larger one with 921 parameters. The residual network is faster to train, but this discrepancy gets smaller for larger networks. The advantage of residual networks was already mentioned by E and Yu \[8\].

The above considerations show the need for a quality measure of the solution that works across architectures and training methods. In the following section we will present numerical examples that demonstrate the usability of the error estimator for controlling the approximation error during training. This estimate can then be used as stopping criterion once a sufficiently low error level is reached.
Figure 3: Training progress for networks of similar size

5 Numerical examples

In this section we will consider two test cases, the Laplace equation on a L-shaped domain that has already been considered previously and the Stokes equations on a disc. We start by showing the neural network Deep Ritz solutions to both test cases in Figure 4. We give the approximation at different stages of the training procedure, at the beginning and after a certain number of epochs (indicated in the figure caption).

5.1 Test Case 1. Laplace equation

As first test case we consider the Poisson equation on the L-shaped domain \( \Omega_L = (-1, 1)^2 \setminus [0,1]^2 \) shown in Figure 5. The functional of interest is the evaluation of the solution in the point \( x_a = (0.5, -0.5) \)

\[
- \Delta u = 1 \text{ in } \Omega_L, \quad u = 0 \text{ on } \partial \Omega_L, \quad J(u) = u(x_a).
\]  

We note that \( J \not\in H^{-1}(\Omega_L) \) is not an admissible functional. The point evaluation should be replaced by averaging over a small neighbourhood of the point \( x_a \). On the other hand, it is well documented that the non-regularized functional gives optimal performance in the context of the dual weighted residual method, see [3, 19]. For comparison, we first determine a reference value by resolved finite element simulations on very fine meshes. We identify it as

\[
J_{ref} = 0.1023612 \pm 0.001953125.
\]

First we demonstrate the performance of the DWR estimator

\[
\eta(u_N, z_h) = (f, z_h)_\Omega - (\nabla u_N, \nabla z_h)_\Omega + \langle \partial_n z_h, u_N \rangle_{\partial \Omega}
\]
as presented in Section 3.2. The adjoint solution $z_h$ will be computed as finite element approximation on very coarse meshes. Training results and estimator values are shown for neural network solutions obtained with the Deep Ritz method and using the strong formulation. Both network architectures of FFNet type and of ResNet type are considered. The complete set of parameters is summarized as follows:

- FFNet: $H = 20, L = 4, \sigma(x) = \text{ELU}(x)$,
- ResNet: $H = 20, L = 2, \sigma(x) = \max(x^3, 0)$.

Note, since ResNet block consists of two layers, both architectures have same number of parameters and the Exponential Linear Unit (ELU) is defined as

$$\text{ELU}(x) = \begin{cases} x & \text{if } x \geq 0 \\ e^x - 1 & \text{if } x < 0. \end{cases}$$

For the Deep Ritz approach and the strong formulation all gradients are computed both with automatic differentiation and finite difference approximation, respectively. We perform 8000 epochs and the estimator is evaluated every 100 epochs, see Figure 6.
Figure 6: Loss, error and estimator for different network architectures and Loss functions.

One can observe that independently of the applied method, the estimator follows the error. Consequently we study the dependence on the coarse mesh size $h \in \{0.5, 0.25, 0.0625\}$ used to approximate the adjoint solution and show the results in Figure 7. Increasing the level of refinement improves the exactness of the estimator. The results are relatively good even for extremely coarse meshes and the evaluation of estimator is computationally cheap. The choice $h = 0.5$ corresponds to only 12 quadrilateral elements, the finest mesh with $h = 0.0625$ corresponds to just 768 elements. Further, many degrees of freedom reside on the boundary of the domain such that the number of unknowns to approximate the adjoint solution ranges from 5 on the coarsest mesh to 640 on the finest mesh and from the results we observe that the intermediate mesh with $h = 0.25$ comprising 16 unknowns is sufficiently accurate.

5.2 Test Case 2. Stokes equations

For the second test case we consider the Stokes equations on a unit circle $\Omega = B((0,0),1)$. We prescribe an analytical solution for comparison with the neural network approxima-
\( L = 1, h = 0.5 \)
\( L = 2, h = 0.25 \)
\( L = 4, h = 0.0625 \)

Figure 7: Loss, error and estimator for different refinement levels of dual solution \( h = 2^{-L} \).

| epoch | \( L=1 \) error | \( L=1 \) estimate | \( L=1 \) eff | \( L=2 \) error | \( L=2 \) estimate | \( L=2 \) eff | \( L=4 \) error | \( L=4 \) estimate | \( L=4 \) eff |
|-------|-----------------|-----------------|----------|-----------------|-----------------|----------|-----------------|-----------------|----------|
| 500   | -0.008480       | -0.014786       | 0.57     | 0.010748        | 0.009397        | 1.14     | 0.018578        | 0.019248        | 0.96     |
| 1000  | -0.003403       | -0.006700       | 0.51     | 0.005855        | 0.007324        | 0.80     | -0.004695       | -0.004719       | 0.99     |
| 1500  | -0.008228       | -0.008022       | 1.03     | -0.007460       | -0.003477       | 2.15     | -0.009242       | -0.009126       | 1.01     |
| 2000  | -0.006424       | -0.004946       | 1.23     | -0.009138       | -0.011058       | 0.83     | -0.006117       | -0.006393       | 0.96     |

Table 1: The values of error and estimator with effectivity index \( \text{eff}_h \), see [25], for different refinement levels of dual solution \( h = 2^{-L} \).

The functional of interest \( J(v) \) is an integral of a \( y \)-component of the velocity on a line segment \([0, 1]\)

\[
J(v) := \int_0^1 v_y(x, 0) \, dx, \quad J_{ref} = -\frac{1}{\pi}.
\]

In Figure 7 we present the loss function and the functional error as well as the error estimator. The training of the Deep Ritz method is performed for 25000 epochs, with the Feedforward Neural Network (FFNet: \( d = 2, c = 2, H = 10, L = 20, \sigma(x) = \text{ELU}(x) \)). The adjoint Stokes problem is approximated with equal order finite elements.
using pressure stabilization on a coarse mesh level $L = 3$ that corresponds to $h \approx 0.04375$. The results for some selected epochs together with effectivity index are summarized in Table 2.

The numerical implementation is realized in the finite element toolkit Gascoigne 3D [5], which is coupled to machine learning framework PyTorch [17].

6 Conclusion

Based on the dual weighted residual method the error estimator of neural network approximations of PDEs is developed. We derive the estimator for a functional of interest and demonstrate its performance for Laplace and Stokes equation. The method is independent of the design of the neural network and the training procedure. The evaluation on a very coarse meshes already shows very good accuracy, such that little computational overhead is brought along. The estimator can be used as accurate and simple to use stopping criterion during the training process. Hereby, we gain a first validation of the neural network approximation and the error controlled training also helps to reduce the computational effort by avoiding excessive training epochs.
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