A priori and a posteriori error estimates for the Deep Ritz method applied to the Laplace and Stokes problem

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Abstract

We analyze neural network solutions to partial differential equations obtained with Physics Informed Neural Networks. In particular, we apply tools of classical finite element error analysis to obtain conclusions about the error of the Deep Ritz method applied to the Laplace and the Stokes equations. Further, we develop an a posteriori error estimator for neural network approximations of partial differential equations. The proposed approach is based on the dual weighted residual estimator. 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.

Keywords: neural networks, finite elements, error estimates, dual weighted residual method, a posteriori error estimates

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 representing the solution to the PDE by a deep neural network. Many of these approaches have demonstrated that they can provide efficient approximations in certain situations. Here we pursue two goals. On the one hand, we try to show commonalities in the analysis of finite element methods and the analysis of solutions represented by neural networks. On the other hand, we develop an a posteriori error estimator which allows testing a once trained network for its accuracy and which can furthermore be used as a termination criterion during the training process. Even though the resulting error estimator provides very high accuracy in practical applications, it is not robust in the sense of a guaranteed upper bound.

Learning solutions of partial differential equations. We consider a neural network function $v_N$ as a (differentiable) function $v_N : \Omega \rightarrow \mathbb{R}^c$, where $\Omega \subset \mathbb{R}^d$ is the computational

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domain of dimension \( d \in \mathbb{N} \) and \( c \in \mathbb{N} \) is the size of the differential system. By \( \mathcal{N} \) we denote the architecture of a neural network, \( v_{\mathcal{N}} \) is then a specific realization within this architecture. Several different approaches have been presented that train the network by integrating the differential equation into a loss function. Here we focus on the Deep Ritz method by E and Yu [1] which aims at minimizing the energy functional and 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

\[
E(u_{\mathcal{N}}) \leq E(v_{\mathcal{N}}) = \frac{1}{2} \int_{\Omega} |\nabla v_{\mathcal{N}}(x)|^2 \, dx - \int_{\Omega} v_{\mathcal{N}}(x) \cdot f(x) \, dx + \lambda \int_{\partial\Omega} |v_{\mathcal{N}}(x) - g(x)|^2 \, dx,
\]

with a parameter \( \lambda > 0 \), where the integrals are approximated by Monte-Carlo integration based on randomly chosen quadrature points within the domain \( \Omega \) and on the boundary \( \partial\Omega \). The optimal network solution \( u_{\mathcal{N}} \) is then identified by minimizing the approximated energy functional \( E(u_{\mathcal{N}}) \leq E(v_{\mathcal{N}}) \). See Section 2.2 and [2] for an overview and further examples on the energy based approach.

Another approach, denoted as DeepXDE (Lu, Meng, Mao and Karniadakis [3]), Unified Deep Artificial Network [4] or Deep Galerkin Method (DGM) [5], see also [6], minimizes the strong residual of the equation, either as collocation method in randomly picked \( N_{\text{in}} \) points within the domain and \( N_{\text{bnd}} \) on the boundary, formulated once more for the Laplace problem,

\[
E(u_{\mathcal{N}}) \leq E(v_{\mathcal{N}}) = \frac{1}{N_{\text{in}}} \sum_{k=1}^{N_{\text{in}}} |-\Delta v_{\mathcal{N}}(x_k) - f(x_k)|^2 + \lambda \, \sum_{j=1}^{N_{\text{bnd}}} |v_{\mathcal{N}}(x_j) - g(x_j)|^2.
\]

This corresponds to a Monte-Carlo integration of the (strong) residual

\[
E(v_{\mathcal{N}}) = \| -\Delta v_{\mathcal{N}} - f \|_{L^2(\Omega)}^2 + \lambda \| g - v_{\mathcal{N}} \|_{L^2(\partial\Omega)},
\]

which could be considered as a natural extension of Deep Ritz to non-symmetric and nonlinear problems.

Finally, a third variant, variational physics-informed neural network VPINN (Kharazmi, Zhang and Karniadakis [7]) is based on the variational formulation

\[
E(u_{\mathcal{N}}) \leq E(v_{\mathcal{N}}) = \left( \int_{\Omega} \nabla v_{\mathcal{N}}(x) \cdot \nabla \phi_k(x) \, dx - \int_{\Omega} f(x) \phi_k(x) \, dx \right)^2
\]

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

The stopping criteria of the training process have not been studied in detail. Commonly a fixed number of epochs is performed, see e.g. [1] or training runs until the mean residual reaches a specified threshold, [3]. According to the authors knowledge, it is the first time that an a posteriori error estimator is utilized as stopping criterion.

Approximation properties and convergence. The common rationale for the three different approaches discussed above is the excellent approximation property of neural networks, in particular, Pinkus [8] 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 [3, 5]. 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 far more challenging computational task.

Learning operators. All approaches mentioned so far have in common that a neural network represents the solution of a specific differential equation problem. If the problem, e.g. the right-hand side, a parameter or the domain, is changed, a new network must be trained. This is also the case for classical simulation methods. Here however the solution is obtained by solving a linear or nonlinear system of equations which can be accomplished with optimal efficiency if, for instance, multigrid methods are available. In contrast, neural network based approaches will call for a retraining of the network, which corresponds to solving an ill-structured optimization problem. The picture changes if e.g. parameter-dependent learning is used or if very high-dimensional problems are investigated [1]. DeepONet [10] extends the above mentioned ideas and directly aims at learning the complete solution operator. This allows reusing the once trained network for solving multiple problems.

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 [11] 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 [12]. The Deep Neural Network Multigrid Method (DNN-MG) [13, 14], uses deep neural networks to locally enrich classical finite element multigrid solutions on coarse meshes with additional fine mesh fluctuations.

One contribution that is similar in terms of the techniques is the use of neural networks to represent dual problems in the context of the DWR method [15].

Outline of the article. In this contribution, which is based on the early preprint [16], we tackle the question of reliability and error control of deep neural network approaches.

After a brief introduction in Section 1 we focus on the Deep Ritz method, and investigate to what extent classical finite element analysis carries over to neural network approximations by analysing different contributions to the approximation error. Section 2 is devoted to the numerical analysis of network approximations to the Laplace and the Stokes problem. We present a priori error estimates that are complete except for the error stemming from the inexact solution of the optimization problem.

Next, in Section 3 we derive a posteriori error bounds for neural network solutions. This error estimator extends to different PINNs and can be used to rate the quality of trained networks. A posteriori error estimation is approached within the concept of the dual weighted residual estimator (DWR) that has been introduced by Becker and Rannacher [17]. 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. For the sake of simplicity, the estimator
is developed for the Deep Ritz method. However, it directly extends to different neural network representations of the solution.

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 the Laplace problem. Let $\Omega \subset \mathbb{R}^d$ be a $d$-dimensional domain. We find the weak solution $u \in V := H^1_0(\Omega)$ to

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

where $f \in L^2(\Omega)$ is the right hand side. By $V = H^1_0(\Omega)$ we denote the space of $L^2$-functions with the first weak derivative in $L^2(\Omega)$ with a vanishing trace on $\partial \Omega$. The solution $u \in V$ is characterized by the variational problem

$$(\nabla u, \nabla v) = (f, v) \quad \forall v \in V,$$

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

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.

By $V_h \subset V$ we denote the finite dimensional (finite element) subspace of $H^1_0(\Omega)$. Then, let $u_h \in V_h$ be the approximation to $u \in V$ given by

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

The finite element error $u - u_h$ is bounded by the interpolation error, yielding the standard estimate

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

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 a convex polygonal for $r = 1$ or locally parametrizable by a $C^{r+1}$-function for $r \geq 1$.  

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2.2. Deep Ritz approximation of the Laplace problem

In principle, the Deep Ritz method as proposed by E and Yu [1] is based on minimizing the energy functional (3) by representing the unknown solution by a neural network \( u_{N, \omega} : \mathbb{R}^d \rightarrow \mathbb{R} \) instead of a finite element function. We denote by \( \mathcal{N} \) the topology of the neural network and by \( \omega \in \mathbb{R}^{\#\mathcal{N}} \) the parameters of the network, where \( \#\mathcal{N} \) is the total number of free parameters. Finally, \( u_{N, \omega} \) 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 \( \omega \) unless it is of relevance in the given context.

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 \( \mathcal{V}_N \) used in the Deep Ritz method is given by

\[
\mathcal{V}_N := \{ u_{N, \omega} : \mathbb{R}^d \rightarrow \mathbb{R} \mid \omega \in \mathbb{R}^{\#\mathcal{N}} \}.
\]

As long as \( \#\mathcal{N} \) is finite and when the activation functions are differentiable it holds \( \mathcal{V}_N \subset H^1(\Omega) \). However, for \( u_N \in \mathcal{V}_N \) it will not hold \( u_N = 0 \) on \( \partial \Omega \) in the general case, hence \( \mathcal{V}_N \not\subset \mathcal{V} = H^1_0(\Omega) \). Further, it is important to note that \( \mathcal{V}_N \) is not a vector space. For \( v_1, v_2 \in \mathcal{V}_N \) it will usually not hold that \( v_1 + v_2 \in \mathcal{V}_N \). We consider the penalized energy functional, compare [1],

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

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 \( v \) toward zero along the boundary. The minimizer of (7) denoted by \( u_\lambda \in H^1(\Omega) \) is characterized by the variational problem

\[
a_\lambda(u_\lambda, v) = (f, v) \quad \forall v \in H^1(\Omega), \quad a_\lambda(u, v) := (\nabla u, \nabla v) + \lambda(u, v)_{\partial \Omega},
\]

where \( (\cdot, \cdot)_{\partial \Omega} \) denotes 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 hence introduces an additional modeling error term \( \| u - u_\lambda \| \) that will depend on the parameter \( \lambda \) and that will converge to zero for \( \lambda \rightarrow \infty \).

Training of the neural network minimizes the modified energy functional (7) expressed in terms of Monte Carlo integration. To be precise: \( N^{\text{inn}} \in \mathbb{N} \) inner quadrature points \( x^{\text{inn}} = \{ x_1^{\text{inn}}, \ldots, x_{N^{\text{inn}}}^{\text{inn}} \} \subset \Omega \) and \( N^{\text{bnd}} \in \mathbb{N} \) boundary quadrature points \( x^{\text{bnd}} = \{ x_1^{\text{bnd}}, \ldots, x_{N^{\text{bnd}}}^{\text{bnd}} \} \subset \partial \Omega \) are chosen, either randomly or based on a mesh of the

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1In [3], the authors discussed a modified setup of the neural network that indeed strongly satisfies the homogeneous Dirichlet condition.
domain. The loss function is given by

\[ E_{\lambda, \text{mc}}(u_N^i; x^{in}, x^{bnd}) := \frac{|\Omega|}{N^{in}} \sum_{k=1}^{N^{in}} \left( \frac{1}{2} |\nabla u_N(x^{in}_k)|^2 - f(x^{in}_k) \cdot u_N(x^{in}_k) \right) + \frac{|\partial \Omega|}{N^{bnd}} \sum_{j=1}^{N^{bnd}} \frac{\lambda}{2} |u_N(x^{bnd}_j)|^2. \]  

(10)

Minimizing (10) identifies the weights \( \omega \in \mathbb{R}^\#N \).

**Error analysis for the Laplace equation.** For the following, we denote by \( u \in H^1_0(\Omega) \) the exact solution to the Laplace problem and by \( u_N \in V_N \) the Deep Ritz solution that is obtained with a numerical optimization routine and which is based on Monte-Carlo integration of the energy functional. The error of the Deep Ritz approximation \((u - u_N)\) is composed of a multitude of different influences: first, as stated above, the energy functional is based on a perturbed problem, and we denote by \( u_\lambda \in H^1(\Omega) \) the exact solution to this perturbed problem. By \((u - u_\lambda)\) we denote the **modeling error**. By \( u_{N, \text{ex}} \in V_N \) we denote the minimum of the energy functional (7) in the set of neural network functions \( V_N \). The error \((u_\lambda - u_{N, \text{ex}})\) is an approximation error. Next, \( u_{N, \text{mc}} \in V_N \) is minimum of the Monte-Carlo approximated energy functional (10). This introduces the **generalization error** \((u_{N, \text{ex}} - u_{N, \text{mc}})\). Finally, the **optimization error** \((u_{N, \text{mc}} - u_N)\) remains. Altogether, four distinct contributions can be identified

\[ \|u - u_N\| \leq \|u - u_\lambda\| + \|u_\lambda - u_{N, \text{ex}}\| + \|u_{N, \text{ex}} - u_{N, \text{mc}}\| + \|u_{N, \text{mc}} - u_N\|. \]

Modeling (1st) and network approximation (2nd) error of the Laplace equation have been studied in the literature, and also quantitative convergence results are available [18, 19], these however do not consider the numerical quadrature of the energy functional. Some first results are also known for nonlinear problems [20]. Also, the generalization error (3rd) has been studied, usually from a stochastic point of view [21]. We start by estimating the model error that depends on the choice of \( \lambda > 0 \), but that is not yet related to the discretization of the equation.

**Lemma 1 (Model error).** Let \( f \in L^2(\Omega) \), \( \lambda \in \mathbb{R}^+ \) and \( \Omega \) be such that the solutions \( u \in H^1_0(\Omega) \) and \( u_\lambda \in H^1(\Omega) \) to

\[ \begin{aligned}
(\nabla u, \nabla \phi) &= (f, \phi), \\
(\nabla u_\lambda, \nabla \phi_\lambda) + \lambda (u_\lambda, \phi_\lambda)_{\partial \Omega} &= (f, \phi_\lambda)
\end{aligned} \]  

(11)

for \( \phi \in H^1_0(\Omega) \) and \( \phi_\lambda \in H^1(\Omega) \) satisfy \( \|u\|_{H^1(\Omega)} + \|u_\lambda\|_{H^1(\Omega)} \leq c_f \|f\| \). 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

\[ -\Delta z = \frac{\nabla (u - u_\lambda)}{\|\nabla (u - u_\lambda)\|} \quad \text{in} \quad \Omega, \quad z = 0 \quad \text{on} \quad \partial \Omega. \]

(12)
Since the right hand side of this problem is in $L^2(\Omega)$, it holds $z \in H^2(\Omega)$ and $\|z\|_{H^2(\Omega)} \leq c_s$ (given that the domain’s boundary is sufficiently smooth or convex polygonal). Multiplication of (12) with the error $u - u_\lambda$ and integration over the domain give the error identity

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

As $u = 0$ and $z = 0$ on $\partial \Omega$ this, together with (11) gives

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

Finally, with (9) and using the trace inequality and the regularity of adjoint and primal solution we obtain

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

\[\square\]

To study the approximation error $u_\lambda - u_{N,ex}$, where $u_\lambda \in H^1(\Omega)$ is the minimizer to $E_\lambda(\cdot)$ in the Hilbert space $H^1(\Omega)$ and $u_{N,ex} \in V_N$ is the minimizer to $E_\lambda(\cdot)$ in the neural network set, we use a generalized version of Cea’s lemma taken from [18, Prop. 3.1]. It holds

$$\|u_\lambda - v_N\|^2 \leq 2(E_\lambda(v_N) - \inf_{\tilde v \in V_N} E_\lambda(\tilde v)) + \inf_{w_N \in V_N} \|u_\lambda - w_N\|^2 \quad \forall v_N \in V_N, (13)$$

where the norm $\| \cdot \|$ is defined via the bilinear form $A$

$$\|u\|_A := a_\lambda(u, u)^{\frac{1}{2}} = \left(\|\nabla u\|^2 + \lambda \|u\|_{\partial \Omega}^2\right)^{\frac{1}{2}}.$$ 

If we choose $v_N = u_{N,ex} \in V_N$, the exact minimum to $E_\lambda(\cdot)$ in the neural network set, it holds

$$\|u_\lambda - u_{N,ex}\| \leq \inf_{w_N \in V_N} \|u_\lambda - w_N\|_A \quad \forall w_N \in V_N,$$

and the error $u_\lambda - u_{N,ex}$ is indeed a neural network approximation error that has already been extensively studied in the literature [22, 9, 18]. Quantitative convergence results $\|u_\lambda - u_{N,ex}\| \to 0$ for increasing network sizes are well known, see for example [9] Theorem 4.1, where the authors state that the bound

$$\|\nabla (u_\lambda - u_{N,ex})\| = O(\epsilon)$$

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

$$\|\nabla (u_\lambda - u_{N,ex})\| = O\left(\frac{\sqrt{\log(N)}}{\sqrt{N}}\right).$$

\[2\] The exact relation is $\epsilon = \sqrt{W_0(N)/\sqrt{N}}$, where $W_0(x)$ is the Lambert $W$-function, the inverse of $f(y) = ye^y$. It holds $W(N) \leq \log(N)$. 

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

In Lemma 3, we will give a unified estimate for this approximation error and the generalization error, i.e. we will estimate $u_\lambda - u_{\lambda,mc}$ at once.

The choice of the numerical quadrature points gives rise to the generalization error of the neural network representation. In the context of Deep Ritz, the generalization error is the error of numerical quadrature, i.e. the error $u_{\lambda,ex} - u_{\lambda,mc}$ where $u_{\lambda,mc} \in V_N$ is the minimum in the neural network set $V_N$ based on Monte-Carlo integration of the energy functional. To estimate this error, one has to quantify the stability of the minimizer with respect to the quadrature of the energy functional. In [23] the authors base the analysis on stability estimates of the underlying partial differential equations. The authors of [24] give bounds on the Rademacher complexity of the energy functions and therefore limit the generalization error.

We will analyze the generalization error based on the best approximation estimate (13) taken from [18, Prop. 3.1] and on estimating the quadrature error between $E_\lambda(\cdot)$ and $E_{\lambda,mc}(\cdot)$. First, we cite a standard result on the Monte Carlo integration error, taken from [25, Theorem 2.1].

**Lemma 2 (Monte Carlo Quadrature).** Let $\Omega \subset \mathbb{R}^d$ be a bounded domain. For large $N$, let $x_1, \ldots, x_N \in \Omega$ be a set of Monte Carlo quadrature nodes. For $f \in C(\Omega)$ it holds

$$\left| \int_{\Omega} f(x) \, dx - \frac{|\Omega|}{N} \sum_{i=1}^{N} f(x_i) \right| = \|f\|_{L^2(\Omega)} O(N^{-\frac{1}{2}} \nu),$$

where $\nu$ is a standard normal random variable.

In a more precise version, the integration error depends on the variance of $f$ and not on the $L^2$-norm of $f$ itself, this simplified version however is sufficient for our purposes.

**Lemma 3 (Generalization and approximation error of the Deep Ritz method for the Laplace problem).** Let $\Omega \subset \mathbb{R}^d$ be a bounded domain, $f \in L^2(\Omega)$ and $V_N \subset C^1(\Omega) \cap C(\overline{\Omega})$ be a neural network set. Let $u_\lambda \in H^1(\Omega)$ be the solution to (8) and $u_{\lambda,mc} \in V_N$ be the neural network minimizer to $E_{\lambda,mc}(\cdot)$. Further, let the network satisfy

$$\inf_{v_N \in V_N} \|u_\lambda - v_N\|_\lambda \leq \epsilon_N$$

for a tolerance $\epsilon_N > 0$. Then, for $N := \min\{N^{in}, N^{bd}\}$ it holds

$$\|\nabla(u_\lambda - u_{\lambda,mc})\|^2 + \lambda \|\nabla(u_\lambda - u_{\lambda,mc})\|^2_{\partial \Omega} \leq C(\epsilon_N^2 + O(N^{-\frac{1}{2}} \nu))$$

where $\nu$ is a standard normal random variable and where $C > 0$ depends on the domain $\Omega$, $\|f\|_{L^2}$, $\|u_{\lambda,mc}\|_{C^1(\Omega) \cap C(\overline{\Omega})}$ and on $\|u_{\lambda,ex}\|_{C^1(\Omega) \cap C(\overline{\Omega})}$.

**Proof.** With the best approximation estimate (13) we get

$$\|u_\lambda - u_{\lambda,mc}\|_\lambda \leq 2(E_\lambda(u_{\lambda,mc}) - \inf_{v_N \in V_N} E_\lambda(v_N)) + \inf_{w_N \in V_N} \|u_\lambda - w_N\|_\lambda.$$ (17)
Here, \( u_{N,mc} \) is not the minimizer of \( E_\lambda(\cdot) \) in \( V_N \), which we denote by \( u_{N,ex} \in V_N \), but the minimizer of \( E_{\lambda,mc}(\cdot) \). Hence, we extend the first term as
\[
E_\lambda(u_{N,mc}) - \inf_{\tilde{v}_N \in V_N} E_\lambda(\tilde{v}_N) =: E_\lambda(u_{N,mc}) - E_\lambda(u_{N,ex})
\]
\[
= (E_\lambda(u_{N,mc}) - E_{\lambda,mc}(u_{N,mc})) + (E_{\lambda,mc}(u_{N,mc}) - E_{\lambda,mc}(u_{N,ex})) + (E_{\lambda,mc}(u_{N,ex}) - E_\lambda(u_{N,ex})).
\]  
(18)

The first and the third terms are quadrature errors, and they can be estimated with Lemma 2 by using \( V_N \subset L^2(\Omega) \cap C(\Omega) \) as well as Young’s inequality
\[
\left| E_\lambda(u_{N,mc}) - E_{\lambda,mc}(u_{N,mc}) \right| \\
= \left( \| \nabla u_{N,mc} \|^2_{L^2(\Omega)} + \| f \|^2_{L^2(\Omega)} \right) + \lambda \| u_{N,mc} \|^2_{L^1(\partial\Omega)} + \| \nabla u_{N,mc} \|^2_{L^\infty(\Omega)} \right) \mathcal{O}(N^{-\frac{1}{2}}) \\
\leq C \left( \| u_{N,mc} \|^2_{W^{1,\infty}(\Omega)} + \lambda \| u_{N,mc} \|^2_{L^\infty(\Omega)} + \| f \|^2_{L^2(\Omega)} \right) \mathcal{O}(N^{-\frac{1}{2}}).
\]

The same argument can be applied to estimate the last term in (18). The second term of (18) is negative as
\[
E_{\lambda,mc}(u_{N,mc}) = \inf_{u_N \in V_N} E_{\lambda,mc}(u_N) \leq E_{\lambda,mc}(u_{N,ex})
\]
and therefore it can be neglected. The last term in (17) is the approximation error and given by (16).

Finally, the optimization error \( u_{N,mc} - u_N \) remains for which there is no a priori error bound.

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 \( v \in V_0 := H^1_0(\Omega) \times H^1_0(\Omega) \) and the pressure \( p \in L := L^2(\Omega) \setminus \mathbb{R} \) such that
\[
\nabla \cdot v = 0, \quad -\Delta v + \nabla p = f \text{ in } \Omega, \quad v = 0 \text{ on } \partial\Omega,
\]  
(19)

where we denote by \( f \in \mathcal{L}^2 := L^2(\Omega) \times L^2(\Omega) \) the right hand side. Considering a discrete pair of subspaces \( V_h \times L_h \subset V \times \mathcal{L} \), the finite element solution is defined by
\[
(\nabla v_h, \xi_h) + (\nabla v_h, \nabla \phi_h) - (p_h, \nabla \cdot \phi_h) = (f_h, \phi_h) \quad \forall (\phi_h, \xi_h) \in V_h \times L_h.
\]  
(20)

Assuming inf-sup stability of the discrete finite element pair, the solution exists uniquely, and standard best approximation results are satisfied, e.g. for the \( P^2 - P^1 \) Taylor-Hood element it holds
\[
\| \nabla (v - v_h) \| + \| p - p_h \| \leq ch^2 \| f \|_{H^1(\Omega)},
\]  
(21)

or, for equal-order linear finite elements for the pressure and the velocity, the solution to the stabilized formulation
\[
(\nabla v_h, \nabla \phi_h) - (p_h, \nabla \cdot \phi_h) + \beta (\nabla p_h, \nabla \xi_h) = (f_h, \phi_h) \quad \forall (\phi_h, \xi_h) \in V_h \times L_h
\]  
(22)
satisfies the estimate
\[ \|\nabla (v - v_h)\| + \|p - p_h\| \leq ch\|f\|. \] (23)

We refer to the literature, e.g. the monograph of John [26] 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 free condition, i.e.
\[ E_{\lambda,\alpha}(v) := \frac{1}{2} \|\nabla v\|^2 - (f, v) + \frac{\alpha}{2} \|\text{div } v\|^2 + \frac{\lambda}{2} |v|^2_{\partial\Omega}, \] (24)

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
\[ v_{\lambda,\alpha} \in V_2 := H^1(\Omega) \times H^1(\Omega), \]
\[ A_{\lambda,\alpha}(v_{\lambda,\alpha}, \phi) = F(\phi) \quad \forall \phi \in H^1(\Omega), \]
\[ A_{\lambda,\alpha}(v, \phi) := (\nabla v, \nabla \phi) + \alpha(\text{div } v, \text{div } \phi) + \lambda(\phi, \phi)_{\partial\Omega}, \] (25)

This variational problem corresponds to the following classical formulation which also reveals a disturbed boundary condition
\[ -\Delta v_{\lambda,\alpha} - \alpha \text{div } v_{\lambda,\alpha} = f \text{ in } \Omega, \quad \lambda v_{\lambda,\alpha} + \alpha \vec{n} \text{div } v_{\lambda,\alpha} - \partial_n v_{\lambda,\alpha} = 0 \text{ on } \partial\Omega. \] (26)

Hereby and similar to Lemma 1 we get

**Lemma 4 (Stokes model error).** Let \( f \in L^2 \), \( \lambda, \alpha \in \mathbb{R} \) with \( \lambda, \alpha > 0 \) and \( \Omega \) be such that the solutions \((v, p) \in V_2 \times L^2 \) and \( v_{\lambda,\alpha} \in V_2 \) to (19) and (25), respectively, satisfy \( \|v\|_{H^2(\Omega)} + \|p\|_{H^1(\Omega)} \leq c_s\|f\| \) and \( \|v_{\lambda,\alpha}\|_{H^2(\Omega)} \leq c_s\|f\| \). It holds
\[ \|\nabla (v - v_{\lambda,\alpha})\| \leq c \min\{\sqrt{\lambda}, \sqrt{\alpha}\} \|f\|, \]

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

**Proof.** Due to its similarity to Lemma 1 we just give a sketch of the proof. Considering the adjoint \((z, p) \in V_2 \times L^2 \), which is the solution to
\[ \frac{\nabla (v - v_{\lambda,\alpha})}{\|\nabla (v - v_{\lambda,\alpha})\|} = -\Delta z - \nabla q, \quad \text{div } z = 0, \]
we obtain the error estimate
\[ \|\nabla (v - v_{\lambda,\alpha})\| = \left| (\nabla z, \nabla (v - v_{\lambda,\alpha})) + (q, \text{div } (v - v_{\lambda,\alpha})) + \langle \partial_n z + q\vec{n}, v_{\lambda,\alpha} \rangle_{\partial\Omega} \right. \]
\[ -\alpha(\text{div } v_{\lambda,\alpha}, \text{div } z) - \lambda(\phi, \phi)_{\partial\Omega} - (p, \text{div } z) \left. \right| = 0 \]
\[ = \left| \langle \partial_n z + q\vec{n}, v_{\lambda,\alpha} \rangle_{\partial\Omega} - (\text{div } v_{\lambda,\alpha}, q) \right| \leq (\|z\|_{H^2(\Omega)} + \|q\|_{H^1(\Omega)}) \cdot (\|\text{div } v_{\lambda,\alpha}\| + |v_{\lambda,\alpha}|_{\partial\Omega}). \] (27)
On the other hand, diagonal testing of (25) gives
\[
\frac{1}{2} \| \nabla v_{\lambda,\alpha} \|^2 + \lambda |v_{\lambda,\alpha}|_{\partial\Omega}^2 + \alpha \| v_{\lambda,\alpha} \|^2 \leq \frac{1}{2} \| f \|^2
\]
and hereby, we obtain the postulated result.

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.

Having these first results at hand we can proceed as in the case of the Laplace problem and define $v_{N,\text{ex}} \in W_N = V_N \times V_N$ as the neural network solution based on exact integration. The numerical neural network solution is obtained by Monte-Carlo quadrature of the energy $E_{\lambda,\alpha}(v)$, see (24), using $N^{\text{in}}$ interior and $N^{\text{bnd}}$ boundary points
\[
E_{\lambda,\alpha,\text{mc}}(v) := \frac{|\Omega|}{N^{\text{in}}} \sum_{k=1}^{N^{\text{in}}} \left\{ \frac{1}{2} \| \nabla v(x_k^{\text{in}}) \|^2 + \frac{\alpha}{2} \| \text{div} v(x_k^{\text{in}}) \|^2 - f(x_k^{\text{in}}) \cdot v(x_k^{\text{in}}) \right\}
+ \frac{|\Omega|}{N^{\text{bnd}}} \sum_{j=1}^{N^{\text{bnd}}} \lambda |v(x_j^{\text{bnd}})|^2. \tag{28}
\]
The structure is comparable to the Laplace problem, see (10) just with the additional penalty term enforcing the divergence condition.

Similar to Lemma 3 we then can estimate the generalization and approximation error of the Stokes problem.

**Lemma 5** (Generalization and approximation error of Deep Ritz (Stokes)). Let $\Omega \subset \mathbb{R}^2$ be a bounded domain, $f \in L^2(\Omega)^2$ and $W_N \subset C^1(\Omega)^2 \cap C(\Omega)^2$ be a neural network set. Let $v_{\lambda,\alpha} \in H^1(\Omega)^2$ be the solution to (24) and (25) and $v_{N,\text{mc}} \in W_N$ be the neural network minimizer to $E_{\lambda,\alpha,\text{mc}}(\cdot)$ given by (28). Further, let the network be such that it holds
\[
\inf_{v_{\lambda,\alpha} \in V_N} \| v_{\lambda,\alpha} - v_{N,\text{mc}} \|_{\lambda,\alpha} \leq \epsilon_N, \tag{29}
\]
for a tolerance $\epsilon_N > 0$, where
\[
\| v \|_{\lambda,\alpha}^2 := \| \nabla v \|^2 + \alpha \| \text{div} v \|^2 + \lambda \| v \|^2_{\partial\Omega}.
\]
Then, for $N := \min\{N^{\text{in}}, N^{\text{bnd}}\}$ it holds
\[
\| v_{\lambda,\alpha} - v_{N,\text{mc}} \|_{\lambda,\alpha}^2 \leq C(\epsilon_N^2 + O(N^{-\nu})),
\]
where $\nu$ is a standard normal random variable and where $C > 0$ depends on the domain $\Omega$, of $\| f \|_{L^2}$, $\| v_{N,\text{mc}} \|_{C^1(\Omega) \cap C(\Omega)^2}$ and on $\| v_{N,\text{ex}} \|_{C^1(\Omega) \cap C(\Omega)^2}$.

The proof follows that of Lemma 3 line by line, just taking into account the additional term $\alpha(\text{div} v, \text{div} \phi)$. 

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3. A posteriori error estimation for neural network solutions

In the following we will derive an a posteriori error estimator for estimating the complete error \( (u - u_N) \) and \( (v - v_N) \) for the Laplace and the Stokes problem, respectively, that includes all the different error contributions discussed above: the model error, the approximation error, the generalization error and also the training error. This estimator is goal oriented: instead of estimating the error in a norm \( \| u - u_N \| \), we estimate scalar quantities of interest \( J : (u - u_N) \mapsto \mathbb{R} \). Examples of such error functionals are the point-wise error of the solution in a certain point \( x_a \in \Omega \)

\[ J_a(u - u_N) = u(x_a) - u_N(x_a), \]

averages of the solution or boundary integrals on \( \Gamma \subset \partial \Omega \)

\[ J_\Omega(u - u_N) = \int_\Omega u(x) - u_N(x) \, dx, \quad J_\Gamma(u - u_N) = \int_\Gamma \partial_n u(x) - \partial_n u_N(x) \, ds. \]

3.1. The dual weighted residual method (DWR)

We start by giving a concise description of the dual weighted residual method, such as presented in [27, 17] for the most simple case of the Laplace problem \(-\Delta u = f\) with homogeneous Dirichlet data \( u = 0 \). In the general case, the dual weighted residual method can be applied to all problems given in a Galerkin formulation based on a bilinear or semilinear form. Applications include problems in fluid dynamics [27, 17] and the approach has been extended to optimization and parameters identification [28], to plasticity [29] to coupled multiphysics problems [30], among many other applications. The estimator is further applicable to the estimation of time-stepping errors [31, 32].

As introduced above, \( V = H^1_0(\Omega) \) and \( V_h \subset V \) is a discrete subspace. Now, let \( J : V \rightarrow \mathbb{R} \) be a linear functional (in the general case, the dual weighted residual estimator also handles nonlinear quantities of interest, see [17]) and let \( z \in V \) be the solution to the adjoint problem

\[-\Delta z = J \text{ in } \Omega, \quad z = 0 \text{ on } \partial \Omega, \quad (30)\]

which, in variational formulation, is given as

\[ z \in V \quad (\nabla v, \nabla z) = J(v) \quad \forall v \in V. \quad (31)\]

This already gives the primal error identity

\[ J(u - u_h) = (\nabla(u - u_h), \nabla z) = (f, z) - (\nabla u_h, \nabla z). \quad (32)\]

By Galerkin orthogonality \( (\nabla(u - u_h), \nabla v_h) = 0 \) for all \( v_h \in V_h \) the corresponding dual error identity reads

\[ J(u - u_h) = (\nabla(u - u_h), \nabla(z - z_h)) = (\nabla u, \nabla(z - z_h)) = J(u) - (\nabla u, \nabla z_h), \quad (33)\]

where \( z_h \in V_h \subset V \) is the discrete solution to the adjoint problem.

Both simple error identities (32) and (33) cannot be used in practice since the adjoint solution \( z \in V \) and the primal solution \( u \in V \) are not known. Applying the DWR method
calls for an approximation of the primal or adjoint solutions in a subspace $V_{hh} \subset V$ which is not a subspace of the discrete space, e.g. $V_{hh} \nsubseteq V_h$ and to approximate the error by

$$J(u - u_h) \approx \eta_h(u_h, z_{hh}) := (f, z_{hh}) - (\nabla u_h, \nabla z_{hh}). \quad (34)$$

By $\eta_h(u_h, z_{hh})$, we denote the error estimator. It only depends on the primal and adjoint discrete solution and it is therefore computable. Likewise, a computable estimator could be defined based on the adjoint error identity $33$. While both formulations are equivalent for linear problems, a combination of primal and dual form is required in the general nonlinear case, see $[17]$.

Various approaches are discussed in $[17]$ Sec. 5] or $[33]$ Sec. 3]. In general, they are based on the higher-order postprocessing of same-space approximations. This reconstruction of higher order information is of an approximative type such that the DWR method usually does not give a rigorous error bound but only a computational measure to estimate the error in practical applications. This approximation is usually highly accurate.

Given that the exact error $J(u - u_h)$ is known, the accuracy of the error estimator can be numerically validated by considering the effectivity index, which is the quotient of estimator value $\eta_h(u_h, z_{hh})$ defined in (34) and real error

$$\text{eff}_h := \frac{\eta_h(u_h, z_{hh})}{J(u - u_h)}. \quad (35)$$

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 and further extensions and various applications have already been demonstrated by Becker and Rannacher $[17]$. 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 $u_N \not\in V = H^1_0(\Omega)$ does not satisfy the Dirichlet condition $u = 0$, the error $\phi := u - u_N$ is no admissible test function for the variational formulation of the adjoint problem $[31]$. Hence, we multiply both sides of the classical formulation $-\Delta z = J$, see (30), with $\phi = u - u_N$, integrate over $\Omega$ and a consistency term on the boundary remains

$$J(u - u_N) = (\nabla (u - u_N), \nabla z) + \langle \partial_n z, u_N \rangle_{\partial \Omega}. \quad (36)$$

With $(\nabla u, \nabla z) = (f, z)$ we derive the error identity

$$J(u - u_N) = (f, z) - (\nabla u_N, \nabla z) + \langle \partial_n z, u_N \rangle_{\partial \Omega}. \quad (37)$$

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 $z_{hh} \not\in V_N$. Since for
the neural network spaces it naturally holds $V_h \nsubseteq V_N$. We will approximate the adjoint solution in coarse finite element spaces, i.e. $z_H \in V_h \subset V$. Hereby, we introduce the a posteriori error estimator $\eta(u_N, z_H)$ as

$$\eta(u_N, z_H) := (f, z_H) - (\nabla u_N, \nabla z_H) + \langle \partial_n z_H, u_N \rangle_{\partial\Omega}. \quad (38)$$

This error estimator is efficiently evaluated on the finite element mesh using a numerical quadrature rule within the domain and along the boundaries. The accuracy of the estimate is measured by means of the effectivity index (35). We finally note that the error estimator (38) is not specific to the Deep Ritz method. Instead it could also be used in the context of DeepXDE [3], or for any other approximation technique that yields a $H^1$-conforming solution.

**Remark 6** (Considering high dimensional problems). The Deep Ritz method [12] has the potential to be more efficient than conventional grid-based methods such as the finite element method, especially for high-dimensional problems. The application of the error estimator to this case will naturally raise doubts, since for very high dimension the approximation of the dual problem would not be feasible. In that case, the dual problem should also be represented using a neural network. Since it is necessary that the reconstruction of the dual solution comes from a space that is not included in the primal space, a different network architecture or, for example, a different activation function should be used for the dual solution.

To be specific, let $A$ be a different network architecture and let $z_A \in V_A$ be the adjoint solution herein. Then, the estimator can be estimates as

$$\eta(u_N, z_A) := (f, z_A) - (\nabla u_N, \nabla z_A) + \langle \partial_n z_A, u_N \rangle_{\partial\Omega}.$$

In high dimensions, these integrals cannot be efficiently evaluated by standard mesh-based quadrature rules. Instead, also the estimator must be approximated using stochastic integration via

$$\eta(u_N, z_A) := \frac{1}{N^{in}} \sum_{k=1}^{N^{in}} f(x_k^{in}) z_A(x_k^{in}) - \nabla u_N(x_k^{in}) \cdot \nabla z_A(x_k^{in}) + \frac{1}{N^{bnd}} \sum_{j=1}^{N^{bnd}} \partial_n z_A(x_j^{bnd}) u_N(x_j^{bnd}).$$

### 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 (24) such as described in Section 2.3. For a linear goal functional $J : H^1_0(\Omega)^2 \to \mathbb{R}$ we introduce the adjoint solution

$$\text{div } z = 0, \quad -\Delta z - \nabla q = J \quad \text{in } \Omega, \quad z = 0 \quad \text{on } \partial\Omega. \quad (39)$$

The error identity for the network solution $v_N$ minimizing (24) is then derived as

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

$$= (f, z) - \langle \nabla v_N, \nabla z \rangle - \text{div } v_N, q \rangle + \langle v_N, \partial_n z + q\vec{n} \rangle_{\partial\Omega}.$$
To evaluate and approximate this error identity we compute a coarse finite element approximation $(z_{H}, q_{H}) \in V_{h} \times L_{h}$

$$-(\operatorname{div} z_{H}, \xi_{H}) + (\nabla z_{H}, \nabla \phi_{H}) + (q_{H}, \operatorname{div} \phi_{H}) = J(\phi_{H}) \quad \forall (\phi_{H}, \xi_{H}) \in V_{h} \times L_{h},$$

and define the Stokes error estimate as

$$\eta(v_{N}, z_{H}, q_{H}) := (f, z_{H}) - (\nabla v_{N}, \nabla z_{H}) - (\operatorname{div} v_{N}, q_{H}) + \langle \partial_{n}z_{H} + q_{H}\vec{n}, v_{N} \rangle_{\partial \Omega}. \quad (40)$$

4. Network architecture and training

Let us recall from the introduction that the network architecture is denoted by $N$ and a specific neural network function by $v_{N} \in V_{N}$. More precisely, we consider fully connected $L$-layer neural networks $N$ 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. First, a standard feed forward neural network (FFNet)

$$v_{N}^{(0)}(x) := x \in \Omega,$$

$$v_{N}^{(l)}(x) := \sigma(W_{l}^{t}v_{N}^{(l-1)}(x) + b_{l}^{t}), \quad l = 1, 2, \ldots, L,$$

$$v_{N}(x) = W_{L+1}v_{N}^{(L)} + b_{L+1}^{L+1}$$

and second a residual neural network (ResNet) that has also been considered in the original formulation of the Deep Ritz method

$$v_{N}^{(0)} = x,$$

$$v_{N}^{(l)}(x) = v_{N}^{(l-2)}(x) + \sigma \left( W_{l}^{t} \sigma \left( W_{l-1}^{t-1}v_{N}^{(l-2)}(x) + b_{l-1}^{t-1} \right) + b_{l}^{t} \right), \quad l = 2, 4, \ldots, L,$$

$$v_{N}(x) = W_{L+1}v_{N}^{(L)} + b_{L+1}^{L+1}.$$
With the employed notation $v^{(0)}_N$ is the input layer with $l_0 = d$ and $v_N$ is the output layer with $N_{t+1} = c$. All hidden layers are of the same size $H$, i.e. $l_H = H$ for $1 \leq l \leq L$.

4.1. Training

This section presents 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 [34].

In Figure 2 we present training progress for residual networks of various sizes. In the left sketch, we show the loss function, i.e. the value of the penalized and approximated energy functional (10) and on the right, we show the $L^2$ error of the resulting approximations $\|u - u_N\|$ during training. In general, the larger 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 increases the size of the network does not improve the solution. To further increase the accuracy, we would also have to adjust the number of quadrature points accordingly. Finally, the network’s training plays an important role, making this optimisation error difficult to control. 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 can yield better approximations.

In Figure 3 we present the training and approximation progress of networks with Feed Forward and Residual architectures and the 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 [1].

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
5. Numerical examples

We will discuss two test cases, the Laplace equation on a $L$-shaped domain and the Stokes equations on a disc. Figure 4 shows the solution to both problems obtained with the Deep Ritz method during the network training.

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 quantity of interest is the evaluation of the approximation error during training. This estimate can be used as a stopping criterion once a sufficiently low error level is reached.
solution in the point \( x_a = (0.5, -0.5) \in \Omega_L \)

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

(41)

Since \( J \not\in H^{-1}(\Omega_L) \) is not an admissible functional it should be replaced by averaging over a small neighbourhood of the point \( x_a \). This is discussed in [33, Sec. 5.2]. Also, the reentrant corner of the L-shaped geometry reduces the regularity of the solution, so that the superapproximation results, which are the basis for reconstructing the solution, cannot be used stringently. On the other hand, it is well documented that the non-regularized functional limited solution regularity nevertheless gives optimal performance in the context of the dual weighted residual method, see [17, 33]. For comparison, we first determine a reference value by finite element simulations on highly refined meshes. We identify it as

\[ J_{ref} = 0.1024 \pm 0.0020. \]

First we demonstrate the performance of the DWR estimator

\[ \eta(u_N, z_h) = (f, z_h) - (\nabla u_N, \nabla z_h) + \langle \partial_n z_h, u_N \rangle_{\partial \Omega} \]

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**: \( H = 20, \ L = 2, \ \sigma(x) = \max(x^3, 0) \).

Since each ResNet block consists of two layers, both architectures have same number of parameters. 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.
we show the loss function (bold green line), the functional error $J(u - u_N)$ (dashed orange line) and the error estimator $\eta(u_N, z_h)$ (dotted blue line). We note that functional errors $J(u) - J(u_N)$ are generally signed. Hence, convergence in Fig. 6 cannot be expected to be monotone and also, errors are not necessarily positive.

One can observe that independently of the applied method, the estimator follows the error and gives a highly accurate error approximation. 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 good even for extremely coarse meshes. The estimator is highly efficient and cheap to evaluate such that it brings along very little computational overhead. This allows to use the estimator as stopping criterion while training the network. 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 the unit circle $\Omega = \{x \in \mathbb{R}^2, |x|^2 < 1\}$. We prescribe an analytical solution for comparison with the neural network approximation given by

$$v(x,y) = \cos \left( \frac{\pi}{2} (x^2 + y^2) \right) \left( \begin{array}{c} y \\ -x \end{array} \right)$$

and compute the corresponding forcing term as

$$f(x,y) = \pi \cos \left( \frac{\pi}{2} (x^2 + y^2) \right) \left( \begin{array}{c} y(x^2 + y^2) + 4(y - x) \tan \left( \frac{\pi}{2} (x^2 + y^2) \right) \\ -x(x^2 + y^2) - 4(x + y) \tan \left( \frac{\pi}{2} (x^2 + y^2) \right) \end{array} \right).$$

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 8 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: $d = 2$, $c = 2$, $H = 10$, $L = 20$, $\sigma(x) =$

| epoch | $L=1$ error estimate eff$_h$ | $L=2$ error estimate eff$_h$ | $L=4$ error estimate eff$_h$ |
|-------|-----------------------------|-----------------------------|-----------------------------|
| 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 1.04    |
| 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 eff$_h$, see (35), for different refinement levels of dual solution $h = 2^{-L}$. 

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

Table 1: The values of error and estimator with effectivity index eff$_h$, see (35), for different refinement levels of dual solution $h = 2^{-L}$. 

| epoch | $L=1$ error estimate eff$_h$ | $L=2$ error estimate eff$_h$ | $L=4$ error estimate eff$_h$ |
|-------|-----------------------------|-----------------------------|-----------------------------|
| 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 1.04    |
| 2000  | -0.006424 -0.004946 1.23    | -0.009138 -0.011058 0.83    | -0.006117 -0.006393 0.96    |
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 error estimator is highly accurate and robust over the complete training process such that it can be used as stopping criterium. In particular for $L = 4$ the effectivities are very close to one and the estimator values deviate by less than 5% from the true error. Given the limited regularity of the problem (reentrant corner and quantity of interest that is not a linear functional in $H^1(\Omega)$) this result is remarkable.

The numerical implementation is realized in the finite element toolkit Gascoigne 3D [35], which is coupled to the machine learning framework PyTorch [36].

6. Conclusion

In this article, we have used different tools from the finite element analysis to get a deeper insight into the neural network approximation of partial differential equations obtained with Physics-Informed Neural Networks. In particular, we used standard tools of error analysis to interpret the generalization error as consistency error arising from faulty numerical quadrature. Further, based on the dual weighted residual method we have derived an a posteriori error estimator that can be used to measure the error of previously defined networks. The efficiency and accuracy of the estimator has been numerically demonstrated in applications to the Laplace and the Stokes problem. 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 an accurate and straightforward stopping criterion during the training process. Hereby, we gain a first validation of the neural network approximation, and the error controlled training also helps reduce the computational effort by avoiding excessive training epochs.

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